Bellasio R. and R. Bianconi 2010. Coupling Meteorological and Air Quality Models. Chapter 5E of AIR QUALITY MODELING - Theories, Methodologies, Computational Techniques, and Available Databases and Software. Vol. IV – Advances and Updates (P. Zannetti, Editor). Published by The EnviroComp Institute (<u>http://www.envirocomp.org/</u>) and the Air & Waste Management Association (<u>http://www.awma.org/</u>).

# **Chapter 5E**

# **Coupling Meteorological and Air Quality Models**

Roberto Bellasio and Roberto Bianconi

*Enviroware srl, via Dante 142, 20049 Concorezzo (MB) (Italy)* <u>info@enviroware.com</u>, <u>http://www.enviroware.com</u>

**Abstract:** Current computational and storage capabilities allow running highly complex computer codes in very short times over large domains with high time resolution over long periods. This computational power has stemmed a series of new developments in the creation of three-dimensional air quality models that are integrated into a meteorological model (online modeling) or can make use of most widely used meteorological models (offline modeling). This chapter presents the main features of meteorological models and the relevant aspects that need to be considered when setting up some software for offline coupling.

Key Words: meteorological models, air quality models, offline coupling, meteorological input.

#### 1 Introduction

Air quality models (AQMs) are computer codes that solve numerically or implement analytical solutions to the conservation equations for pollutant masses. They are a necessary tool for evaluating and predict air quality at different scales in space and time.

The dispersion of pollutants in the atmosphere is strongly influenced by meteorological conditions that, in turn, can be observed or estimated. While there are conditions where meteorology does not change significantly over the domain of interest, in several applications it is important to account for the variations of meteorological variables in space and time. These latter cases are where using a meteorological model is a need.

In general, the model complexity that should guarantee the more precise accounting of the physics (and chemistry) of atmospheric processes comes at a higher cost of meteorological input complexity. For this reason it is important to select the right type of air quality model depending on the problem that is faced.

In fact, the great success of simpler analytical models, such as the Gaussian one, is also due to the limited set of meteorological variables needed and their homogeneity. For example, it is sufficient to only have a single measurement of the average wind speed and direction and an estimate of atmospheric stability in terms of Pasquill-Gifford class, to compute with acceptable precision the concentration close to the source of an inert pollutant emitted from a non-buoyant source. This applies when the atmospheric stability is neutral or stable so that the planetary boundary layer height does not play a main role in first approximation.

There are, however, many situations where more measurements must be used and fed into a meteorological model that can compute three-dimensional fields of meteorological variables over a large area. These meteorological data can then drive complex non-stationary and non-homogeneous dispersion models.

Air quality and meteorology modeling were traditionally separated prior to the 1970's (Zhang, 2008). The three-dimensional chemical transport models until that time were driven by either measured or analyzed meteorological fields at a time resolution of 1-6 h from a mesoscale meteorological model on urban/regional scales, or by outputs at a much coarser time resolution (e.g., 6-h or longer) from a global circulation model (GCM). This technique is referred to as offline coupling or offline modeling. Offline modeling refers to when there is no feedback from the atmospheric chemistry in the CTM to the meteorological simulations, as would occur with the impacts of particulate matter on radiation, clouds, and precipitation. This absence of feedback is the main disadvantage, together with the large amount of data exchange, of the offline modeling, because it may result in a loss of important process information that occurs at a time scale smaller than that of the outputs from the offline meteorology models. Such feedbacks, on the other hand, can be simulated in *fully-coupled online models*, without space and time interpolation of meteorological fields but commonly with higher computational costs.

Both offline and online models are actively used in current regional and global models. Offline models are frequently used in ensembles, operational forecasting and sensitivity simulations. Online models are increasingly used for applications in which the feedbacks become important (e.g., locations with high frequencies of clouds and large aerosol loadings) and when the local scale wind and circulation systems change quickly. For online models, the coupled meteorology-air quality

modeling is essential for accurate model simulations (e.g., real-time operational forecasting or simulating the impact of future climate change on air quality).

This chapter deals with offline modeling. Some examples of online-coupled modeling are described by Zhang (2008). In this chapter, meteorological models are discussed, presenting for both diagnostic and prognostic, which are the relevant features. Also discussed are the advantages and disadvantages of their use compared to the other models. The discussion then focuses on the coupling, pointing out the relevant aspects to be tackled whereupon examples of couplings are then introduced. At the end of this chapter we provide some useful resources of geophysical and meteorological data located on the Internet.

# 2 Meteorological Data

Meteorology is a primary factor affecting actual and simulated air quality, therefore it is very important to measure and assess it in a reliable way. In a limited number of situations, meteorological observations can be used directly as input to AQMs. Instead, meteorological measurements are generally used as input to meteorological models, integrated when necessary with parameterizations of processes that are not measured.

# 2.1 Meteorological Observations

The simplest interfacing between meteorology and AQMs are based on the direct use of measurements. This is typically limited to Gaussian models.

Meteorological observations can be made at ground level and aloft. They are either routinely made (e.g. meteorological and air quality stations, airports) or on the spot for specific needs (e.g. measuring campaigns). While measurements at ground are generally available with hourly resolution, measurements aloft are made in general up to two times per day (at main airports).

Most meteorological measurements carried out at surface level (typically 10 m AGL for wind and 2 m AGL for temperature) give information about wind speed and direction, temperature, relative humidity, precipitation and pressure. Some also include net radiation and cloud cover (this last especially at airports). Sonic anemometers, which can take measurements with very fine temporal resolution (20 Hz or better and are therefore suited for turbulence and heat exchange measurements), are not so diffuse in routine meteorological stations. These hourly routine meteorological observations are almost always carried out at a single level above the ground, and therefore the vertical profile of the variables is missed.

Routine measurements aloft are made with rawinsondes that measure wind speed and direction, temperature, relative humidity and pressure. Other measurements that include turbulence are made with SODARs. These measurements at surface and aloft are often enough to characterize the meteorological conditions for applying simpler dispersion models. In fact, starting from a limited set of observed parameters (wind speed, temperature, cloud cover and land use) it is possible to apply some schemes that define the structure of the surface layer.

The characterization obtained, however, is site-specific and it is only valid close to the location where measurements are taken. When an evaluation of a wider area is required, especially when measurements show clearly that observations within the area significantly differ; it is necessary to rely on a meteorological model.

#### 2.2 Meteorological Models

There are many situations where the use of a meteorological model must be preferred to the use of meteorological measurements. This is when the meteorological conditions are not homogeneous over the domain of interest, for example in presence of complex terrain as well as on coastal areas.

The resulting complex wind circulation affects the transport and diffusion of pollutants and recirculation patterns can develop. Also, the extent of the mixing layer can change abruptly, especially at coastal sites where a thermal internal boundary layer (TIBL) develops. These features are not described by point measurements.

At a bare minimum, in order for models to catch these circulation features it is necessary that they adequately describe the terrain elevation and the land use with sufficient accuracy. This is generally obtained with small enough grid cells.

As pointed out in Brode and Anderson (2008), it is important to recognize that while a 3D meteorological model can generate spatially varying three dimensional wind fields, this does not guarantee that the wind fields generated by said model will provide a more appropriate treatment of plume transport and dispersion. This also does not necessarily result in an improved estimate of concentrations compared to a dispersion model based on single meteorological station measurements.

Meteorological models can be broadly divided into diagnostic and prognostic categories and in these terms they are described hereafter.

<u>Diagnostic meteorological models</u> reconstruct the three-dimensional wind and temperature field over domains extending up to thousands of square kilometers. They are called diagnostic because they try to reconstruct a dynamically consistent wind field starting from "observations" at surface and aloft. These observations are either real measurements or data coming from another meteorological model output at a larger scale. The consistency is often found by

applying the continuity equation in order to estimate the vertical wind components starting from the horizontal ones and imposing the conservation of mass (minimization of divergence).

These models start from sparse values at ground level of meteorological variables including at least wind speed and direction, temperature and cloud cover. The input also includes upper air data (height above ground, wind speed and direction, temperature). Diagnostic models also use as input, the terrain height and the land use for each cell of their regularly gridded computational domain.

Typically an initial guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce a first wind field estimate. Then an objective analysis procedure is used to introduce observational data into the previous step wind field to produce a final wind field, also based on mass conservation. Measured winds contribute to grid points where the wind is reconstructed with a weight that decreases with distance.

Diagnostic models include micrometeorological modules for the computation of the sensible heat flux, the Monin-Obukhov length and the velocity scales in the planetary boundary layer. These variables are used to compute the height of the planetary boundary layer and the turbulent dispersion coefficients for the dispersion models.

Diagnostic models can also receive as input relative humidity and precipitation rate values from sparse points and interpolate them to the regular output grid.

Prognostic (or dynamical) meteorological models are based on the complete solution of all the equations for the hydrodynamic flow. This set of equations is numerically solved after the introduction of some simplifications. The most important simplification is perhaps the one, which distinguishes the models in hydrostatic and non-hydrostatic. Hydrostatic models are those in which the vertical equation of motion contains only gravity and the vertical pressure gradient while the vertical acceleration is ignored (vertical acceleration is maintained in non hydrostatic models). The hydrostatic assumption is acceptable at scales greater than about 10 km, while it is not acceptable at smaller scales. Prognostic models have the advantage to be able, in theory, to predict all the meteorological fields, even at small scales, independently form the set of measures (which is instead fundamental for diagnostic models). This strength is also a weak point for prognostic models because after a simulation has started, during the simulation, there is no more comparison with the measurements; therefore possible numerical errors cannot be solved. The Four Dimensional Data Assimilation (FDDA) technique has been recently introduced in some prognostic models to use observations in order to correct possible prediction errors.

Prognostic models solve the conservation equations in Eulerian framework and they can be applied at any scale in space and time. They require a proper initialization and the correct description of boundary conditions for the whole duration of the simulation.

Prognostic models include the calculation of the PBL evolution as well as all the description of convective precipitation, distribution of atmospheric water vapor content and cloud physics.

The higher complexity of prognostic models comes at a computational cost that might not be convenient for some air quality applications that require results in relatively short time periods.

#### 2.3 Comparison of Diagnostic and Prognostic Model Features

Both diagnostic and prognostic meteorological models have some important favorable characteristics, one compared to the other. Considering diagnostic models, since they are "reinitialized" by the measures at each hour, there is no accumulation of errors as the time evolves. On the other hand, since they need observations that are carried out at hourly intervals (when not at longer times), their time resolution can be not less than 1 hour.

Diagnostic meteorological models are easier to get acquainted with and less consuming in terms of computational times and input/output data storage. This is particularly important in air quality studies. In fact, air quality legislation establishes limits that often require the analysis of the hourly concentrations for at least one full year. The European legislation, for example, in order to protect the human health, establishes that the 1-hour average concentration of NO<sub>2</sub> must not exceed 200  $\mu$ g/m<sup>3</sup> more than 18 times in one year. This means that AQMs, in order to be useful planning tools, must be capable of estimating the 1-hour pollutant(s) concentration for a whole year over a fine grid mesh. Therefore the input meteorological variables to AQMs must be available at least with the same space and time resolution, and must be reliable.

The capability to obtain the 3D meteorological fields for one or more years with hourly time resolution and fine grids (e.g. 250 m) is of fundamental importance in obtaining the statistics of interest from the AQMs.

Moreover, the fact that these models directly use as input, the meteorological observations guarantees that the model output will almost reproduce the input at the same location. This is particularly important when a measurement is available close to an emission source of interest because it guarantees that the initial dispersion is based on the observed values.

Diagnostic models however have some limitations. These are mainly the limited physics they describe and the fact that they do not have prediction capabilities. In fact they can only run with past observations or using the output of a prognostic model as a provider of forecast meteorological input.

A generic limitation of all the gridded models is related to their ability to simulate terrain generated wind fields (Brode and Anderson, 2008). This ability is limited by the horizontal resolution of terrain and land use data on the model grid. For example, a river valley that is about 1 kilometer wide from peak to peak and about 500 meters deep would not be adequately resolved by a 250-meter grid spacing. This is because a single grid cell could span the entire valley wall from ridge top to river level, such that the slopes of the valley walls represented by gridded terrain elevations could be highly reduced. This effect significantly affects the gravity driven slope flows and other diagnostic wind field adjustments.

Also, diagnostic models do not compute turbulence and can only provide some parameters that can be used as input for parameterizations that were found from the analysis of datasets of observations and are reported in literature.

The prognostic wind fields in some cases have the advantage to better represent regional flows and certain aspects of sea breeze circulations along with slope/valley circulations where dynamical consistency is required.

Also, they can incorporate the dispersion equations for one or more species, and this allows accounting for feedback effects that pollutants can have on meteorology. An example of this is the attenuation of solar radiation due to the presence of particulate matter with variable size.

The complexity and more exhaustive description of the involved physical processes make these models more prone to numerical errors. Also this requires a large set of input parameters and data that might be more difficult to collect and store as opposed to the requirements for diagnostic models.

Some pros and cons of diagnostic and prognostic models are summarized in the following table.

	PROS	CONS
DIAGNOSTIC	<ul> <li>no error propagation</li> <li>fast computer codes meteo input and output are locally consistent</li> </ul>	<ul> <li>high frequency of input data</li> <li>reduced set of equations</li> <li>no predictive capabilities</li> <li>turbulence of wind not computed limited capability of producing effects that were not observed</li> </ul>
PROGNOSTIC	<ul> <li>prognostic capabilities</li> <li>computation of turbulence</li> <li>more complete description of physical processes</li> <li>possibility to integrate a dispersion model (online modeling)</li> </ul>	<ul> <li>heavier computational costs</li> <li>propagation of errors unless complex FDDA is incorporated</li> </ul>

Table 1. Pros and	Cons of diagnostic and	prognostic models.

The choice of a diagnostic or a prognostic model is not straightforward. For example, Hu et al. (2010) predicted the  $PM_{2.5}$  concentrations for the California Regional Particulate Air Quality Study (CRPAQS) using the CIT/UID (Kleeman and Cass, 2001) air quality model run. Plus, using meteorological output from a diagnostic objective analysis method and the output of the prognostic WRF model (Skamarock et al., 2008) initialized with that analysis and, as a third option, integrated with four-dimensional data assimilation (FDDA).

The results using the diagnostic analysis as meteorological input were superior to those of the prognostic model alone. When the FDDA was used it gave better results than the diagnostic input configuration.

Seaman (2000) describes a number of features of the meteorological models for air quality applications.

# 3 The Coupling

As discussed before, while the online modeling has a number of advantages, the offline modeling offers the possibility to use one of the state-of-the-art meteorological models with any given air quality model. Also, an offline coupling is necessary when the time-space domain of the application of the air quality model is smaller than that of the meteorological model.

Due to all the differences among meteorological models as well as among air quality models, it is necessary - for offline modeling - to develop some ad-hoc software that can transfer the meteorological output to the air quality model, completing the required information that is missing with some computed fields.

The common issues that must be considered when coupling a meteorological three-dimensional model with an air quality model include:

- Data format conversion
- Effects of boundaries
- Sub-domain selection
- Interpolation in horizontal and vertical directions
- Coordinate system conversion
- Conversion of classification schemes
- Conversion of units
- Calculation of additional parameters
- Integration with additional observations

Models can have standard formats for their input/output files (e.g. GRIB, NetCDF, GDAS) but often they have a proprietary format that requires one to incorporate in the coupling code the routines that can decode the meteorological model output and make the *data format conversion* required by the air quality model.

While this is a mere software task, all other issues are not limited to the development of a generally complex software, but they involve a number of considerations on the physics of the models and the scope of the application.

Meteorological models are all based on an Eulerian formulation. They solve the conservation equations and boundary effects thus affect them. This is especially true for mass conservation. For this reason it is always a good choice to locate the domain of the dispersion model within the domain of the meteorological model, so that no information is missing and the boundary effects that may be present in the meteorological model output do not influence the extracted meteorological fields. The need for an appropriate *sub-domain extraction* holds for both the horizontal and the vertical direction: the top of dispersion model must be well below the top of the meteorological model.

The horizontal and vertical cell sizes might not match the sizes of the dispersion model. For this reason it may be necessary to apply an *interpolation in horizontal and vertical directions* to obtain the meteorological model output at different locations in space.

Along the *horizontal*, since the domain of the dispersion model is smaller than the meteorological model domain, there might be cases where the coordinate systems are different. For example, coordinates are in longitude/latitude degrees for the meteorological model (where the distance between adjacent grid points is not

conserved) and the coordinates are in metric for the dispersion model. Moreover, meteorological models running at large scale, as in case of regional models that may cover a portion of an entire continent or more, generally use longitude and latitude coordinates. Since there are a number of existing projections, the coupling software should be able in such cases to make a *coordinate system conversion*.

The interpolation along the *vertical* can be more complex than for the horizontal: there are in fact many vertical coordinate systems that are not necessarily based on the height above some reference but they can be in expressed in terms of pressure. This means that the vertical coordinate system can even be time variable at a given location (mass coordinates), as for example in the case of the meteorological model WRF.

For this reason it is important that the coupler, in the case of an Eulerian air quality model, can guarantee the mass conservation. This is especially important in presence of complex terrain. Usually conservation is obtained with the adjustment of vertical velocity with numerical schemes of different complexity that can even be incorporated in the air quality model (Hu and Odman, 2008).

Interpolations along the vertical may also require that the profile of height dependence of variables is known. There are in fact several variables that do not have a linear-with-height profile. For example, the mixing ratio or the vertical potential temperature in the PBL during typical daytime conditions are almost uniformly distributed along the vertical in the bulk of the mixed layer, but their profile is different in the surface layer and in the entrainment zone at the top (e.g. Stull, 1988). This might require that the coupling software incorporate some equations that allow estimating the elevation of the mixing layer and some parameters that allow identifying the stability conditions (e.g. Monin-Obukhov length, Richardson bulk number, etc.).

Both the meteorological and the dispersion model may use some input data that are described in terms of classes with corresponding values for one or more parameters. One clear example is the land use type, which is categorized in a number of discrete classes, each of them characterized by a specific value of albedo, roughness length, Bowen ratio, leaf area index (LAI) and others. If any of these parameters is used by the air quality model, it might be necessary to perform a *conversion of classification schemes* to assign the land use classes of the meteorological model to those that are in use in the air quality model. This conversion may include some modification to one or more of the parameters so that they are consistent with the classification that is in use in the air quality model.

Care must be given to *units* in use by the models, so that the values are always properly converted, if needed.

In some cases it is necessary to implement the *calculation of additional parameters*. In fact, depending on the meteorological model, there are many variables that might not be computed or produced in output. For example when coupling an air quality model such as AERMOD that bases the diffusion schemes on the scaling parameters of the boundary layer to a meteorological model as WRF, it is necessary to compute from available output fields some variables as convective scale velocity and mechanical mixing height that are then used for the calculation of the vertical and lateral turbulent fluctuations (Kesarkar et al., 2007). The available output from the meteorological model drives the choice of the approach. For example the calculation of turbulent fluctuations for AERMOD using MM5 or the Eta model (Black, 1994) can go through parameterizations based on the turbulent kinetic energy (Isakov et al., 2007).

Depending on the application of the air quality model and the processes implemented, it is sometimes useful to include in the coupler the *integration with additional observations* as well as the incorporation of datasets that are not included in the meteorological model output. For example this is the case of clouds information that can be acquired from satellite imaging and used in the air quality model in wet deposition and photolysis calculations.

# 4 Examples of Coupling Processors

The general concepts of the previous paragraph are discussed here in specific context, with description of software couplers that are commonly used.

Air Quality Models (AQMs) require different meteorological input variables depending on their type. Simple Gaussian models require basically only the horizontal components of wind field (wind speed and wind direction), mixing height, Pasquill-Gifford stability classes and temperature for plume rise calculation. Advanced Gaussian models are capable of estimating dry and wet deposition, and for this purpose they require additional meteorological data such as precipitation, mechanical and convective scale velocities (u\* and w\*) and a few others. Moreover Gaussian models require the meteorological variables for a single point, which must (should) be representative for the whole simulation domain.

A broad distinction among more complex air quality models is generally made on the reference frame used to develop the equations that describe the fate of pollutants. There are two different approaches, the Eulerian and the Lagrangian one. The Eulerian framework is fixed and the equations are expressed in terms of fluxes while the Lagrangian one is linked to each portion of fluid considered and moves with it.

The Eulerian gridded approach is based on the mass conservation of the species under the assumption that velocity and temperature of the fluid are not influenced by the concentration of the pollutant, so that the mass balance equation is not coupled to the energy and momentum conservation equations. The calculation domain is made of computational volumes within which all the conservation equations are numerically solved. The basic equations of the Eulerian gridded models are reported, for example, in Zannetti (1990) and Seinfeld and Pandis (1998).

Eulerian and Lagrangian numerical models require additional meteorological variables, such as the vertical wind component and the Monin Obukhov length to describe turbulence (in place of the Pasquill Gifford Classes). These variables must be available for a 3-D domain.

Very complex AQMs, capable of predicting the formation of secondary pollutants, both in gas and aerosol phase, require even more variables such as the solar actinic flux and the water vapor mixing ratio.

# 4.1 MM5CAMX and WRFCAMX Processors

The Comprehensive Air quality Model with extensions (CAMx) is a publicly available open-source computer modeling system for the integrated assessment of gaseous and particulate air pollution (<u>http://www.camx.com</u>). CAMx is designed to simulate air quality over many geographic scales, treat a wide variety of inert and chemically active pollutants (ozone, inorganic and organic  $PM_{2.5}/PM_{10}$ , mercury and toxics), provide source-receptor sensitivity and process analyses, and be computationally efficient along with easy to use.

The meteorological inputs needed by CAMx are 3-dimensional gridded fields of: horizontal wind components, temperature, pressure, water vapor, vertical diffusivity, clouds and rainfall; which should be generated by self-consistent meteorological models (MM5, WRF, RAMS, etc.).

The MM5 mesoscale model of PSU/NCAR (<u>http://www.mmm.ucar.edu/mm5/</u>) is a limited-area, non-hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale atmospheric circulation. The model is supported by several pre- and post-processing programs, which are referred to collectively as the MM5 modeling system.

MM5 can be used for a broad spectrum of theoretical and real-time studies, including applications of both predictive simulation and four-dimensional data assimilation to monsoons, hurricanes and cyclones. On the smaller meso-beta and meso-gamma scales (2-200 km), MM5 can be used for studies involving mesoscale convective systems, fronts, land-sea breezes, mountain-valley circulations and urban heat islands.

The Weather Research and Forecasting (WRF) model (<u>http://wrf-model.org</u>) is a NWP and atmospheric simulation system designed for both research and operational applications. The model is suitable for a broad span of applications across scales ranging from large-eddy to global simulations, and can be configured for both research and operational applications.

The development of WRF has been a collaborative effort among the National Center for Atmospheric Research's (NCAR) Mesoscale and Microscale Meteorology (MMM) Division, the National Oceanic and Atmospheric Administration's (NOAA) National Centers for Environmental Prediction (NCEP) and Earth System Research Laboratory (ESRL), the Department of Defense's Air Force Weather Agency (AFWA) and Naval Research Laboratory (NRL), the Center for Analysis and Prediction of Storms (CAPS) at the University of Oklahoma and the Federal Aviation Administration (FAA) with the participation of university scientists.

WRF is maintained and supported as a community model to facilitate wide use internationally, for research, operations, and teaching. There are thousands of WRF users around the World.

The WRF software framework provides the infrastructure that accommodates the dynamics solvers, physics packages that interface with the solvers and programs for initialization (WRF-Var and WRF-Chem).

There are two dynamics solvers in the WRF software framework: the Advanced Research WRF (ARW) solver (originally referred to as the Eulerian mass or "em" solver) developed primarily at NCAR, and the NMM (Non-hydrostatic Mesoscale Model) solver developed at NCEP. The software framework includes also the WRF-Chem model, which provides capabilities for air chemistry modeling.

An Arakawa C horizontal grid characterizes the WRF model along with terrainfollowing hydrostatic-pressure vertical coordinates.

One of the activities in coupling meteorology models and CTM is to interpolate the variables on the same grid scheme. For example, MM5 data are on an Arakawa B grid with flip of i, j indices from standard configuration, while CAMx data are on an Arakawa C grid. These two Arakawa grid schemes are graphically illustrated in Figure 1 where scalars are calculated at the center of the grid cells in both schemes, while the difference is the position where wind components are calculated. Considering WRF, both WRF and CAMx data are calculated on Arakawa C grids.

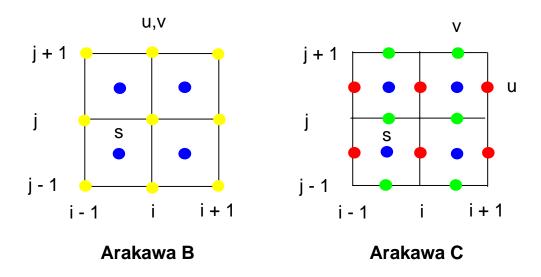


Figure 1. A simple graphical illustration of the Arakawa B (left) and the Arakawa C (right) horizontal grids. Scalars are in the center of the grids for both schemes (blue circles); u and v wind components are at the corners of the grids in Arakawa B (yellow circles); u and v components are at the center of the vertical and horizontal grid faces respectively in Arakawa C (red and green circles respectively).

After the variables interpolation, the vertical dispersion coefficient must be calculated. This procedure can be done using three routines based on the O'Brian (1970) methodology (KVCALC\_OB70), the CMAQ ACM2 methodology (KVCALC\_ACM2) described by Pleim (1997), and the TKE methodology (KV\_TKE) employed in RAMS (Mellor and Yamada, 1974/1982; Helfand and Labraga, 1988).

After these processes, followed by operations on cloud fields, water contents, cells with snow, topography and renormalization of land use, output files with CAMx format are produced.

#### 4.2 CMAQ Meteorology-Chemistry Interface Processor (MCIP)

The Community Multiscale Air Quality modeling system (Byun and Schere, 2006), best known as CMAQ (<u>http://www.cmaq-model.org</u>) simulates atmospheric processes and air quality (including gas-phase chemistry, heterogeneous chemistry, particulate matter, and airborne toxic pollutants) over a broad range of spatial and temporal scales using a comprehensive computational framework based on first-principles solutions. The CMAQ modeling system is considered to be the state-of-the-science for Eulerian air quality modeling. It is widely used for a variety of retrospective, forecasting, regulatory, climate, atmospheric process-level and emissions control applications. CMAQ is used by local, state, and national government agencies, at academic institutions and in private industry.

MCIP uses MM5 or WRF-ARW output files to create netCDF based input meteorology for the emissions model and the CCTM. The CMAQ CTM uses Arakawa C horizontal staggering (Figure 1), where the horizontal wind components are on perpendicular cell faces and all other prognostic fields are defined at the cell centers. MCIP performs the following functions (Otte and Pleim, 2010):

- Extracts meteorological model output for the CTM horizontal grid domain. MM5 data are on an Arakawa B grid; therefore there is a difference in the physical locations of the wind components between the MM5 and CMAQ. Interpolating the raw MM5 wind components in MCIP from the cell corners to the cell faces is necessary to use them in CMAQ. On the contrary both WRF-ARW and CMAQ use an Arakawa C-staggered horizontal grid, so horizontal interpolation is in principle not required. Since the plume rise calculations in the emissions processor still expect wind components on the cell corners regardless of the input meteorological model, wind components are interpolated to the Arakawa B grid to satisfy this requirement (Otte and Pleim, 2010).
- Processes all required meteorological fields for the CTM and the emissions model.
- Collapses meteorological model fields, if coarser vertical resolution data are desired for the CTM. MCIP uses mass-weighted averaging on higher vertical-resolution meteorological model output.
- Optionally computes surface and planetary boundary layer (PBL) fields using output from the meteorological model.
- Computes dry-deposition velocities for important gaseous species using the surface and PBL parameters. MCIP can compute dry deposition using two methods: the RADM dry deposition method (Wesely, 1989) calculates deposition velocities of 13 chemical species using friction velocities and aerodynamic resistances. Inputs required for this method include temperature, humidity, and horizontal wind component profiles. The surface exchange aerodynamic method (Pleim et al., 2001) uses

surface resistance, canopy resistance, and stomatal resistance to compute dry deposition velocities.

- Computes cloud top, cloud base, liquid water content, and cloud coverage for cumuliform clouds using simple convective schemes.
- Outputs meteorological/geophysical files in the I/O API format, which is standard within the Models-3 framework.

Appel et al. (2010) presented a comparison of the operational performances of two CMAQ simulations that utilize input data from MM5 and WRF meteorological models. Two sets of CMAQ model simulations were performed for January and August 2006, one set utilized MM5 meteorology (MM5-CMAQ) and the other utilized WRF meteorology (WRF-CMAQ), while all other model inputs and options were kept the same. The results of the simulations have shown some differences, which are primarily caused by the differences in the calculation of wind speed, planetary boundary layer height, cloud cover and friction velocity in the MM5 and WRF model simulations. Differences in the calculation of vegetation fraction and several other parameters result in smaller differences in the predicted CMAQ model concentrations.

#### 4.3 The CALMET Meteorological Processor of CALPUFF

CALPUFF (Scire et al., 2000b) is a multi-layer, multi-species non-steady-state puff dispersion modeling system that simulates the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. CALPUFF is intended for use on scales from tens of meters from a source to hundreds of kilometers. It includes algorithms for near-field effects such as stack tip downwash, building downwash, transitional buoyant and momentum plume rise, rain cap effects, partial plume penetration, subgrid scale terrain and coastal interactions effects and terrain impingement. It also has longer range effects such as pollutant removal due to wet scavenging and dry deposition, chemical transformation, vertical wind shear effects, overwater transport, plume fumigation and visibility effects of particulate matter concentrations.

CALPUFF is appropriate for long-range transport (source-receptor distances of 50 to several hundred kilometers) of emissions from point, volume, area, and line sources. The meteorological input data should be fully characterized with timeand-space-varying three-dimensional wind and meteorological conditions using CALMET. CALPUFF may also be used on a case-by-case basis when the model is more appropriate for the specific application. The purpose of choosing a modeling system like CALPUFF is to fully treat stagnation, wind reversals, and time and space variations of meteorological conditions on transport and dispersion.

Beside the 3-D meteorological fields developed by the CALMET diagnostic meteorological model, CALPUFF can use single station meteorological data stored in format used by other dispersion models (ISC3ST, AUSPLUME,

CTDMPLUS). However single station meteorological files do not allow CALPUFF to take advantage of its capabilities to treat spatially varying meteorological fields.

CALPUFF produces files of hourly concentrations of ambient concentrations for each modeled species, wet deposition fluxes, dry deposition fluxes, and for visibility applications and extinction coefficients.

CALMET (Scire et al., 2000a) is a diagnostic meteorological model that reconstructs the 3-D wind and temperature fields starting from meteorological measurements, orography and land use data. Besides the wind and temperature fields, CALMET determines the 2-D fields of micro meteorological variables needed to carry out dispersion simulations (mixing height, Monin-Obukhov length, friction velocity, convective velocity and others). CALMET uses a terrain following vertical coordinate system. The vertical wind component w is defined at the vertical cell faces, while the other variables are defined at grid centers.

The boundary layer module of CALMET allows for calculating 2D gridded fields of surface friction velocity, convective velocity scale, Monin-Obukhov length, mixing height and Pasquill-Gifford-Turner (PGT) stability classes.

CALMET adopts two different boundary layer algorithms for applications overland and overwater. The energy balance method of Holtslag and van Ulden (1983) is used over land surfaces to calculate the sensible heat flux, the surface friction velocity, the Monin-Obukhov length and the convective velocity scale. The mixing layer height is then calculated starting from the computed sensible heat flux and the temperature radiosoundings (Carson, 1973; Maul, 1980). The boundary layer parameters overwater are calculated using a different algorithm, which also requires the air-sea temperature difference.

The boundary layer parameters calculated by CALMET are used in CALPUFF to determine the horizontal and vertical dispersion coefficients of a puff. Different algorithms are used according to the stability conditions and to the position of the puff within the planetary boundary layer (Weil, 1985; Briggs, 1985; Panofsky et al., 1977; Hicks, 1985; Arya, 1984; Nieustadt, 1984).

The flow diagram of the CALMET model is illustrated in Figure 2. The diagnostic wind field module uses a two-step approach for the computation of the wind field. In the first step an initial guess wind field is adjusted for kinematic effects of terrain, slope flows and terrain blocking effects to produce a Step 1 wind field. The second step consists of an objective analysis procedure to introduce observational data into the Step 1 wind field to produce a final wind field. CALMET can optionally use the output of prognostic meteorological models such as MM5 in three different ways:

- As a replacement for the initial guess field,
- As a replacement for the Step 1 field,
- As pseudo observations in the objective analysis procedure.

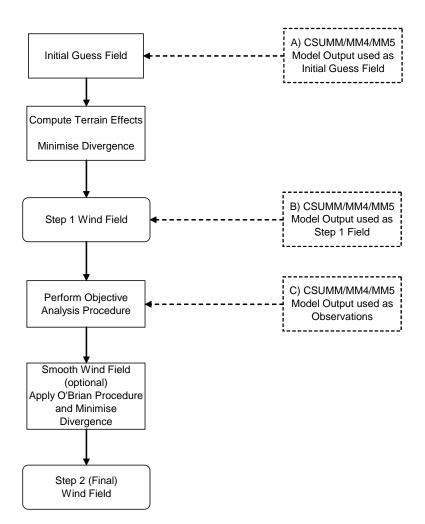
The prognostic wind fields in some cases have the advantage of better representing regional flows and certain aspects of sea breeze circulations and slope/valley circulations.

CALMET needs meteorological observations at surface and upper air data. At surface the following variables are needed with hourly resolution: wind speed, wind direction, temperature, cloud cover, ceiling height, surface pressure, relative humidity and precipitation rate. The upper air data, needed at least twice daily, must contain for each vertical level: wind speed, wind direction, temperature, pressure and height.

The output of the CALMET model is directly interfaced with dispersion models such as CALPUFF (Lagrangian puff model), CALGRID (Eulerian photochemical model) and KSP (Lagrangian particle model).

Brode and Anderson (2008) critical review of the CALPUFF application in near fields pointed out some important issues about CALMET. These limitations are largely due to its inability to ensure dynamical consistency in the simulated wind field. An example of the potential importance of this limitation is given by the phenomenon of drainage flows that often occur in valley situations under lightwind stable conditions. The three-dimensional structure of gravity-driven wind fields within a valley is very complex. These wind fields are often associated with complex thermal structures within the valley that develop as cold air drains down from the ridge tops and accumulate within the valley. A transition from downslope to down-valley flows will typically develop over time and with distance from the ridge, creating significant lateral and vertical gradients of wind and temperature. CALMET is not able to simulate the thermal structures within the valley that are associated with these complex flows. The three-dimensional temperature fields computed within CALMET are based on either available upper air soundings and surface measurements or gridded prognostic model inputs, depending on user-specified options. The three-dimensional temperature fields are not adjusted to reflect the influence of these drainage flows. As a consequence, for example, the lapse rate used to compute plume rise in CALPUFF would not reflect the stable stratification generated by drainage flows. Therefore CALPUFF would overestimate the plume height for buoyant releases and underestimate the ground-level concentrations.

Reducing the horizontal grid resolution could face some of the CALMET issues. However this would increase the computational burden, unless the overall domain size is decreased, which could limit the applicability of the results by excluding important synoptic or mesoscale features that influence the complex winds. Recent studies have shown significant sensitivity to grid resolution, with some



evidence of a possible bias toward lower concentrations as grid resolution increases.

Figure 2. Flow diagram of the CALMET model.

Finally, CALMET does not include algorithms to account for the differential heating that occurs during the daytime as the sun heats one side of the valley wall while the other side is shaded, which generate complex cross-valley circulations. These circulation patterns will vary depending upon the orientation of the valley and solar elevation angle (based on time of day and season), and may significantly affect plume transport plus dispersion depending on the location of the source relative to the valley orientation. Some new algorithms for calculating the solar radiation over sloping surfaces and improving the temperature interpolation considering different terrain heights have been introduced in a modified version of CALMET that is not publicly available (Bellasio et al., 2005).

#### 4.4 CALMET and LAPMOD

The basic assumption of Lagrangian particle models is that the mass of pollutant is divided in a number of particles moving within the atmospheric fluid with the same velocity of the fluid itself. This velocity is made by the sum of a mean vector (the mean wind) and a fluctuation around the mean. The trajectory of each particle describing a portion of the mass of the pollutant is reconstructed by evaluating the position of the particle at discrete time intervals:

$$\overline{x}_{t+dt} = \overline{x}_t + \overline{u} \, dt$$
$$\overline{u} = u_{mean} + \overline{u}'$$

The mean wind is estimated from measurements or from a meteorological model. The fluctuation of the wind velocity has a distribution with zero mean and it is estimated using a meteorological model, or through parameterizations coming from observation campaigns. The time evolution of this stochastic variable is a first-order Markov process and it is described by the non-linear Langevin equation:

$$d\overline{u}' = a(\overline{u}', \overline{x}, t)dt + b(\overline{x}, t)dW$$

where a is the deterministic acceleration and dW is a random forcing from a normal distribution with dt standard deviation.

When coupling a Lagrangian particle model with some meteorological model output most of the issues to be considered are the same faced with Eulerian air quality models. The main specific issue for Lagrangian particle models is the definition of the distribution of the probability function for the wind velocity fluctuations.

LAPMOD is a new Lagrangian particle dispersion model evolved from the model PLPM (Vitali et al., 2006). It is a full three-dimensional model capable of simulating the release of multiple sources with different shapes (point, line, area, volume) with arbitrary emission rates of multiple substances, including radionuclides. LAPMOD accounts for buoyant point sources as well as linear decay of radionuclides and includes the algorithms for dry and wet deposition.

The meteorological input for LAPMOD is provided by CALMET. LAPMOD can directly read the binary output file of CALMET to acquire the three-dimensional fields of wind and temperature as well as the two-dimensional fields of friction velocity, convective velocity, Monin-Obukhov length and boundary layer height. Some input fields to CALMET (directly input or estimated internally from landuse classification) are also transferred to LAPMOD: terrain elevation, leaf area index, roughness length and precipitation.

The relevant part of the coupling (that is implemented internally into the LAPMOD code) is the calculation of the higher moments of the distribution of the wind velocity. There are several schemes for this task. An effective one, implemented in LAPMOD, is based on the first 4 moments of the distribution of the probability density function of the Eulerian turbulent velocity, under the assumption that it has a quadratic form (Franzese et al., 1999):

$$a = \alpha w^2 + \beta w + \gamma$$

Routine meteorological measurements do not provide higher moments of the distribution of the wind fluctuations. At the same time, these are not standard output variables from meteorological models and for this reason they need to be incorporated in the software that prepares the meteorological input.

For this reason it is necessary to rely on parameterizations available in literature. A possible set of these, the one implemented in LAPMOD, is given hereafter, where the following variables are used:

$Ri = L / z_i$	bulk Richardson number (-)
L	Monin-Obukhov length (m)
z <sub>i</sub>	boundary layer height (m)
$C_0$	Kolmogorov universal constant $(m^{-1}s^{3/2})$
Е	eddy dissipation rate (m <sup>2</sup> s <sup>-3</sup> )

#### Vertical Component

a and b coefficients in convective conditions (Ri < -1)

$$\alpha(z) = \frac{(1/3)\partial \overline{w^3}/\partial z - \overline{w^3}/2\overline{w^2} \left[\partial \overline{w^3}/\partial z - C_0 \varepsilon(z)\right] - \overline{w^2} \partial \overline{w^2}/\partial z}{\left(\overline{w^4} - \overline{w^3}^2\right) / \left(\overline{w^2} - \overline{w^2}^2\right)}$$
$$\beta(z) = \frac{1}{2\overline{w^2}} \left[\frac{\partial \overline{w^3}}{\partial z} - 2\overline{w^3}\alpha(z) - C_0\varepsilon(z)\right]$$
$$\gamma(z) = \frac{\partial \overline{w^2}}{\partial z} - \overline{w^2}\alpha(z)$$
$$a = \alpha w^2 + \beta w + \gamma$$

$$b = C_0 \varepsilon$$

For the moments of the distribution (overbar terms above) there are several parameterizations available in literature coming from observations. For example (Hanna et al., 1982a; Franzese et al., 1999):

$$\overline{\frac{w^2}{w_*}^2} = a_1 + a_2 \left(\frac{z}{z_i}\right)^{2/3} \left(1 - \frac{z}{z_i}\right)^{4/3}$$
$$\overline{\frac{w^3}{w_*}^3} = a_3 + \left(\frac{z}{z_i}\right) \left(1 - \frac{z}{z_i}\right)^2$$
$$\overline{w^4} = 3.5 \overline{w^2}^2$$
$$\varepsilon = 0.4 \frac{w_*}{z_i}^3$$

Where  $a_1$ ,  $a_2$  and  $a_3$  are fitting parameters.

a and b coefficients in stable and neutral conditions ( $Ri \ge -1$ )

$$\alpha(z) = 0.5 \frac{1}{\left(\overline{w^2}\right)^2} \frac{\partial \left(\overline{w^2}\right)^2}{\partial z} = \frac{1}{\left(\overline{w^2}\right)} \frac{\partial \overline{w^2}}{\partial z}$$
$$\beta(z) = -\frac{1}{T_L}$$
$$\gamma(z) = 0.5 \frac{\partial \left(\overline{w^2}\right)^2}{\partial z} = \overline{w^2} \frac{\partial \overline{w^2}}{\partial z}$$
$$b(z) = \overline{w^2} \sqrt{\frac{2}{T_L}}$$

#### Horizontal Components

#### Any stability condition

$$a = \alpha w^2 + \beta w + \gamma$$

with:

$$\alpha = 0$$
$$\beta(z) = -\frac{1}{T_L}$$
$$\gamma = 0$$
$$b(z) = \sigma \sqrt{\frac{2}{T_L}}$$

where  $\sigma$  is the alongwind (*U*) or crosswind (*V*) standard deviation of the distribution of the wind speed fluctuations along those directions and  $T_{LU}$  and  $T_{LV}$  are the corresponding Lagrangian times.

*Convective conditions* 

$$T_{LU} = T_{LV} = 0.15 \frac{z_i}{\sigma_V}$$
$$\sigma_V = u_* \left(12 - 0.5 \frac{z_i}{L}\right)^{\frac{1}{3}}$$

Neutral conditions

$$\sigma_U = 2u_* \exp\left(1 - \frac{z}{z_i}\right) \qquad \sigma_V = \sigma_W = 1.3u_* \exp\left(-\frac{2f z}{u_*}\right)$$
$$T_{LU} = T_{LV} = T_{LW} = -\frac{0.5 z}{\sigma_W \left(1 + 15\frac{f z}{u_*}\right)}$$

Stable conditions

$$\sigma_U = 2u_* \left( 1 - \frac{z}{z_i} \right) \qquad \sigma_V = \sigma_W = 1.3u_* \left( 1 - \frac{z}{z_i} \right)$$

$$T_{LU} = 0.15 \frac{z_i}{\sigma_U} \sqrt{\frac{z}{z_i}} \qquad T_{LV} = 0.07 \frac{z_i}{\sigma_V} \sqrt{\frac{z}{z_i}} \qquad T_{LV} = 0.10 \frac{z_i}{\sigma_W} \left(\frac{z}{z_i}\right)^{0.8}$$

The scaling parameters that appear in these equations can be computed, for example, with the scheme of Holtslag and Van Ulden (1983).

Alternatively, prognostic models can directly provide the standard deviations of the wind components, the planetary boundary layer height and the eddy dissipation rate so that these can be used in the above equations.

#### 4.5 FLEXPART and the ECMWF Data

FLEXPART (e.g. Stohl et al., 2005) is a Lagrangian particle dispersion model designed for calculating the long-range and mesoscale dispersion of air pollutants.

The ECMWF meteorological fields on a latitude/longitude grid feed the FLEXPART model. The first action that must be done on the meteorological files is their transformation from the Gridded Binary (GRIB) format.

The model needs five three-dimensional fields: horizontal and vertical wind components, temperature and specific humidity. The meteorological input data are located on ECMWF model levels, which are defined by a hybrid coordinate system  $\eta$ . These coordinates are then converted into pressure coordinates.

The two-dimensional meteorological fields needed by the model are: surface pressure, total cloud cover, 10 m horizontal wind components, 2 m temperature and dew point temperature, large scale and convective precipitation, sensible heat flux, east/west and north/south surface stress.

Starting from the surface stress and the air density, FLEXPART determines the friction velocity  $u^*$ . If surface stress and sensible heat flux are not available, the friction velocity, the Monin-Obukhov length and other scaling parameters are calculated using the Berkowicz and Prahm method (1982). The mixing layer height is calculated according to Vogelezang and Holtslag (1996) methodology.

Once calculated for each ECMWF point (0.5 or 0.25 degree) and time (6 hours), the mixing layer height must be adequately processed in order to consider spatial and temporal variations on scales not resolved by the ECMWF model. These scales play an important role in determining the thickness of the layer over which a tracer is effectively mixed (Stohl et al., 2005). The height of the convective mixing layer reaches its maximum value in the afternoon before a much shallower stable mixing layer forms. If, for example, meteorological data are available at 12:00 and 18:00, the simple linear interpolation of the mixing height calculated for these two times might result in overestimation of the calculated concentration for tracers released at the surface shortly before the breakdown of the convective

mixing layer. A similar problem is also encountered for spatial variations of mixing layer due to complex topography and variability in land use or soil wetness. In order to consider these problems, FLEXPART adopts an "envelope" mixing height obtained from the mixing height calculated at each point, the standard deviation of the ECMWF model subgrid topography, the wind speed at height of the original mixing layer, and the Brunt-Vaisala frequency.

The boundary layer parameters calculated as explained above are then used for calculating the standard deviations of the wind speed components and the Lagrangian times by means of the Hanna (1982b) parameterization scheme, modified accordingly to Ryall and Maryon (1997) for the standard deviation of the vertical wind component.

#### 4.6 Measurements and Gaussian Models

Gaussian models are widely described in literature (e.g. Zannetti, 1990; Seinfeld and Pandis, 1998). Well-known advanced Gaussian models are ISC3 and AERMOD. Most of these models require meteorological variables at surface (e.g. 10 m AGL) and at a single point. An exception is AERMOD, which also can take into account variables that are measured at upper levels. The surface meteorological variables needed by Gaussian models are essentially wind speed and direction, temperature, stability conditions and height of the mixing layer.

Measurements carried out at surface must be vertically extrapolated in order to determine their values at the heights of the sources. This operation is usually done within the dispersion model using algorithms based on the scaling properties of the planetary boundary layer. A more precise indication would come from upper air measurements, but these are costly and not always available, especially for long periods with high temporal frequency of measurement (e.g. rawinsondes or SODAR).

When a reliable and representative meteorological station is available close to the source, its data must be used to produce the model input file. Rarely the meteorological monitoring stations have information about cloud cover, which is fundamental information. Cloud covers can be obtained from METAR data, which are available from the most important airports. Cloud cover, solar radiation and wind speed allow determination of the Pasquill Gifford stability class (e.g. Zannetti, 1990). The mixing layer height at each hour can be estimated starting from the surface radiation budget (e.g. Hostlag and van Ulden, 1983). The surface radiation budget also allows acquisition of the friction velocity  $u^*$ , the Monin-Obukhov length L and other scaling parameters.

Under stable conditions the mixing height can be estimated with diagnostic equations, which depend only from  $u^*$  and L. Under neutral conditions the mixing height depends only from the mechanical turbulence, which means  $u^*$  (e.g. Zilitinkevich, 1972; Zilitinkevich, 1989). During daytime unstable conditions the

mixing height must be estimated by means of prognostic equations as, for example, the one proposed by Batchvarova and Grining (1991). An exhaustive review of the equations needed to estimate the mixing height is given in (Seibert et al., 2000).

One of the main problems when using dispersion models that are fed by a single meteorological station is that the meteorological station closest to the dispersion domain is often tenths of km far away. Such a station therefore might not be representative for the area. A possible approach to overcome the problem could be the use of a 3-D prognostic or a diagnostic meteorological model for determining the meteorological field over a wide domain, then the extraction of the variables from a single model grid close to the sources of interest. This approach would also solve the problem of possible missing data present in a single meteorological station, because the model would fill the gaps. Moreover, for dispersion models that require both surface and upper air variables, such as AERMOD, this approach has the advantage that all the variables would refer to the same point (grid). Some variables needed by the atmospheric dispersion model (Monin-Obukhov length, friction velocity, convective velocity, etc.) might be calculated by specific routines, if not directly available from the dispersion model. The US-EPA, for example, is planning to develop specific processors, for using AERMOD starting from the MM5 prognostic models (US-EPA 9th Modeling Conference Presentations). The US-EPA is also planning to develop some processors to use CALPUFF starting from MM5 or WRF, therefore bypassing the use of the CALMET diagnostic meteorological model. An example of methodology for the application of AERMOD with incomplete input data has been presented by Turtos et al. (2010).

#### 4.7 Other Couplers

Apart from those already cited, there are several software packages that were developed for coupling meteorological and dispersion models. On a global scale, a recent example of interesting coupling (Flemming et al., 2010) is the one between the ECMWF's integrated forecast system (IFS) and the global chemistry and transport models (CTMs) MOCAGE (Josse et al., 2004; Bousserez et al., 2007), MOZART-3 (Kinnison et al., 2007) and TM5 (Krol et al., 2005). This is a special type of coupling, since the resulting modeling system has the IFS taking care of the transport of the reactive gases and one of the CTMs providing the chemical transformations based on the meteorological predictions of the IFS. The system however includes a feedback so that the changes of concentration of the chemical species are assimilated by the IFS itself.

Apart from the availability of the meteorological input for each of these models, an additional advantage of the coupling of the same meteorological input with more CTM models is that these can be used to produce ensemble forecasts of air quality isolating the variability within the chemistry and transport part of the system.

# **5** Sources of Data over the Internet

One of the most difficult tasks in running air quality models is to find all the input data needed. Generally the number of input data increases with the model complexity. This paragraph contains some hints about Internet sites, which contain useful data for the whole World. Once downloaded from Internet, the data cannot be used as they are but they need to be processed in order to find possible gaps, missing values or to average them on the model grid mesh. Scripting languages, such as Perl, are very useful and powerful in this phase.

#### 5.1 Land Cover

Land cover data are important for meteorological and AQ models for many reasons. For example, because they are related to the roughness length and to deposition velocity of some pollutants they are also needed during emission inventories.

At the European level, the land cover data can be obtained from the CORINE land cover project, which is part of the CORINE program and is intended to provide consistent localized geographical information on the land cover of the Member States of the European Community. Two useful Internet sites to browse these data are:

http://www.eea.europa.eu/publications/COR0-landcover

#### http://image2000.jrc.ec.europa.eu/

Global land cover data are available from the University of Maryland Department of Geography (<u>http://glcf.umiacs.umd.edu/data/landcover</u>). Imagery from the AVHRR satellites acquired between 1981 and 1994 were analyzed to distinguish fourteen land cover classes (Hansen et al., 2000). The land cover data are available at three spatial scales: 1 degree, 8 kilometer and 1 kilometer pixel resolutions.

#### 5.2 Orography

The Shuttle Radar Topography Mission (SRTM) obtained elevation data on a near-global scale to generate the most complete high-resolution digital topographic database of Earth. SRTM consisted of a specially modified radar system that flew onboard the Space Shuttle Endeavour during an 11-day mission in February of 2000. SRTM is an international project spearheaded by the National Geospatial-Intelligence Agency (NGA), NASA, the Italian Space Agency (ASI) and the German Aerospace Center (DLR). There are three resolution outputs available, including 1-kilometer and 90-meter resolutions for the world and a 30-meter resolution for the US. The SRTM data are available from <a href="http://glcf.umiacs.umd.edu/data/srtm">http://glcf.umiacs.umd.edu/data/srtm</a>.

Orography data are also available from the National Geophysical Data Center of NOOA at this address:

http://www.ngdc.noaa.gov/cgi-bin/mgg/ff/nph-ewform.pl/mgg/topo/customdatacd

# 5.3 Meteorology

Meteorological data at upper levels are available from two different Internet sites of NOAA:

The Integrated Global Radiosonde Archive (IGRA) consists of radiosonde and pilot balloon observations at over 1,500 globally distributed stations (<u>http://www.ncdc.noaa.gov/oa/climate/igra/index.php</u>). Observations are available for standard, surface, tropopause and significant levels for many variables, among which are: wind direction and speed, pressure, temperature, geopotential height and dew point. The period of record varies from station to station, with many starting from 1970.

The Radiosonde Observation (RAOB) Internet site (http://www.esrl.noaa.gov/raobs/) allows the download of upper air meteorological data by specifying the time interval, the wind units and selecting the stations by their WMO code, by country or by coordinates.

Other meteorological data at surface and at upper levels are the GDAS (Global Data Assimilation System), which is one of the operational systems of the National Weather Service's National Centers for Environmental Prediction (NCEP). These data are available at <u>http://www.arl.noaa.gov/gdas1.php</u> with 1-degree space resolution and 3-hour time resolution.

Surface data are available from many Internet sites as METAR data, which is a weather format predominantly used by pilots as a part of fulfilling a pre-flight weather briefing. Meteorologists also use aggregated METAR information to assist in weather forecasting. METAR data are available at many points of the World, practically at all the main airports. The METAR phrase is not so clear at first glance for non-expert people. For example the string

KFDW 110215Z AUTO 06016G21KT 7SM -DZ OVC003 17/17 A3001 RMK AO1

indicates a report issued by the airport with ICAO code KFWD (Fort Worth, TX) at 02:15 UTC of day 11 of some month (month and year are not specified). At such hour both temperature and dew point are 17°C (62.6°F), there is a solid overcast at 300ft, a light drizzle is present, visibility is 7 statute miles, wind speed is 16 knots and wind direction is 60 degrees. A wind gust of 21 knots has also been observed. It is clear that METAR strings must be automatically processed by software before they can be used in AQ models. One of the possible sources of METAR data is <u>http://weather.noaa.gov/weather/metar.shtml</u>.

#### Acronyms

- AFWA Department of Defense's Air Force Weather Agency
- AGL above ground level
- AQM air quality model
- CAPS Center for Analysis and Prediction of Storms
- CRPAQS California Regional Particulate Air Quality Study
- CTM chemical transport model
- ECMWF European Centre for Medium Range Weather Forecasting
- ESRL Earth System Research Laboratory
- FAA Federal Aviation Administration
- FDDA Four Dimensional Data Assimilation
- GCM global circulation model
- GDAS global data assimilation system
- GRIB gridded binary
- LAI leaf area index
- METAR METeorological Aerodrome Report
- NCAR National Center for Atmospheric Research
- NCEP National Centers for Environmental Prediction
- NOAA National Oceanic and Atmospheric Administration
- NRL Naval Research Laboratory
- NWP numerical weather prediction
- PBL planetary boundary layer
- PSU Penn State University
- TIBL thermal internal boundary layer
- SODAR SOnic Detection And Ranging

#### References

Appel K. W., S. J. Roselle, R. C. Gilliam, and J. E. Pleim. Sensitivity of the Community Multiscale Air Quality (CMAQ) model v4.7 results for the eastern United States to MM5 and WRF meteorological drivers. Geosci. Model Dev., 3, 169–188, 2010

Arya S.P.S. (1984) Parametric relations for the atmospheric boundary layer. Boundary Layer Meteorology, 30, 57-73.

Batcharova, E., Gryning, S. E., 1991. Applied model for the growth of the daytime mixed layer. Boundary Layer Meteorology, 56, 261 274.

Bellasio R., G. Maffeis, J. Scire, M.G. Longoni, R. Bianconi and N. Quaranta (2005) Algorithms to account for topographic shading effects and surface temperature dependence on terrain elevation in diagnostic meteorological models. Boundary-Layer Meteorology, 114: 595-614.

Berkowicz, R. and Prahm, L. P.: Evaluation of the profile method for estimation of surface fluxes of momentum and heat, Atmos. Environ., 16, 2809–2819, 1982.

Black T. (1994) The new NMC mesoscale eta model: description and forecast examples. Weather Forecasting, 9, 265-278.

Bousserez, N., Atti'e, J.-L., Peuch, V.-H., Michou, M., and Pfister, G. (2007) Evaluation of the MOCAGE chemistry and transport model during the ICARTT/ITOP experiment, J. Geophys. Res., 112, D10S42, doi: 10.1029/2006JD007595.

Briggs G.A. (1985) Analytical parameterization of diffusion: the convective boundary layer. J. Clim. And Appl. Meteor., 24, 1167\_1186.

Brode R.W. and Anderson B. (2008) Technical Issues Related to CALPUFF Near-field Applications. US-EPA.

Byun, D. W. and Schere, K. L. (2006) Review of the governing equations, computational algorithms, and other components of the Models3 Community Multiscale Air Quality (CMAQ) Modeling System, Appl. Mech. Rev., 59, 51–77.

Carson D.J. (1973) The development of a dry, inversion-capped, convectively unstable boundary layer. Quart. J. Roy. Meteor. Soc., 99, 450-467.

Flemming J., A. Inness, H. Flentje, V. Huijnen, P. Moinat, M. G. Schultz, and O. Stein (2010). Coupling global chemistry transport models to ECMWF's integrated forecast system

Franzese P., A.K. Luhar and M.S. Borgas (1999) An efficient Lagrangian stochastic model of vertical dispersion in the convective boundary layer. Atm. Env., 33, 2337-2345.

Hanna S.R., Briggs G.A. and Hosker R.P. (1982a) Handbook on atmospheric diffusion. Technical Information Center, U.S. Department of Energy, pp. 102

Hanna, S. R. (1982b) Applications in air pollution modeling, in: Atmospheric Turbulence and Air Pollution Modelling, edited by: Nieuwstadt, F. T. M. and van Dop, H., D. Reidel Publishing Company, Dordrecht, Holland.

Hansen, M., R. DeFries, J.R.G. Townshend, and R. Sohlberg (2000), Global land cover classification at 1km resolution using a decision tree classifier, International Journal of Remote Sensing. 21: 1331-1365.

Helfand, H. M., M. J. C. Labraga, 1988: Design of non singular level 2.5 second order closure model for the prediction of atmospheric turbulence. J. Atmos. Sci., 45, 113-132.

Hicks B.B. (1985) Behavior of turbulence statistics in the convective boundary layer. J. Clim. And Appl. Meteor., 24, 607-614.

Holtslag, A.A.M., A.P. Van Ulden. 1983. A simple scheme for daytime estimates of the surface fluxes from routine weather data. J. Climate Applied Meteorology, 22, 517-529.

Hu Y. and M. T. Odman (2008) A comparison of mass conservation methods for air quality models. Atmospheric Environment, 42, 35, 8322-8330.

Hu J., Q. Ying, J. Chen, A. Mahmud, Z. Zhao, S.H. Chen and M.J. Kleeman (2010) Particulate air quality model predictions using prognostic vs. diagnostic meteorology in central California Atmospheric Environment, 44 (2), 215-226

Isakov V., A. Venkatram, J. S. Toumaa, D. Koračinc and T. L. Otte (2007). Evaluating the use of outputs from comprehensive meteorological next term models in air quality modeling applications. Atmospheric Environment, 41, 8, 1689-1705.

Josse, B., Simon, P., and Peuch, V.-H. (2004) Rn-222 global simulations with the multiscale CTM MOCAGE, Tellus B, 56, 339–356.

Kesarkar A.P., M. Dalvi, A. Kaginalkar and A. Ojha (2007) Coupling of the Weather Research and Forecasting Model with AERMOD for pollutant dispersion modeling. A case study for PM10 dispersion over Pune, India. Atmospheric Environment, 41, 9, 1976-1988.

Kinnison, D. E., Brasseur, G. P., Walters, S., Garcia, R. R., Marsh, D. R., Sassi, F., Harvey, V. L., Randall, C. E., Emmons, L., Lamarque, J. F., Hess, P., Orlando, J. J., Tie, X. X., Randel, W., Pan, L. L., Gettelman, A., Granier, C., Diehl, T., Niemeier, U., and Simmons, A. J. (2007) Sensitivity of Chemical Tracers to Meteorological Parameters in the MOZART-3 Chemical Transport Model, J. Geophys. Res., 112, D03303, doi: 10.1029/2008JD010739.

Kleeman M.J and G.R. Cass (2001) A 3D Eulerian source-oriented model for externally mixed aerosol. Environmental Science & Technology, 35, 4834-4848.

Krol, M., Houweling, S., Bregman, B., van den Broek, M., Segers, A., van Velthoven, P., Peters, W., Dentener, F., and Bergamaschi, P. (2005) The two-way nested global chemistry-transport zoom model TM5: algorithm and applications, Atmos. Chem. Phys., 5, 417–432. http://www.atmos-chem-phys.net/5/417/2005/.

Maul P.R. (1980) Atmospheric transport of sulphur compound pollutants. Central Electricity Generating Bureau MID/SSD/80/0026/R. Nottingham, England.

Mellor, G.L. and T. Yamada, 1974: A hierarchy of turbulence closure models for planetary boundary layers. J. Atmos. Sci., 31, 1791-1806.

Mellor, G. L. and Yamada, T., 1982: Development of a turbulence closure model for geophysical fluid problems. *Rev. Geophys. Space Phys.*, **20**, 851-875.

Nieuwstadt F.M.T. (1984) The turbulent structure of the stable, nocturnal boundary layer. J. Atmos. Sci., 41, 2202-2216.

O'Brien J.J. (1970) A note on the vertical structure of the eddy exchange coefficient in the planetary boundary layer. J. Atmos. Sci., 27, 1213-1215.

Otte T. L. and J. E. Pleim (2010) The Meteorology-Chemistry Interface Processor (MCIP) for the CMAQ modeling system: updates through MCIPv3.4.1. Geosci. Model Dev., 3, 243–256.

Panofsky H.A., H. Tennekes, D. H. Lenschow and J.C. Wyngaard (1977). The characteristics of turbulent velocity components in the surface layer under convective conditions. Boundary Layer Meteorology, 11, 355-361.

Pleim, J. E., A. Xiu, P. L. Finkelstein, and T. L. Otte, 2001: A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes. Water Air Soil Pollut. Focus, 1, 243–252.

Ryall, D. B. and Maryon, R. H.: Validation of the UK Met Office's NAME model against the ETEX dataset, in: ETEX Symposium on Long-Range Atmospheric Transport, Model Verification and Emergency Response, edited by: Nodop, K., European Commission, EUR 17 346, 151–154, 1997.

Scire J.S., Robe F.R., Fernau M.E. and Yamartino R.J. (2000a) A user's guide for the CALMET dispersion model. Earth Tech, Inc.

Scire J.S., Strimaitis D.G. and Yamartino R.J. (2000b) A user's guide for the CALPUFF dispersion model. Earth Tech, Inc.

Seaman N.L. (2000) Meteoological modeling for air-quality assessments. Atmospheric Environment, 34, 2231-2259.

Seibert, P., Beyrich, F., Gryning, S.-E., Joffre, S., Rasmussen, A., Tercier, P., 2000. Review and intercomparison of operational methods for the determination of the mixing height. Atmospheric Environment, 34, 7, 1001-1027.

Seinfeld J. And Pandis S. (1998) Atmospheric Chemistry and Physics, from Air Pollution to Climate Change. John Wiley, New York, 1326 pp.

Skamarock, W. C., Klemp, J. B., Dudhia, J., Gill, D. O., Barker, D. M., Duda, M. G., Huang, X.-Y., Wang, W., and Powers, J. G. (2008) A description of the Advanced Research WRF Version 3, National Center for Atmospheric Research, Tech. Note, NCAR/TN-475+STR, 113 pp.

Stohl A., C. Forster, A. Frank, P. Seibert, and G. Wotawa. Technical note: The Lagrangian particle dispersion model FLEXPART version 6.2. Atmos. Chem. Phys., 5, 2461–2474, 2005

Stull R.B. (1988) An introduction to boundary layer meteorology. Kluwer Press. ISBN 90-277-2768-6

Turtos Carbonell L.M., M.S. Gacita, J.R. Oliva, L.C. Garea, N.D. Rivero, E. M. Ruiz (2010) Methodological guide for implementation of the AERMOD system with incomplete local data, Atmospheric Pollution Research, 1, 102-111

US-EPA 9th Modeling Conference Presentations. http://www.epa.gov/scram001/9thmodconfpres.htm (visited April 26, 2010)

Vitali L., F. Monforti, R. Bellasio, R. Bianconi, V. Sacchero, S. Mosca and G. Zanini (2006) Validation of a Lagrangian dispersion model implementing different kernel methods for density reconstruction. Atmospheric Environment, 40, 40, 8020-8033.

Vogelezang, D. H. P. and A. A. M. Holtslag (1996) Evaluation and model impacts of alternative boundary-layer height formulations. Bound. Layer Meteor., 81, 245-269.

Weil J.C. (1985) Updating applied diffusion models. J. Clim. And Appl. Meteor, 24, 1111-1130.

Wesely, M. L., 1989: Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models. Atmos. Environ., 23, 1293–1304.

Zannetti P. (1990) Air pollution modeling: theories, computational methods, and available software. Van Nostrand, New York, 444 pp.

Zhang Y. Online-coupled meteorology and chemistry models: history, current status, and outlook. Atmos. Chem. Phys., 8, 2895–2932, 2008

Zilitinkevich S.S. (1972) On the determination of the height of the Ekman boundary layer. Boundary Layer Meteorology, 3, 141-145. Zilitinkevich, S.S., 1989. Velocity profile, the resistance law and the dissipation rate of mean flow kinetic energy in a neutrally and stably stratified planetary boundary layer. Boundary Layer Meteorology, 46, 367-387.