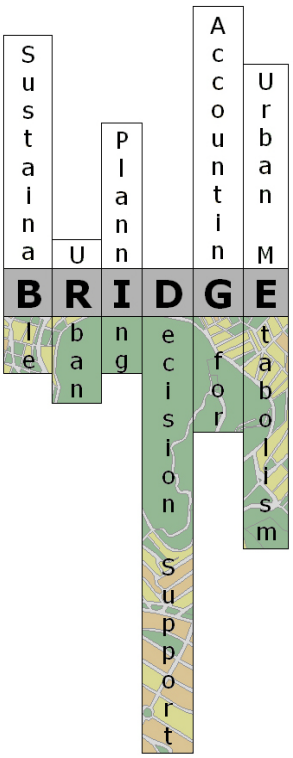
SEVENTH FRAMEWORK PROGRAMME

THEME 6: Environment (including climate change)

Contract for: **Collaborative Project**

D.4.1
Model Selection Report



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1.0	November, 30, 2009	J.L. Pérez & R. San José (UPM)	Add new changes from other partners and format changes

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1. Introduction

The modelling approach within BRIDGE integrates different types of models for mesoscale air quality models to urban canopy models. The cascade modelling technique from large to local scale is the main methodology to be applied under BRIDGE. This approach will allow estimating the pollutant concentrations and the fluxes associated to different urban development scenarios and strategies. Mesoscale meteorological models such as MM5 and WRF are considered within BRIDGE for simulating the meteorological variables through the numerical simulation of the atmospheric flows based on the Navier-Stokes equations. MM5 and WRF models simulate the atmospheric flow (meteorology only) in a 3D cube with spatial resolutions on about 1 – 100 km with domains between 20-50 km (urban domain) to thousands of km (Europe). These models require as input the meteorological boundary conditions coming from the outer domain. This information is typically obtained from Global Meteorological Models such as GFS, AVN or ECMWF. MM5 and WRF models give detailed information of all meteorological variables and fluxes involved in the atmospheric flow. They also require land use and topographic information which should be adequate to the specific spatial resolution that they are run. These meteorological models provide input information (meteorological fluxes and variables) to chemical transport models such as CAMx and CMAQ, which estimate the pollutant concentrations in the atmosphere. CAMx and CMAQ require additional input data such as emission data (amount of pollutant emitted in a grid cell per second). The chemical transport models simulate the atmospheric chemistry based on lumped carbon mechanisms (such as CB-IV or CB05 or RADM) and a detailed description of the photochemistry. CAMx and CMAQ can estimate the ozone concentrations (and other secondary pollutants) in the atmosphere. In addition, CAMx and CMAQ models use different aerosol models to estimate primary and secondary PM concentrations in the atmosphere.

In addition we have a representative of the most modern generation of meteorological and chemical models named WRF/CHEM. This is an on-line model which simultaneously simulates the meteorology and the chemistry (being closer to the atmospheric reality). WRF/CHEM is based on the same principles than MM5 and WRF but including the chemical solver in every time-step together with the meteorology. The computer demand in substantially higher than using MM5-CMAQ or MM5-CAMx or WRF-CMAQ/CAMx.

At the local scale, of a few hundred meters, we have a large suit of models with different objectives. We have two models named: MICROSYS and VADIS, which are CFD codes based on similar principles than MM5 and WRF (based on the Reynolds-averaged Navier-Stokes equations formulation) so that these models are receiving boundary conditions and initial conditions from the mesoscale models (MM5 and WRF). MICROSYS and VADIS are applied to a microscale domain and they can include buildings, roads, sidewalks, trees, etc. to simulate the closest urban domain with a 4D interaction between biosphere and atmosphere. These models are “nested” into the mesoscale models as explained before. MICROSYS and VADIS can obtain detailed information related to the biosphere-atmosphere heat flux exchange at surface level and simulate the passive and chemically active pollutants in the micro-scale urban domain. These models require also information related to emission data which is usually produced by a traffic model in an urban context. Within BRIDGE the traffic models CAMO and TREM will be applied.

In BRIDGE at microscale level other models will also be applied regarding different turbulence schemes usually in one dimension, such as LUMPS - UWB - SUES - NARP – OHM or TEB models. These models are already suited to produce comfort index or energy indexes. These models are simpler than the actual CFD codes but they are integrating many other aspects in more detail such as hydrological processes, urban management processes, etc.

At urban scale the URBAIR model will be used to evaluate air quality and dispersion patterns. This is a second generation Gaussian plume model intended to be used for distances up to about 10 km from the source. URBAIR is a steady state atmospheric dispersion model, based on boundary layer scaling parameters, instead of relying on Pasquill stability classification. The model was developed for simulating passive or buoyant gas dispersion and deposition at local and urban scales. It is designed to allow consideration of dispersion in rural or urban areas, including the treatment of building effects. This model is also suitable to run on-line and thus to be included in DSS.

We also have the ACASA model which incorporates higher-order closure principles for turbulent statistics to predict effects that higher-order turbulent kinetic and thermodynamic processes have on the surface microenvironment and associated fluxes of heat, moisture, and momentum. ACASA simulates the microscale urban metabolism as a stand-alone model (surface-atmosphere interactions and the distribution of trace gases). ACASA calculates, each independently, the output quantities (and associated vertical gradients) often used for output comparisons (at each model layer throughout the air, soil, or snowpack domains). The domain extends maximally to 100m above the city and plant canopy elements to ensure applicability of the turbulence assumptions. ACASA is also nested in the mesoscale model WRF to provide spatial information of energy and mass fluxes. The ACASA domain for the WRF coupling is the region that exists between this sigma-level and three meters belowground.

Finally, two models focusing only on the hydrological processes (SIMGRO) and a model of a complete different nature (based on neural networks) named NKUA NN are also considered. SIMGRO can produce detailed information on all the hydrological processes present in an urban environment (these aspects are not yet integrated in the mesoscale models in detail but there are some versions – such as MM5 urban – which includes some of these aspects). NKUA NN has been mainly applied for urban heat island experiments. A lot of research is currently being done with CFD codes on this aspect and including satellite data assimilation.

A Regional Climate Model (RCM3) is also integrated in BRIDGE modeling setup which can be used for producing information on the climate evolution for future scenarios, to provide climate variables (temperature, wind, humidity, PBL height, etc.) and fluxes under climate change.

Some models such as WRF-UCM/CHEM, MICROSYS, CAMx, CMAQ and RCM3 cannot be integrated in the DSS to be run “on-line” because of its complexity, size and computer demands and these models will be run “off-line” or in-house to produce the accurate results for the different alternatives (scenarios and control base run). Other models like LUMPS and TEB (on-line models) will be integrated into the DSS to be run by the user when enough input data is available. The DSS user will integrate the results of the off-line and online models.

1.1 Definitions and Acronyms

Acronyms

ACASA	Advanced Canopy-Atmosphere-Soil Algorithm (CMCC)
CAMO	Cellular Automata Traffic Model (UPM)
CAMx	Comprehensive Air quality Model with extensions (ENVIRON)
CMAQ	Community Multiscale Air Quality Modelling System (US EPA)
EMIMO	An emission model (UPM)
MICROSYS	Microscale Air Quality Simulation System (UPM)
MM5 NCAR	Mesoscale Meteorological Models (US NCAR)
TREM	Transport Emission Model for Line Sources (UAVR)
URBAIR	Urban air quality model (UAVR)
VADIS	Microscale air quality model (UAVR)
WRF W of Oklahoma)	eather Research & Forecasting Model (US NCAR, NCEP, FSL, AFWA, FAA, University

1.2 Purpose of the document

This document, in line with the EC requirements, is the Model Selection Report of the BRIDGE (sustainaBle uRban plannIng Decision support accountinG for urban mEtabolism) Project. It contains information and description of the different models, their characteristics and functionalities, the required input data and the characteristics of the results or output data. It also contains descriptions of the relations between models selected in WP4 and the rest of the WP's in BRIDGE.

This document also intends to present the details of the different models to be used in BRIDGE and the applicability of the models. It also contains a description of the physics, chemistry and mathematics of the models with a list of references associated to each model and the way that the models will be used in BRIDGE.

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1.4 Project Overview

Urban metabolism considers a city as a system and distinguishes between energy and material flows. "Metabolic" studies are usually top-down approaches that assess the inputs and outputs of food, water, energy, etc. from a city, or that compare the metabolic process of several cities. In contrast, bottom-up approaches are based on quantitative estimates of urban metabolism components at local scale, considering the urban metabolism as the 3D exchange and transformation of energy and matter between a city and its environment. Recent advances in bio-physical sciences have led to new methods to estimate energy, water, carbon and pollutants fluxes. However, there is poor communication of new knowledge to end-users, such as planners, architects and engineers.

BRIDGE aims at illustrating the advantages of considering environmental issues in urban planning. BRIDGE will not perform a complete life cycle analysis or whole system urban metabolism, but rather focuses on specific metabolism components (energy, water, carbon, pollutants). BRIDGE's main goal is to develop a Decision Support System (DSS) which has the potential to propose modifications on the metabolism of urban systems towards sustainability.

BRIDGE is a joint effort of 14 Organizations from 11 EU countries. Helsinki, Athens, London, Firenze and Gliwice have been selected as case study cities. The project uses a "Community of Practice" approach, which means that local stakeholders and scientists of the BRIDGE meet on a regular basis to learn from each other. The end-users are therefore involved in the project from the beginning. The energy and water fluxes are measured and modelled at local scale. The fluxes of carbon and pollutants are modelled and their spatio-temporal distributions are estimated. These fluxes are simulated in a 3D context and also dynamically by using state-of-the-art numerical models, which normally simulate the complexity of the urban dynamical process exploiting the

power and capabilities of modern computer platforms. The output of the above models lead to indicators which define the state of the urban environment. The end-users decide on the objectives that correspond to their needs and determine objectives' relative importance. Once the objectives have been determined, a set of associated criteria are developed to link the objectives with the indicators. BRIDGE integrate key environmental and socio-economic considerations into urban planning through Strategic Environmental Assessment. The BRIDGE DSS evaluates how planning alternatives can modify the physical flows of the above urban metabolism components. A Multi-criteria Decision Making approach has been adopted in BRIDGE DSS. To cope with the complexity of urban metabolism issues, the objectives measure the intensity of the interactions among the different elements in the system and its environment. The objectives are related to the fluxes of energy, water, carbon and pollutants in the case studies. The evaluation of the performance of each alternative is done in accordance with the developed scales for each criterion to measure the performance of individual alternatives.

Several studies have addressed urban metabolism issues, but few have integrated the development of numerical tools and methodologies for the analysis of fluxes between a city and its environment with its validation and application in terms of future development alternatives, based on environmental and socio-economic indicators for baseline and extreme situations. The innovation of BRIDGE lies in the development of a DSS integrating the bio-physical observations with socio-economic issues. It allows end-users to evaluate several urban planning alternatives based on their initial identification of planning objectives. In this way, sustainable planning strategies will be proposed based on quantitative assessments of energy, water, carbon and pollutants fluxes.

2. Description of Models

2.1 The role of numerical modelling in the scope of BRIDGE

Numerical air quality modelling is a powerful tool for air quality evaluation and management. Its application has been defined and recommended throughout EU's air quality legislation [96/62/EC, COM(2001), 2008/50/EC] to provide an adequate level of information on ambient air quality. In the framework of CAFE, modelling techniques have been used to study the repercussions of emission reduction scenarios in air quality levels, namely on ozone and particulate matter concentrations and their impacts on human health and vegetation [Thunis et al., 2007; Vautard et al., 2007].

An atmospheric numerical model is a computerized mathematical representation of the dynamical, physical, chemical and radiative processes in the atmosphere. Modern atmospheric science is a field that combines meteorology, physics, mathematics, chemistry, and computer sciences; other sciences such as geology, biology and oceanographic sciences are also involved to a lesser extent in the so called Earth System Models.

Until the 1940s scientific studies of the atmosphere were limited to the weather, since then the growing awareness of air pollution problems lead to a rapid increase of air pollution studies, and computer modelling of meteorology and air pollution slowly emerged [Jacobson, 1999].

In the 1950's laboratory work was undertaken to better understand the formation of photochemical and London-type smog; also the emergence of computers allowed the implementation of box models for the simulation of atmospheric chemical reactions. Between the 1950's and the 1970's air quality models were expanded to three dimensions, and included the treatment of transport, deposition, emissions, and chemistry [Jacobson, 1999]. In the beginning these models used observed meteorological data as input; shortly after outputs from meteorological models were used as inputs to air quality models [Pielke et al., 1992].

Nowadays the majority of the modelling systems for the study of air pollution comprise a meteorological model and an air quality model. These can be linked off-line or on-line: in the first the meteorological simulation is performed first and its outputs are fed into the chemical model; whereas in the second both the meteorology and chemistry simulations are performed at the same time on the same grid, therefore existing feed-back mechanisms between the two models.

The primary meteorological variables in a model are wind speed, wind direction, air temperature, air density, air pressure and water content. These variables are simulated by solving a set of partial differential equations and parameterized equations, including the momentum equation, the thermodynamic energy equation, the continuity equation of air, the equation of state, and the continuity equation for total water. Changes in concentrations of gaseous and particulate species are found by solving ordinary differential equations that describe chemistry and physics and partial differential equations that describe transport [Jacobson, 1999].

Over the past few years there has been a growing need to simulate meteorological fields for complex situations at higher spatial resolutions. This has been partly stimulated by the scientific and technological advances and partly by policy pressures requiring more detailed assessment of air pollution on urban to regional scales. As a consequence, complex dynamical models have been

increasingly used in Europe and the USA for meteorological and air pollution applications [COST728, 2005].

Atmospheric problems can be simulated over a variety of spatial scales. Molecular-scale motions occur over distances much smaller than 2 mm (ex. molecular diffusion); microscale motions occur over distances of 2 mm to 2 km (ex. swirling motions of air); mesoscale motions occur over distances 2-2000 km (ex. thunderstorms); and finally the synoptic scale covers motions or events on a scale of 500-10000 km (ex. pressure systems) [Jacobson, 1999]. Mesoscale studies spatial scales range from tens of kilometres (urban scale) to some thousands (regional scale); this is the scale representative of many of the air pollution problems [Moussiopoulos, 1996].

There is currently a wide variety of models steaming from the diversity in spatial and temporal scales, since different scales demand different approximations and parameterizations. For a classical Gaussian model, surface data from a single meteorological station are enough, since this type of model considers that these are applicable to the entire simulation domain and no variations with height are found. Most updated Gaussian models – the so called second generation – allows dispersion parameters to have a continuous variation with the atmospheric stability. Using vertical measurements of meteorological parameters, such as upper air soundings, the models calculates the parameters that describes the PBL: friction velocity, Monin-Obukhov length, convective velocity scale, temperature scale, mixing height and surface heat flux. This parameters are then used to calculate wind vertical profiles, turbulent fluctuations, potential temperature gradient and potential temperature, allowing a more realistic dispersion formulation.

Lagrangean and Eulerian models allow the variation of meteorological conditions along the domain, horizontal and vertically. For the simulation of complex meteorological conditions three-dimensional models are advised; these can be classified as diagnostic or prognostic models. Diagnostic models use available local meteorological to determine meteorological variables over the simulation domain through interpolation or extrapolation techniques; meteorological fields calculated for each time step are independent on previous time-steps results. Prognostic meteorological models are initialized by large scale synoptic analysis, and numerically solve atmospheric dynamics equations in order to determine local meteorological conditions [Seinfeld and Pandis, 1998]. Often these models have nesting capabilities that allow the consideration of a first regional domain (500–1000 km) with a coarse resolution, and afterwards successive smaller nests to cover a specific area (1-10 km) at higher resolutions.

Meteorological models able to resolve mesoscale processes (1-200 km) are considered to be important tools in future air pollution assessments because they allow for sufficiently high spatial and temporal resolution and can trace back the linkages between sources and impacts of long travel distances and times. Additionally they can accommodate a wide range of specific local conditions. However, the meso-meteorological capabilities of meteorological models are generally not specifically optimized for pollution applications, namely in urban areas. For example, meteorological models contain options for treating processes which the users must select themselves, such as the boundary layer parameterization to use. Also, situations which present huge challenges for meteorological models include dispersion in very stable, or low wind speed conditions, as well as very unstable conditions, which generally lead to the production of secondary pollutants, such as ozone [COST728, 2005].

Meteorological mesoscale models have been developed in most European countries for flow simulations and for dispersion studies. Public/research domain versions are available from

European and US National Weather Services (NWS) and other agencies. Models such as MM5 [Dudhia et al., 1993] are more commonly employed as meteorological pre-processors/drivers for photochemical models and have demonstrated their usefulness for air pollution assessment down to spatial resolutions of 1 km and temporal resolutions of 1 hour [COST728, 2005]. Other research models which have been similarly employed include WRF [Grell et al., 2005], ALADIN [URL7], RAMS [Pielke et al., 1992], MEMO [Moussioupoulos et al., 1994], MESO-NH [Cousin et al., 2005], and METRAS [Schlünzen, H. K., 1988].

Air quality models simulate the transport, dispersion and chemical transformation of pollutants, therefore allowing the assessment of a variety of emission sources in a given region in the concentration and deposition of reactive and inert chemical species. Air quality models can be further classified according to their mathematical formulation as Lagragean or Eulerian models. Lagrangean models consider that the air parcel moves with the local wind so that there is no mass exchange that is allowed to enter the air parcel and its surroundings (except of species emissions). The air parcel moves continuously and the length and direction of the dislocation are determined through the average wind speed and direction for each time step of the calculation [Draxier and Hess, 1998]. Eulerian models consider a fixed three-dimensional cartesian grid as a frame of reference rather than a moving frame of reference; these models are also known as grid models due to their three-dimensional grid. The emission of pollutants is considered for each cell, and the pollutants go through the grid under the influence of the atmospheric flow, undergoing physical and chemical transformations.

Eulerian models are therefore more demanding in computational terms than Lagrangean models. The treatment of individual processes in Eulerian models can be more or less complex, thus these vary widely in vertical resolution, parameterizations, initialization methods and boundary conditions, and also in the used numerical techniques [Reid et al., 2007].

Three-dimensional air quality Eulerian models were firstly developed and applied extensively to study ozone related pollution [Moussiopoulos, 1996]; more recently, developments have focused on the chemical simulation of aerossols [Hass et al., 2003; Bessagnet et al., 2004; Van Dingenen et al., 2004]. The simulation of photochemical processes demands the inclusion of a group of chemical reactions responsible for ozone formation and the respective parameterization of reaction rates. These, together with the integration of transport, diffusion and deposition processes (dictated by meteorology) and anthropogenic and biogenic emissions, allow the estimation of several air pollutants [Seinfeld and Pandis, 1998].

Air quality models need to be evaluated in order to be used with confidence at the scientific and policy levels, therefore its application must always be accompanied by a set of quality control and quality assurance procedures, and preferably an uncertainty estimation analysis should be conducted [Borrego et al., 2008]. Currently, many air quality models exist for the simulation of gaseous and particulate chemistry at regional scales. Some examples are the European models EMEP, LOTOS-EUROS and CHIMERE [Van Loon, 2004; Vautard et al., 2007], the American models CMAQ and CAMx [Tesche et al., 2006] or the Australian model TAPM [Hurley et al., 2003]. However, this type of models doesn't have the capability for describing in detail the behaviour of flow and pollutants dispersion within urban areas, especially inside the street-canyons. In fact, the street scale is of particular interest for urban air quality as it is the smallest scale that encompasses one of the main pollutant sources, the vehicles, and an important receptor, the citizens. The term street canyon ideally refers to a relatively narrow street with buildings lined

up continuously along both sides [Nicholson, 1975]. However, the same term has been used to refer to larger streets, also called avenue canyons. In the real world, a broader definition of the term has been applied, including urban streets that are not necessarily flanked by buildings continuously on both sides, allowing thus for some openings on the walls of the canyon.

A street canyon constitutes the basic geometric unit of urban areas. This unit is also bounded by the ground surface at the bottom and the roof level at the top. It has a distinct climate where micro-scale meteorological processes dominate [Oke, 1988] and the air ventilation and pollutant removal are mainly through the roof level. The most important features of street-canyon micro-climate are the wind-induced flow patterns, such as air recirculation. These unique micro-scale meteorological processes not only affect the local air quality but also the comfort of the city inhabitants [Bottema, 1993].

The average level of the pollutant concentrations within the street canyon is a balance between the emissions within the canyon, and the exchange of pollutants between the street canyon and the flow above, and/or with other streets. The exchange is a two-way process with street-sourced material being removed and material from other sources upwind being brought into the street [Britter, 2003].

There is a plethora of different air quality models specially developed for, or simply used, in local or street canyon applications with domain sizes of several tens of metres to a few kilometres (street canyons, city quarters). For the urban area it is thus possible to distinguish different local scale models: statistical, receptor, screening, box, street canyon, Gaussian and computational fluid dynamics (CFD). The physical and/or mathematical principles allow distinguishing between the different models.

With the continuous increase of hardware capabilities and the optimisation of numerical methods, CFD has become an attractive tool to predict flow and concentration fields near buildings. CFD modelling is a general term used to describe the analysis of systems involving fluid flow, heat transfer and associated phenomena (e.g. chemical reactions) by means of computer-based numerical methods. It is a powerful modelling technique spanning a wide range of industrial, environmental and even biomedical applications [Gosman, 1999]. Many works can be found in the literature reporting on the use of computational fluid dynamics techniques to model flow and pollutant dispersion around isolated buildings or groups of buildings [Borrego *et al.*, 2003; Li *et al.*, 2006; Neofytou *et al.*, 2006; Sabatino *et al.*, 2007]. CFD's are the only models that allow a detailed estimation of spatial and temporal distribution of air pollutants in complex urban areas, contributing to the identification of sensitive urban areas in terms of air quality and with potential harmful effects to human health.

CFD can be divided into Reynolds averaged Navier-Stokes equation (RANS) modelling and Large Eddy Simulation (LES). RANS is a CFD method that uses turbulence models to simulate the turbulent flow. This type of model is currently the industrial standard in engineering practice. RANS can be modified to handle urban and microscale wind flow problems and are the most commonly adopted CFD models in calculating street-canyon wind flow.

The home-made CFD codes VADIS (Borrego et al., 2003), CHENSI (Levi Alvares and Sini, 1992), MISKAM (Eichhorn, 1995) and MIMO (Ehrhard et al., 2000) are examples of RANS models that were specially designed to simulate pollutant dispersion at local scale. Furthermore, there are a number of commercially general-purpose CFD codes available (FLUENT, STAR-CD

and CFX-TASCflow) that have been used for the simulation of pollutants dispersion within complex urban geometries (Martins et al., 2009; Riddle et al., 2004). In LES modelling the time-dependent flow equations are solved for the mean flow and the largest eddies, whereas the effects of the small eddies are modelled. Compared with RANS models, LES has the advantage of describing the large scale turbulent structures and hence, can be used in a more accurate and reliable way in the prediction of the flows over bluff bodies that involve unsteady separation and vortex shedding [Yang, 2004]. However, this technique is presently at the research stage and the calculations are too costly to merit consideration in the current computation capabilities.

2.2 Air Quality Models

2.2.1 Mesoscale Modelling

Mesoscale meteorological and air quality models have had a substantial advance during the last decades. Nowadays, we have complex and accurate models which can simulate the air quality concentrations in large areas with a good spatial resolution. Essentially, global models are currently simulating the air concentrations at global scale with a resolution of about 1º or 0.5º. Global models are traditionally run in supercomputer environment and they are separate into two different areas: meteorology and dispersion of pollutants (chemical models). There is a group of global meteorological and chemical models. Global Climate Models (GCMs) are a particular branch of the general global modeling area. Global climate models are running for hundreds or thousands of years reproducing the past times and forecasting the future climate. Short term meteorological and chemical models are used up to a few weeks or months in the future. Examples of global meteorological and chemical models are: CCM3, MOZART and GISS. Mesoscale models are using boundary conditions provided by the global modeling tools. The spatial resolution for mesoscale models is ranging between a few hundreds of meters and several kilometers. Examples of mesoscale meteorological models are: MM5 and WRF. The last version of WRF (WRF-UCM) includes a module called “urban canopy model” which describes the partition of surface heat fluxes and the changes in vertical meteorological variables (T, q, w,v, w) due to the urban canopy layer which is created as a consequence of the urban roughness and the canyon streets. UCM is an idealized urbanized model which assumes an averaged idealized canyon street into grid cells of about 200 x 200 m with a specific inclination. Chemical and dispersion mesoscale models are represented by CMAQ, CHIMERE or CAMx models which include several carbon chemical mechanisms to estimate the formation/destruction of secondary pollutants such as ozone or PAN. WRF/CHEM is a meteorological and chemical mesoscale model (including UCM) which belongs to the so-called “on-line” models in the sense that chemistry is calculated in every meteorological time step with the feedback effects on solar radiation and other meteorological aspects. The computer demand is much higher than in the case of pure meteorology (WRF) and the dispersion (CMAQ) running apart (Figure 1). There are mesoscale applications of climate models such as RCM3. The next step is to use the so-called CFD (Computational Fluid Dynamics) models which can be run over limited areas with a very high spatial resolution (a few meters). All models are based on the Navier-Stokes Equation System and the numerical solution. Examples of CFD models are: MICROSYS based on the MEMO model (University of Karlsruhe, Germany) and EULAG model (UCAR). The computational requirements for the CFD codes are very high and they can only be used for limited periods of time and spatial domains.

The classical mesoscale meteorological models – such as MM5 or WRF - use a dynamics solver which integrated the compressible, non-hydrostatic Euler equations. The equations are usually written in flux form using variables that have conservation properties, following the philosophy of Ooyama (1990). The equations are formulated using terrain-following mass vertical coordinate (Laprise, 1992). The models usually support four projections to the sphere – the Lambert conformal, the polar stereographic, the Mercator grids and latitude-longitude projections. The transformations are isotropic for three of these projections – the Lambert conformal, polar stereographic and Mercator grids. Before constructing the discrete solver, it is advantageous to recast the governing equations using perturbation variables to reduce truncation errors in the horizontal pressure gradient calculations. For this purpose, new variables are defined as perturbations from a hydrostatically-balanced reference state, and we define reference state variables that are a function of height only and that satisfy the governing equations for an atmosphere at rest. The model solver uses a time-split integration scheme. Generally speaking, slow or low-frequency (meteorologically significant) modes are integrated using a third-order Runge-Kutta (RK3) time integration scheme, while the high-frequency acoustic modes are integrated over smaller time steps to maintain numerical stability. The horizontally propagating acoustic modes (including the external mode present in the mass-coordinate equations using a constant-pressure upper boundary condition) and gravity waves are integrated using a forward-backward time integration scheme, and vertically propagating acoustic modes and buoyancy oscillations are integrated using a vertically implicit scheme (using the acoustic time step). The time-split integration for the flux-form equations is described and analyzed in Klemp et al. (2007). The time-splitting is similar to that first developed by Klemp and Wilhelmson (1978) for leapfrog time integration and analyzed by Skamarock and Klemp (1992). This time-split approach was extended to the RK3 scheme as described in Wicker and Skamarock (2002). The primary differences between the earlier implementations described in the references and the ARW implementation are associated with our use of the mass vertical coordinate and a flux-form set of equations, as described in Klemp et al. (2007), along with our use of perturbation variables for the acoustic component of the time-split integration. The acoustic-mode integration is cast in the form of a correction to the RK3 integration. The spatial discretization of the model uses typically a C grid staggering That is, normal velocities are staggered one-half grid length from the thermodynamic variables. The diagnostic variables used in the model, the pressure *p* and inverse density ′, are computed at mass points. See Figure 2.2.1.1.

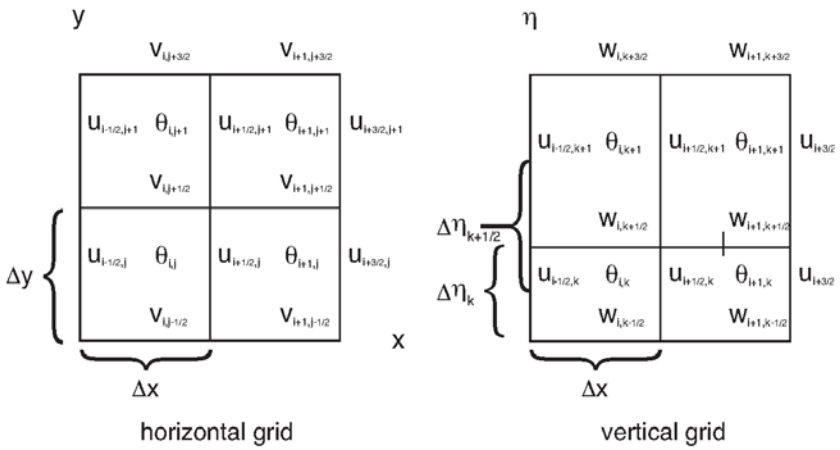

Figure 2.2. 1.1 Horizontal and vertical grids in WRF (ARW) model.

In WRF(ARW) the The RK3 time step is limited by the advective Courant number $u\Delta t/\Delta x$ and the user's choice of advection schemes— users can choose 2^{nd} through 6^{th} order discretizations for the advection terms. The time-step limitations for 1D advection in the RK3 scheme using these advection schemes is given in Wicker and Skamarock (2002), and is reproduced here.

Time Scheme	Spatial order			
	3rd	4th	5th	6th
Leapfrog	Unstable	0.72	Unstable	0.62
RK2	0.88	Unstable	0.30	Unstable
RK3	1.61	1.26	1.42	1.08

Table 2.2.1.1 Maximum stable Courant numbers for one-dimensional linear advection. From Wicker and Skamarock (2002).

As is indicated in the table, the maximum stable Courant numbers for advection in the RK3 scheme are almost a factor of two greater than those for the leapfrog time-integration scheme. For advection in three spatial dimensions, the maximum stable Courant number is 1/ 3 times the Courant numbers given in Table 3.1.1.1.. For stability, the time step used in the ARW should produce a maximum Courant number less than that given by theory. Thus, for 3D applications, the time step should satisfy the following equation:

$$\Delta t_{max} < \frac{Cr_{theory}}{\sqrt{3}} \cdot \frac{\Delta x}{u_{max}},$$

Where Cr_{theory} is the Courant number which has been taken from RK3 method in Table 3.1.1.1. and the u_{max} is the maximum velocity expected during the simulation. For example in real-data applications, where jet stream winds may reach as high as 100 ms^{-1}, the maximum time step would be approximately 80 s on a $\Delta x = 10$ km grid using 5^{th} order advection. For convection-permitting resolutions (typically $\Delta x \leq 5$ km), the vertical velocities in convective updrafts produce the stability-limiting Courant numbers. Given additional constraint from the time splitting, and to provide a safety buffer, we usually choose a time step that is approximately 25% less than that given in above expression. In MM5 model, the rule of thumb for choosing a time step is that the time step, in seconds, should be approximately 3 times the horizontal grid distance, in kilometers. For the WRF (ARW), the time step (in seconds) should be approximately 6 times the grid distance (in kilometers).

The nesting capabilities we mentioned before are generally restricted to a few of possibilities according to the following schemes:

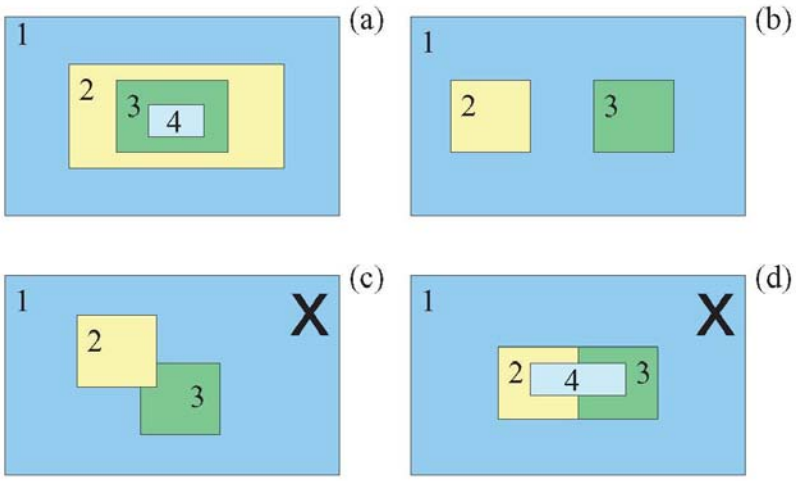

Figure 2.2.1.2. Various nest configurations for multiple grids. (a) Telescoping nests. (b) Nests at the same level with respect to a parent grid. (c) Overlapping grids: not allowed (d) Inner-most grid has more than one parent grid: not allowed.

The WRF model (and similar models) includes several microphysics schemes such as Kessler, Purdue Lin, WSM3, WSM5, WSM6, Eta GCP, Thompson, Goddard and Morrisson 2-Moment. It also includes cloud schemes which are responsible for the sub-grid scale effects of convective and/or shallow clouds. The schemes are intended to represent vertical fluxes due to unresolved updrafts and downdrafts and compensating motion outside the clouds. They operate only on individual columns where the scheme is triggered and provide vertical heating and moistening profiles. Some schemes additionally provide cloud and precipitation field tendencies in the column, and future schemes may provide momentum tendencies due to convective transport of momentum. The schemes all provide the convective component of surface rainfall. Several cumulus parameterization schemes can be chosen such as: Kain-Fritsch scheme, Betts-Miller-Janjic scheme, Grell-Devenyi ensemble scheme and Grell-3 scheme.

The surface layer schemes calculate friction velocities and exchange coefficients that enable the calculation of surface heat and moisture fluxes by the land-surface models and surface stress in the planetary boundary layer scheme. Over water surfaces, the surface fluxes and surface diagnostic fields are computed in the surface layer scheme itself. The schemes provide no tendencies, only the stability-dependent information about the surface layer for the land-surface and PBL schemes. Currently, each surface layer option is tied to particular boundary-layer options, but in the future more interchangeability and options may become available. Note that some boundary layer schemes (YSU and MRF) require the thickness of the surface layer in the model to be representative of the actual surface layer (e.g. 50-100 meters). Several schemes are available such as: Similarity Theory (MM5, Eta, Px) from contributions from: Paulson (1970), Dyer and Hicks (1970), (Janjic, 1996, 2002) mand (Pleim, 2006).

The land-surface model (LSMs) use atmospheric information from the surface layer scheme, radiative forcing from the radiation scheme, and precipitation forcing from the microphysics and convective schemes, together with internal information on the land's state variables and land-surface properties, to provide heat and moisture fluxes over land points and sea-ice points. These fluxes provide a lower boundary condition for the vertical transport done in the PBL

schemes (or the vertical diffusion scheme in the case where a PBL scheme is not run, such as in large-eddy mode). The landsurface model provides no tendencies, but does update the land's state variables which include the ground (skin) temperature, soil temperature profile, soil moisture profile, snow cover, and possibly canopy properties. There is no horizontal interaction between neighboring points in the LSM, so it can be regarded as a one-dimensional column model for each WRF land grid-point, and many LSMs can be run in a stand-alone mode. Several Land-surface models are available such as: 5-layer thermal diffusion, Noah LSM, Rapid update Cycle (RUC) model, the Ocean mixed layer model and the Pleim-Xiu model. The urban canopy model will be described separately.

The planetary boundary layer (PBL) is responsible for vertical sub-grid-scale fluxes due to eddy transports in the whole atmospheric column, not just the boundary layer. Thus, when a PBL scheme is activated, explicit vertical diffusion is de-activated with the assumption that the PBL scheme will handle this process. The most appropriate horizontal diffusion choices are those based on horizontal deformation or constant *Kh* values where horizontal and vertical mixing are treated independently. The surface fluxes are provided by the surface layer and land-surface schemes. The PBL schemes determine the flux profiles within the well-mixed boundary layer and the stable layer, and thus provide atmospheric tendencies of temperature, moisture (including clouds), and horizontal momentum in the entire atmospheric column. Most PBL schemes consider dry mixing, but can also include saturation effects in the vertical stability that determines the mixing. The schemes are one-dimensional, and assume that there is a clear scale separation between sub-grid eddies and resolved eddies. This assumption will become less clear at grid sizes below a few hundred meters, where boundary layer eddies may start to be resolved, and in these situations the scheme should be replaced by a fully three-dimensional local sub-grid turbulence scheme such as the TKE diffusion scheme. Several schemes are available such as: Medium Range Forecast Model (MRF), Yonsei University Model (YSU), Mellor-Yamada_Janjic Model (MYJ) and Asymetrical Convective Model version 2 (ACM2).

The atmospheric radiation models provide atmospheric heating due to radiative flux divergence and surface downward longwave and shortwave radiation for the ground heat budget. Longwave radiation includes infrared or thermal radiation absorbed and emitted by gases and surfaces. Upward longwave radiative flux from the ground is determined by the surface emissivity that in turn depends upon land-use type, as well as the ground (skin) temperature. Shortwave radiation includes visible and surrounding wavelengths that make up the solar spectrum. Hence, the only source is the Sun, but processes include absorption, reflection, and scattering in the atmosphere and at surfaces. For shortwave radiation, the upward flux is the reflection due to surface albedo. Within the atmosphere the radiation responds to model-predicted cloud and water vapor distributions, as well as specified carbon dioxide, ozone, and (optionally) trace gas concentrations. All the radiation schemes in WRF are column (one-dimensional) schemes, so each column is treated independently, and the fluxes correspond to those in infinite horizontally uniform planes, which is a good approximation if the vertical thickness of the model layers is much less than the horizontal grid length. This assumption would become less accurate at high horizontal resolution. Several schemes are available such as: Rapid Radiative Transfer Model (RRTM) longwave, Eta Geophysical Fluid Dynamics Laboratory (GFDL) longwave model, CAM Longwave model, Eta Geophysical Fluid Dynamics Laboratory (GFDL) shortwave model, MM5 Dudhia shortwave model, Goddard shortwave model and CAM shortwave model.

The MM5 and WRF models include also Four Dimensional Data Assimilation schemes, also known as nudging, which is a method of keeping simulations close to analyses and/or observations over the course of an integration. There are two types of FDDA that can be used separately or in combination. Grid- or analysis-nudging simply forces the model simulation towards a series of analyses grid-point by grid-point. Observational or station-nudging locally forces the simulation towards observational data. These methods provide a four-dimensional analysis that is somewhat balanced dynamically, and in terms of continuity, while allowing for complex local topographical or convective variations. Such datasets can cover long periods, and have particular value in driving off-line air quality or atmospheric chemistry models.. Several assimilation methods can be selected such as: Grid nudging or Analysis nudging, Observational or station nudging, 3d-Var and 4-D Var.

2.2.2 Local scale Modelling

As we have mentioned, local scale modelling is dealing with those scales in a range between 1 – 30 km. The spatial resolution of the models dealing with this scale is a few meters and there are a large number of models involved on the study of this atmospheric scale. As we have also mentioned, atmospheric process are occurring simultaneously and there is only “one atmosphere”. The need to impose several scales and somehow different approaches for studying each scale is imposed because of the computer limitations and limited knowledge on atmospheric parameterizations. However, the tendency is to use one approach to model all scales from global to street level. Numerical models appear to be the best option to have a comprehensive approach to this huge task however several simple parameterizations and models continue to be used because of the simplicity and the capability to provide fast responses to complex problems particularly when the objective is quite specific or require very long term simulations. Nowadays, global scale models require the use of supercomputers and a considerable amount of skills and computer capability (processors). The nesting capability of the numerical models based on the Navier-Stokes equations is one of the key solutions found to keep a high level of consistency between global and continental scales with meso and micro (local) scales. This consistency should be kept not only on the numerics (mass balance maintenance) but also in the physical and chemical parameterizations used to perform the simulations. Local scale modeling is using models which have been born in the context of the computational fluid dynamics (CFD) area which has many applications in the architecture, engineering, etc.

The adaptations of these models to be used as part of the local atmospheric simulations has been done during the last decade or so. Computational fluid dynamics (CFD) is one of the branches of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. Computers are used to perform the millions of calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. Even with high-speed supercomputers only approximate solutions can be achieved in many cases. Ongoing research, however, may yield software that improves the accuracy and speed of complex simulation scenarios such as transonic or turbulent flows. Initial validation of such software is often performed using a wind tunnel with the final validation coming in flight test.

The nesting capability of the numerical models based in Navier-Stokes equations, is used to link the global and continental scales with the meso and micro scales. The nesting capability is based on the proper interpolation in vertical and horizontal axes of the different fields involved in the atmospheric process. The interpolation techniques are not a mass conservative technique unless special care is put to assure this important law. The elegant approach of using similar models to simulate the process in all scales is also held by the reality of the atmospheric process which are not divided in scales by definition ("one atmosphere"). However, nowadays our computer platforms and limited knowledge of the physics and chemistry of the atmospheric process imposes the use of different scales. The distance between microscale process and mesoscale process is still very important and we should keep in mind this important fact when modelling all scales at once (by using the nesting capability of the numerical models).

The stability of the chosen discretization or the spatial resolution is generally established numerically rather than analytically as with simple linear problems. Special care must also be taken to ensure that the discretization handles discontinuous solutions gracefully. The Euler equations and Navier-Stokes equations both admit shocks, and contact surfaces.

Some of the discretization methods being used are:

- Finite volume method (FVM). This is the "classical" or standard approach used most often in commercial software and research codes. The governing equations are solved on discrete control volumes. FVM recasts the PDE's (Partial Differential Equations) of the N-S equation in the conservative form and then discretize this equation. This guarantees the conservation of fluxes through a particular control volume. Though the overall solution will be conservative in nature there is no guarantee that it is the actual solution. Moreover this method is sensitive to distorted elements which can prevent convergence if such elements are in critical flow regions. This integration approach yields a method that is inherently conservative (i.e. quantities such as density remain physically meaningful):

$$\frac{\partial}{\partial t}\iiint Q\,dV + \iint F\,d\mathbf{A} = 0,$$

where Q is the vector of conserved variables, F is the vector of fluxes (see Euler equations or Navier-Stokes equations), V is the cell volume, and $\mathbf{A}$ is the cell surface area.

- Finite element method (FEM). This method is popular for structural analysis of solids, but is also applicable to fluids. The FEM formulation requires, however, special care to ensure a conservative solution. The FEM formulation has been adapted for use with the Navier-Stokes equations. Although in FEM conservation has to be taken care of, it is much more stable than the FVM approach. Subsequently it is the new direction in which CFD is moving. Generally stability/robustness of the solution is better in FEM though for some cases it might take more memory than FVM methods.

  In this method, a weighted residual equation is formed:

$$R_i = \iiint W_i Q \, dV^e$$

where R_i is the equation residual at an element vertex i , Q is the conservation equation expressed on an element basis, W_i is the weight factor and V_e is the volume of the element.

- Finite difference method. This method has historical importance and is simple to program. It is currently only used in few specialized codes. Modern finite difference codes make use of an embedded boundary for handling complex geometries making these codes highly efficient and accurate. Other ways to handle geometries are using overlapping-grids, where the solution is interpolated across each grid.

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = 0$$

Where *Q* is the vector of conserved variables, and *F*, *G*, and *H* are the fluxes in the *x*, *y*, and *z* directions respectively.

- Boundary element method. The boundary occupied by the fluid is divided into surface mesh.
- High-resolution schemes are used where shocks or discontinuities are present. To capture sharp changes in the solution requires the use of second or higher order numerical schemes that do not introduce spurious oscillations. This usually necessitates the application of flux limiters to ensure that the solution is total variation diminishing.

2.2.3 Turbulence models

Turbulent flow produces fluid interaction at a large range of length scales. This problem means that it is required that for a turbulent flow regime calculations must attempt to take this into account by modifying the Navier-Stokes equations. Failure to do so may result in an unsteady simulation. When solving the turbulence model there exists a trade-off between accuracy and speed of computation.

2.2.3.1 Direct numerical simulation

Direct numerical simulation (DNS) captures all of the relevant scales of turbulent motion, so no model is needed for the smallest scales. This approach is extremely expensive, if not intractable, for complex problems on modern computing machines, hence the need for models to represent the smallest scales of fluid motion.

2.2.3.2 Reynolds-averaged Navier–Stokes

Reynolds-averaged Navier-Stokes (RANS) equations are the oldest approach to turbulence modeling. An ensemble version of the governing equations is solved, which introduces new *apparent stresses* known as Reynolds stresses. This adds a second order tensor of unknowns for which various models can provide different levels of closure. It is a common misconception that the RANS equations do not apply to flows with a time-varying mean flow because these equations are 'time-averaged'. In fact, statistically unsteady (or non-stationary) flows can equally be treated. This is sometimes referred to as URANS. There is nothing inherent in Reynolds averaging to

preclude this, but the turbulence models used to close the equations are valid only as long as the time scale of these changes in the mean is large compared to the time scales of the turbulent motion containing most of the energy.

RANS models can be divided into two broad approaches:

Boussinesq hypothesis

This method involves using an algebraic equation for the Reynolds stresses which include determining the turbulent viscosity, and depending on the level of sophistication of the model, solving transport equations for determining the turbulent kinetic energy and dissipation. Models include k-ε (Spalding), Mixing Length Model (Prandtl) and Zero Equation (Chen). The models available in this approach are often referred to by the number of transport equations they include, for example the Mixing Length model is a "Zero Equation" model because no transport equations are solved, and the k-ε on the other hand is a "Two Equation" model because two transport equations are solved.

Reynolds stress model (RSM)

This approach attempts to actually solve transport equations for the Reynolds stresses. This means introduction of several transport equations for all the Reynolds stresses and hence this approach is much more costly in CPU effort.

2.2.3.3 Large eddy simulation

Large eddy simulations (LES) is a technique in which the smaller eddies are filtered and are modeled using a sub-grid scale model, while the larger energy carrying eddies are simulated. This method generally requires a more refined mesh than a RANS model, but a far coarser mesh than a DNS solution.

2.2.3.4 Detached eddy simulation

Detached eddy simulations (DES) is a modification of a RANS model in which the model switches to a subgrid scale formulation in regions fine enough for LES calculations. Regions near solid boundaries and where the turbulent length scale is less than the maximum grid dimension are assigned the RANS mode of solution. As the turbulent length scale exceeds the grid dimension, the regions are solved using the LES mode. Therefore the grid resolution for DES is not as demanding as pure LES, thereby considerably cutting down the cost of the computation. Though DES was initially formulated for the Spalart-Allmaras model (Spalart et al., 1997), it can be implemented with other RANS models (Strelets, 2001), by appropriately modifying the length scale which is explicitly or implicitly involved in the RANS model. So while Spalart-Allmaras model based DES acts as LES with a wall model, DES based on other models (like two equation models) behave as a hybrid RANS-LES model. Grid generation is more complicated than for a simple RANS or LES case due to the RANS-LES switch. DES is a non-zonal approach and provides a single smooth velocity field across the RANS and the LES regions of the solutions.

2.2.3.5 Vortex method

The Vortex method is a grid-free technique for the simulation of turbulent flows. It uses vortices as the computational elements, mimicking the physical structures in turbulence. Vortex methods

were developed as a grid-free methodology that would not be limited by the fundamental smoothing effects associated with grid-based methods. To be practical, however, vortex methods require means for rapidly computing velocities from the vortex elements – in other words they require the solution to a particular form of the N-body problem (in which the motion of N objects is tied to their mutual influences). A long-sought breakthrough came in the late 1980's with the development of the Fast Multipole Method (FMM), an algorithm that has been heralded as one of the top ten advances in numerical science of the 20th century. This breakthrough paved the way to practical computation of the velocities from the vortex elements and is the basis of successful algorithms.

Software based on the Vortex method offer the engineer a new means for solving tough fluid dynamics problems with minimal user intervention. All that is required is specification of problem geometry and setting of boundary and initial conditions. Among the significant advantages of this modern technology;

- It is practically grid-free, thus eliminating numerous iterations associated with RANS and LES.
- All problems are treated identically. No modeling or calibration inputs are required.
- Time-series simulations, which are crucial for correct analysis of acoustics, are possible.
- The small scale and large scale are accurately simulated at the same time.

2.2.4 Two phase flow

The modeling of two-phase flow is still under development. Different methods have been proposed. The Volume of fluid method gets a lot of attention lately, but Level set and front tracking are also valuable approaches Most of these methods are either good in maintaining a sharp interface or at conserving mass. This is crucial since the evaluation of the density, viscosity and surface tension in based on the values averaged over the interface.

2.2.5 Solution algorithms

Discretization in space produces a system of ordinary differential equations for unsteady problems and algebraic equations for steady problems. Implicit or semi-implicit methods are generally used to integrate the ordinary differential equations, producing a system of (usually) nonlinear algebraic equations. Applying a Newton or Picard iteration produces a system of linear equations which is nonsymmetric in the presence of advection and indefinite in the presence of incompressibility. Such systems, particularly in 3D, are frequently too large for direct solvers, so iterative methods are used, either stationary methods such as successive overrelaxation or Krylov subspace methods. Krylov methods such as GMRES, typically used with preconditioning, operate by minimizing the residual over successive subspaces generated by the preconditioned operator.

Multigrid is especially popular, both as a solver and as a preconditioner, due to its asymptotically optimal performance on many problems. Traditional solvers and preconditioners are effective at reducing high-frequency components of the residual, but low-frequency components typically require many iterations to reduce. By operating on multiple scales, multigrid reduces all components of the residual by similar factors, leading to a mesh-independent number of iterations.

For indefinite systems, preconditioners such as incomplete LU factorization, additive Schwarz, and multigrid perform poorly or fail entirely, so the problem structure must be used for effective preconditioning. The traditional methods commonly used in CFD are the SIMPLE and Uzawa algorithms which exhibit mesh-dependent convergence rates, but recent advances based on block LU factorization combined with multigrid for the resulting definite systems, have led to preconditioners which deliver mesh-independent convergence rates.

2.3 Urban canopy models

Mesoscale meteorological models are often modified to analyze urban heat islands (e.g., Seaman et al., 1989; Kimura and Takahashi, 1991; Ichinose et al., 1999; Taha, 1999; Kusaka et al., 2000; Kanda et al., 2001). According to Taha (1999), there are two ways to modify the models: (i) Vary the soil constants (e.g., heat capacity and thermal conductivity) and parameters (e.g., surface albedo, roughness length, and moisture availability) that are used in the heat balance equation at the surface; (ii) couple an urban canopy-layer model with an atmospheric model. The first approach is the more common, and most of the above studies used the slab model in a mesoscale model. The actual WRF model includes a Urban Canopy model (UCM) which includes several of the following characteristics. The slab model treats the urban geometry as a flat surface with a large roughness length and small albedo. Hence, approach (i) assumes that buildings and roads have the same temperature, and treats the building height and coverage ratio implicitly in the surface layer. However, to increase the accuracy, more explicit estimates of the effects of urban geometry on the heat island are needed. But, a new approach should contain easily set-up parameters. Such urban geometric effects include the building coverage ratio and differences in physical constants between buildings and roads. For these improvements, approach (ii), an urban canopy-layer model for atmospheric models, is needed. Many canyon models have been developed to study the influence of canyon characteristics on facet energy budgets, surface temperatures, or winds within canyons (Johnson et al., 1991; Mills, 1993; Arnfield et al., 1998). Hence, most were not designed specifically for atmospheric models. Recently, Kondo and Liu (1998), Kondo et al. (1999), and Vu et al. (1999) developed multi-layer urban canopy models.

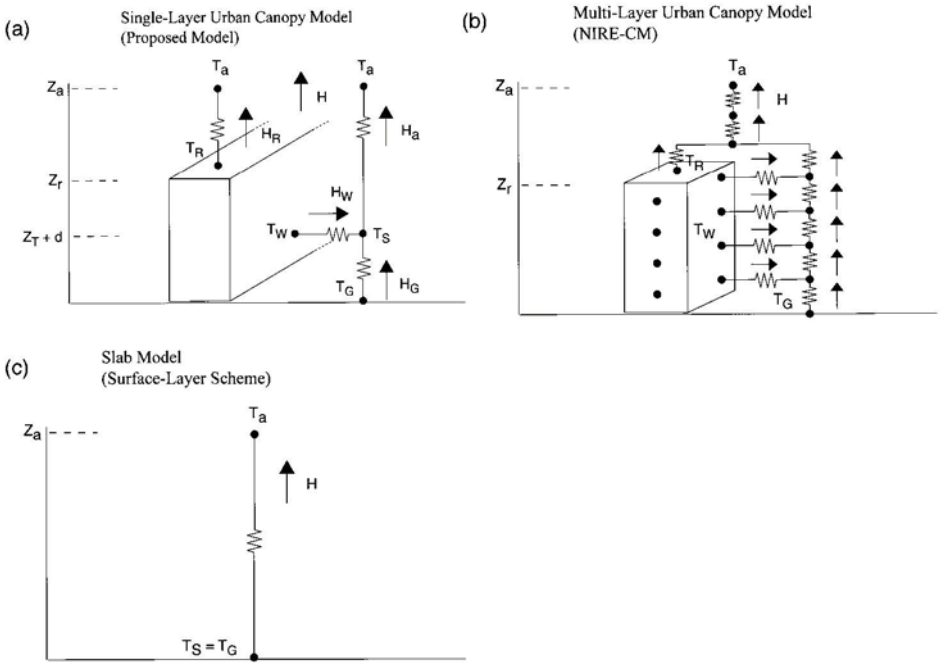

Figure 2.3.1 Energy fluxes and temperatures for the three models. (a) The proposed single-layer urbancanopy model: *Ta* is the air temperature at reference height *za*, *TR* the building roof temperature, *TW*the building wall temperature, *TG* the road temperature, and *TS* the temperature defined at *zT+ d*. *H* is the sensible heat exchange at the reference height. *Ha* is the sensible heat flux from the canyonspace to the atmosphere; similarly, *HW* is that from wall to the canyon space, *HG* that from roadto the canyon space, and *HR* that from roof to the atmosphere. This model includes the 2-D streetcanyons shown in Figure 2. (b) Multi-layer urban canopy model (NIRE-CM): *Ta* is the air temperatureat reference height *za*, *TR* the building roof temperature, *TW* the building wall temperature,and *TG* the road temperature. *H* is the sensible heat exchange at the reference height. This modelincludes 3-D buildings. (c) Slab model (surface-layer scheme): *Ta* is the air temperature at referenceheight *za* and *TG* is the road temperature. *H* is the sensible heat exchange at the reference height.

In contrast, Masson (2000) developed a simpler, single-layer urban canopy model that is similar to single-layer vegetation canopy models (e.g., Deardorff, 1978; Dickinson, 1986; Garratt, 1978; Bonan, 1996), which allow different soil surfaces and foliage temperatures. Kusaka et al. (1999) ran a mesoscale meteorological model that included such a simple single-layer urban canopy model. Our model is similar to Masson's (2000) because it is also developed as an analogy of a vegetation model, but there are signnficant differences: our model includes the canyon orientation and diurnal change of solar azimuth angle, and the surface consists of several canyons with different orientation. Other differences are relatively minor. Despite the need for a simple urban canopy model, there are currently few reports about development of such a model and few comparisons between a single-layer model (Figure 1a), a multi-layer model (Figure 1b), and a slab model (Figure 1c) to evaluate the usefulness of such a model. In table 3.2.1 we show the atmospheric input for standard urban canopy models. Here, Rn,i , Hi, lEi ,and Gi, are the net radiative flux density to the surface, the sensible and latent heat fluxes from the surface, and the heat flux into the ground, which is interpreted as the ground heat flux at the surface. The subscript i indicates the type of surface, which can be roof, wall, or road. A simple hydrological process is considered. The UCM model has a very thin bucket scheme, i.e., roof and road surfaces are

covered with an impermeable layer and the city has a very adequate drainage system. Latent heat flux from street trees along the road and grass in the open spaces are calculated from a single-layer vegetation model. Total latent heat flux from the urban surface is obtained by the average of fluxes on each model (Kimura, 1989). The present case assumes no cloud and no precipitation in order to compare between three models under an identical clear summer day. Test runs against observation also assume no cloud.

Atmospheric input to the present single-layer urban canopy model.

Input data	Symbol	Unit
Reference height	z_a	[m]
Temperature at z_a	T_a	[K]
Zonal wind at z_a	u_a	[m s^{-1}]
Meridional wind at z_a	v_a	[m s^{-1}]
Specific humidity at z_a	q_a	[kg kg^{-1}]
Downward direct solar radiation on a horizontal surface	S_D	[W m^{-2}]
Downward diffuse solar radiation on a horizontal surface	S_Q	[W m^{-2}]
Downward longwave radiation on a horizontal surface	$L^{\downarrow}$	[rad]
Latitude	ϕ	[rad]
Solar declination	δ	[rad]

Table 2.3.1 Atmospheric input to the urban canopy models

Building height has a significant effect on surface temperatures. The larger shadows of taller buildings tend to cool the surface; however, because each surface receives solar and longwave radiation, taller buildings can also trap radiative heat. Consequently, the effects of the shadows, and the reflected solar and longwave radiation, are included in the model. The model is assumed to be a Lambertian surface. In figure 3.2.2 we show a scheme of the solar radiation (SD) incident on a horizontal surface. w is the normalized road width, h is the normalized building height (w + r = 1).Here r is the normalized roof width. Ishadow is the normalized shadow length on the road θz is solar zenith angle.

The energy balance of an urban system (hereafter referred to as urban energy balance (UEB)) can be determined in a micrometeorological sense by considering the energy flows in and out of a control volume. For such a control volume reaching from ground to a certain height above the buildings, the energy balance equation reads as (Oke 1987; Offerle et al. 2005):

$$Q^* + Q_F = Q_H + Q_E + \Delta Q_E + \Delta Q_S + S$$

with,
Q^* as the net radiation,
Q_F as the anthropogenic heat flux,
Q_H as the turbulent sensible heat flux,
Q_E as the turbulent latent heat flux,
ΔQ_S as the net storage change within the control volume,
ΔQ_A as the net advected flux (QA in - QA out),
S as all other sources and sinks.

All terms are usually expressed as energy flux density per horizontal or vertical area (typically W m-2, also MJ m-2 d-2 for temporal sums).

For comparisons between sites it is also common to non-dimensionalize fluxes by expressing individual terms as a percentage of the net radiation which is besides the comparatively small and difficult to determine QF the main input term into the system. In the following sections we will examine each of the UEB terms separately. Studies or models often refer to the surface energy balance (SEB) (e.g. Grimmond & Oke 2002) instead of the UEB. The SEB is distinct from the UEB in the fact that it considers the natural or built surface of the earth as the border or plane where exchange processes take part and not the top of a building-air box volume. Storage change in this case is the flux into or out of the ground. The advection term falls out of the equation. The urban atmosphere usually is divided into vertical layers. The whole part of the lower atmosphere that is influenced by the urban structure is called the Urban Boundary Layer (UBL). From the ground up to roughly the average height of roughness elements like buildings or trees (zH) we speak of the urban canopy layer (UCL). It is produced by micro-scale processes which characterize their immediate surroundings. The UCL is part of the roughness sublayer (RS) which is dependent on the height and density of roughness elements and extends to $z^* = a \cdot zH$, where a ranges between 2 and 5 (Raupach et al. 1991). Above is the inertial sublayer (IS) where under ideal conditions the Monin-Obukhov Similarity Theory (MOST) may be expected to apply within – which is normally not the case in urban areas as we will see later. The upper part of the UBL, which is to a large extent determined by meso-scale advective processes, may be referred to as the outer urban boundary layer (OUBL) (Rotach et al. 2005).

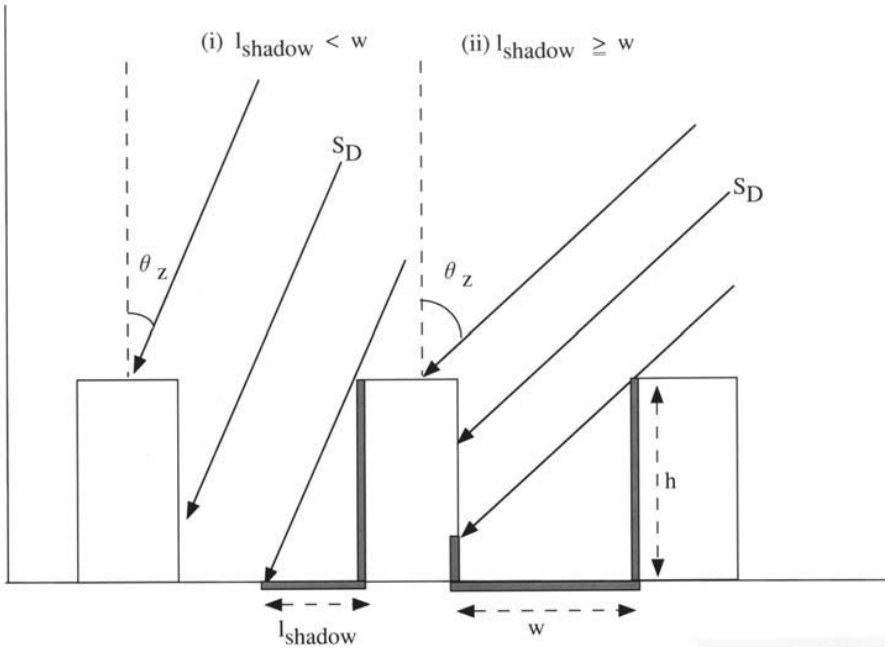

Figure 2.3.2 Explanation how tha shadowing effects are taken into account into the Urban Canopy Model included into WRF.

2.4 Hydrological models

The accurate representation of the urban water balance through modeling is imperative for the assessment of future sustainable urban water management practices, realistic simulation of urban surface processes and for predicting the effects of climate change. A review of the literature identified three general types of urban water balance models each with varying degrees of complexity and spatial extent.

The first type of model is dedicated to the determination of the urban water balance for use in urban hydrology and water management technique assessment applications. These models utilize the mass balance based approach used by Grimmond et al. (1986) in their Urban Water Balance model and combine both natural and anthropogenic hydrological systems. The Urban Water Balance model (Grimmond et al. 1986) utilizes a number of empirical relations to determine the flows and storage of the urban system over a desired spatial and temporal scale, with the later depending on data availability and resolution (typically daily data is used). The model was demonstrated and evaluated using observations from Vancouver, Canada (Grimmond & Oke 1986) and suggested uses include investigation into urban irrigation and the urban energy budget (through the link with evapotranspiration).

Two urban water balance models developed in Australia based on the assessment of water management techniques are Aquacycle (Mitchell et al. 2001) and the Urban Volume and Quality model, UVQ (Mitchell & Diaper 2005). UVQ is essentially an expanded version of Aquacycle with the added ability to model contaminant fluxes and was developed for an urban water resource modeling toolbox during AISUWRS (Diaper & Mitchell 2007). Both models are based on the mass balance principle and are formed of inputs, outputs, flows and stores. Site specific input values are required to calibrate and run the models with three nested spatial scales in each (unit block (property), cluster (neighborhood) and the study area as a whole (Wolf et al. 2007)). Unlike the Urban Water Balance model there is less focus on required meteorological data with only daily precipitation and potential evapotranspiration values needed. Aquacycle contains options to apply water management techniques to the urban water balance and was evaluated using data from Woden Valley, Canberra, Australia (Mitchell et al. 2003). UVQ was utilized to investigate the urban water balance and transport of contaminants for a number of cities around the world as part of the AISUWRS research project (Wolf et al. 2007).

The second type of model identified are urban parameterization schemes used in global and mesoscale numerical weather models. The parameterization schemes identified are the Urban Hydrological Element model, UHE (Berthier et al. 2004, 2006), the urbanized Submesoscale Soil Model, SM2-U (Dupont et al. 2006) and the combined Town Energy Balance and Interaction Soil-Biosphere-Atmosphere scheme, TEB-806 ISBA (Lemonsu et al. 2007). Each scheme differs in complexity and focus but in essence are formed of a number of surface and subsurface layers with the aim of modeling the surface water balance using inputs from a numerical model (typically net radiation and precipitation) and generating output for use in the next model time step (evapotranspiration). All the schemes presented have mixed land uses (urban and natural surface types) each which have individual surface and hydrologic properties weighted by their relative areal coverage of a particular grid box. Unlike the dedicated urban water balance models these parameterizations focus only on the external water system. The UHE model (Berthier et al. 2004, 2006) is a water budget model which simulates storm water runoff and soil infiltration. It is formed of two main layers a surface layer with three possible land use types (natural, paved and

building roof) and a soil layer (formed of an upper and lower sub layer for infiltration purposes) which takes the form of a fine mesh grid. In addition to these layers there is a storm water drainage system which is represented as a trench collecting all available runoff as well as seepage from soil water (this acts in both directions depending on soil moisture conditions). The original version of the model (Berthier et al. 2004) considered evapotranspiration (and infiltration) by applying a 'mixed' boundary condition on modeled soil moisture, observed rainfall and potential evapotranspiration. This model was further developed to include an dual evapotranspiration scheme based on the Penman-Monteith-Rutter-Shuttleworth equation (Grimmond & Oke 1991) for paved and roof surfaces and a scheme based on Feddes et al., (1988) to calculate the potential evaporation and transpiration for the natural surface types (Berthier et al. 2006). The model was then evaluated with data from the Reze field site using site specific parameters and observed meteorological and hydrological variables.

SM2-U is a mesoscale model surface parameterisation scheme (Dupont et al. 2006) formed of four levels (lower atmosphere, surface layer, root zone and deep soil) and a rudimentary drainage network as used in Berthier et al. (2004). It is an extension of Noilhan & Planton's (1989) ISBA scheme with the addition of four artificial urban surface types each with their own surface properties they are building roofs, paved surfaces, vegetation over paved surfaces and paved surfaces under vegetation (Dupont et al. 2006). The addition of these extra surface types which resulted in the modification to a number of terms related to the water balance. The scheme was evaluated with data from three measurement sites two rural and the suburban site at Reze which also allowed comparison of the runoff running through the drainage network with the original version the UHE (Berthier et al. 2004). It was concluded that the SM2-U scheme performed well annually and in summer storm events in comparison to UHE but was poor at simulating winter storms due to moisture infiltration to and from the drainage network not being modeled.

A second surface parameterization scheme that used the ISBA 846 scheme was Lemonsu et al. (2007) who undertook the opposite exercise to Dupont et al. (2006) by adding ISBA to the existing Town Energy Balance (TEB) urban surface parameterization scheme (Masson 2000) to create the TEB-ISBA scheme. The scheme is formed of three layers (the surface and two soil layers) and four surface types, the three ISBA vegetation surfaces (bare soil, soil between vegetation and vegetation) and an urban surface which in TEB is a modeled as a three dimensional urban canyon. An off-line simulation of the TEB-ISBA water balance was undertaken using meteorological data to force the model and input parameters from the literature relevant to a suburban area. The results were then compared with data from the Reze study area to determine required improvements in the scheme, it was decided that further work was required in the parameterization of surface infiltration through roads due to discrepancies between modeled and observed runoff (Lemonsu et al. 2007).

The third type of model identified that considers the water balance of urban areas are hydrology models. The hydrology models identified, Semi-Urbanised Runoff Flow, SURF (Rodriguez et al. 2000), the Water and Energy transfer Processes (WEP) model (Jia et al. 2001), the Urban-Runoff Branching Structure MOdel, URBS-MO (Rodriguez et al. 2008) , the SIMGRO-model (Walsum and Groenendijk, 2008) and the Urban FORest Effects-Hydrology (UFORE-Hydro) model (Wang et al. 2008) are typically composed of two parts: a surface scheme and a hydrological flow model (described as a natural, anthropogenic or a combination drainage system) that moves water

through the study catchment. These models are typically used for studying sewer and drain performance during rainfall events (Rodriguez et al. 2008), assessing impacts of runoff pollution (Rodriguez et al. 2000), the simulation of the effects of urban areas on natural catchment flows and flooding (Jia et al. 2001) and the impact of urban trees and canopy interception on runoff and evapotranspiration (Wang et al. 2008, Walsum and Groenendijk, 2008). The data inputs and parameters required for the models include physical land cover properties (e.g. fraction of impervious land cover and aerodynamic roughness length), surface and subsurface hydrologic properties (e.g. soil storage capacity), water use information (e.g. mean water use), initial conditions in terms of storage in the study area (e.g. soil moisture) and a range of averaged (period of choice) meteorological data (e.g. net radiation and precipitation). The processes described by the SIMGRO model are depicted in Figure 3.3.1 *The urban water cycle in the SIMGRO model (Walsum and Groenendijk, 2008)* The SIMGRO model also includes a dual evapotranspiration scheme based on the Penman-Monteith-Rutter-Shuttleworth equation (Grimmond & Oke 1991) for paved and roof surfaces and a scheme based on Feddes et al., (1988) to calculate the potential evaporation and transpiration for the natural surface types.

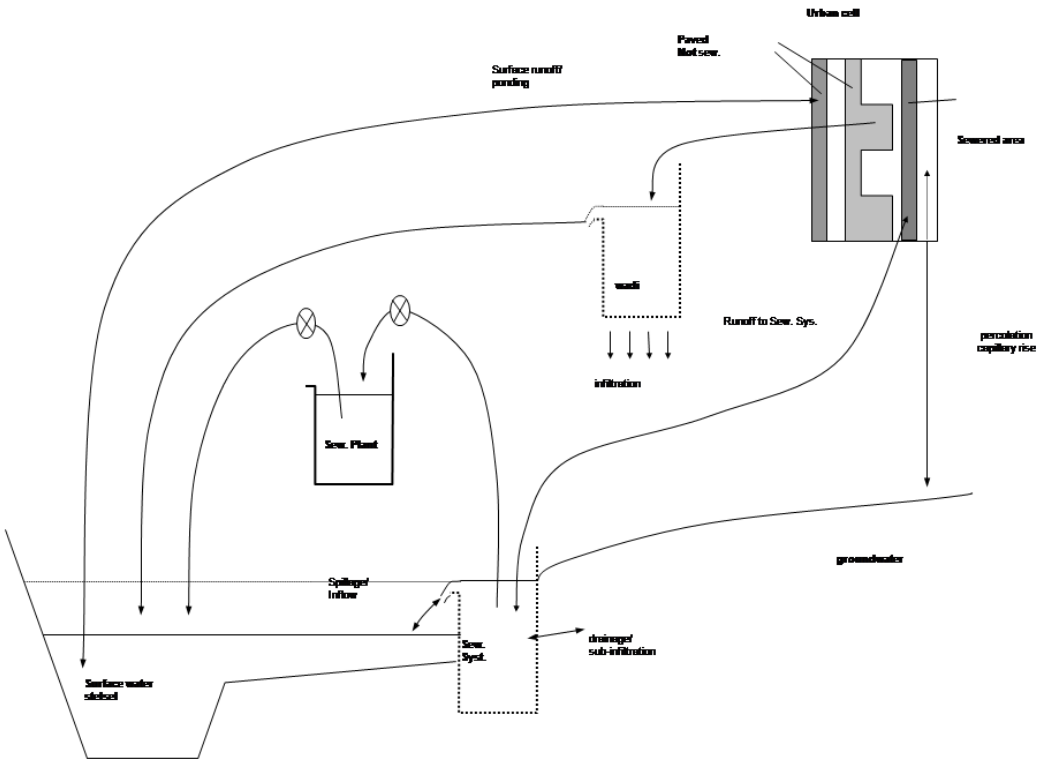

Figure 2.4.1 The urban water cycle in the SIMGRO model (Walsum and Groenendijk, 2008)

3. Partners and Models involved

1. UPM
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Models: WRF-UCM, MICROSYS (CFD), RCM3, MM5-CMAQ and WRF/CHEM

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Models: Neural Network (NKUA)

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4. Models used in BRIDGE

4.1 UPM Models

4.1.1 MM5-CMAQ & WRF/CHEM

UPM will use two mesoscale models: MM5-CMAQ and WRF/CHEM. MM5-CMAQ is a model composed by a mesoscale meteorological non-hydrostatic model (MM5) developed by PSU/NCAR (US) and a chemical transport model CMAQ (Community Multiscale Air Quality Modelling System) developed by EPA (US). In addition UPM will use a so-called WRF/CHEM models which is an on-line chemical and meteorological mesoscale model which is a new generation of mesoscale models based on the on-line simulation of chemical and meteorological processes which is more suitable for climate studies. These models can reproduce the atmospheric process and interaction biosphere/atmosphere in a mesoscale domain (domains range between 10000 km to a few km). The atmospheric flow is solved by using numerical methods with a specific time and spatial resolution in 4D environment. The Boundary conditions are taken from global models or models running over larger domains. The input data for these models is morphological information of the surface, land use types, topography, BC's and IC's (boundary conditions and initial conditions), observed data to be assimilated during or at initial stage of the simulation and emission data (emission per pollutant per grdi per time unit). These models provide detailed information, at mesoscale level, of the flux exchange between atmosphere and soil and pollutant concentrations in the air as an average per grid cell and time unit in a 4D (space + time) environment. Figure 1 shows some visual representation of the different layers of these models.

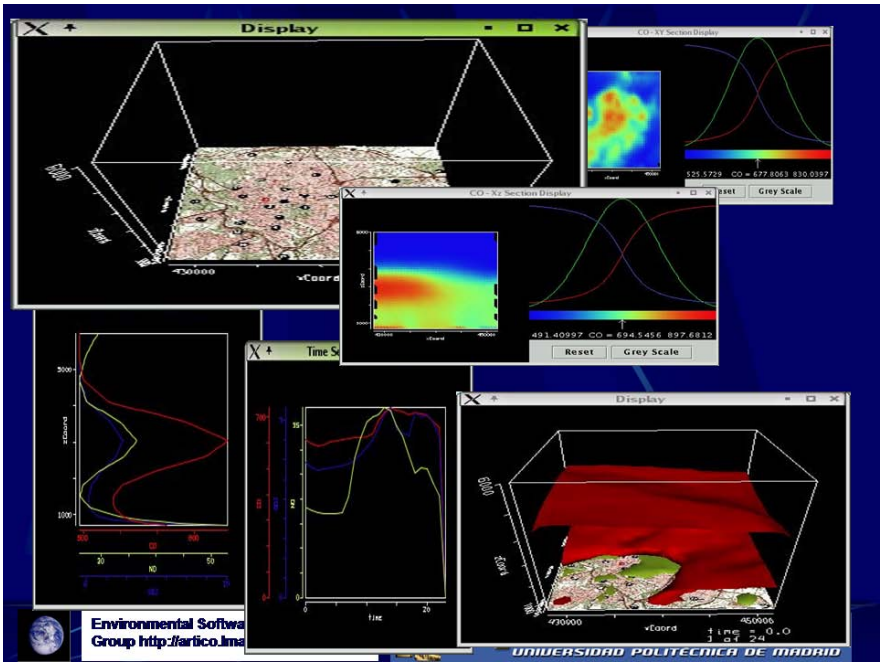


Figure 4.1.1.1. Visual representation of outputs of different mesoscale models such MM5-CMAQ or WRF/CHEM

4.1.1.1 The MM5 Model

The PSU/NCAR mesoscale model is a limited-area, nonhydrostatic or hydrostatic (Version 2 only), terrain-following sigma-coordinate model designed to simulate or predict mesoscale and regional-scale atmospheric circulation. It has been developed at Penn State and NCAR as a community mesoscale model and is continuously being improved by contributions from users at several universities and government laboratories. The Fifth-Generation NCAR / Penn State Mesoscale Model (MM5) is the latest in a series that developed from a mesoscale model used by Anthes at Penn State in the early 70's that was later documented by Anthes and Warner (1978). Since that time, it has undergone many changes designed to broaden its usage. These include (i) a multiple-nest capability, (ii) nonhydrostatic dynamics, which allows the model to be used at a few-kilometer scale, (iii) multitasking capability on shared- and distributed-memory machines, (iv) a four-dimensional data-assimilation capability, and (v) more physics options. The model (known as MM5) is supported by several auxiliary programs, which are referred to collectively as the MM5 modeling system. Figure 2 provides information to facilitate discussion of the complete modeling system.

Terrestrial and isobaric meteorological data are horizontally interpolated (programs TERRAIN and REGRID) from a latitude-longitude mesh to a variable high-resolution domain on either a Mercator, Lambert conformal, or polar stereographic projection. Since the interpolation does not provide mesoscale detail, the interpolated data may be enhanced (program RAWINS or little_r) with observations from the standard network of surface and rawinsonde stations using either a successive-scan Cressman technique or multiquadric scheme. Program INTERPF performs the vertical interpolation from pressure levels to the sigma coordinate system of MM5. Sigma surfaces near the ground closely follow the terrain, and the higher-level sigma surfaces tend to approximate isobaric surfaces. Since the vertical and horizontal resolution and domain size are variable, the modeling package programs employ parameterized dimensions requiring a variable amount of core memory. Some peripheral storage devices are also used.

Since MM5 is a regional model, it requires an initial condition as well as lateral boundary condition to run. To produce lateral boundary condition for a model run, one needs gridded data to cover the entire time period that the model is integrated.

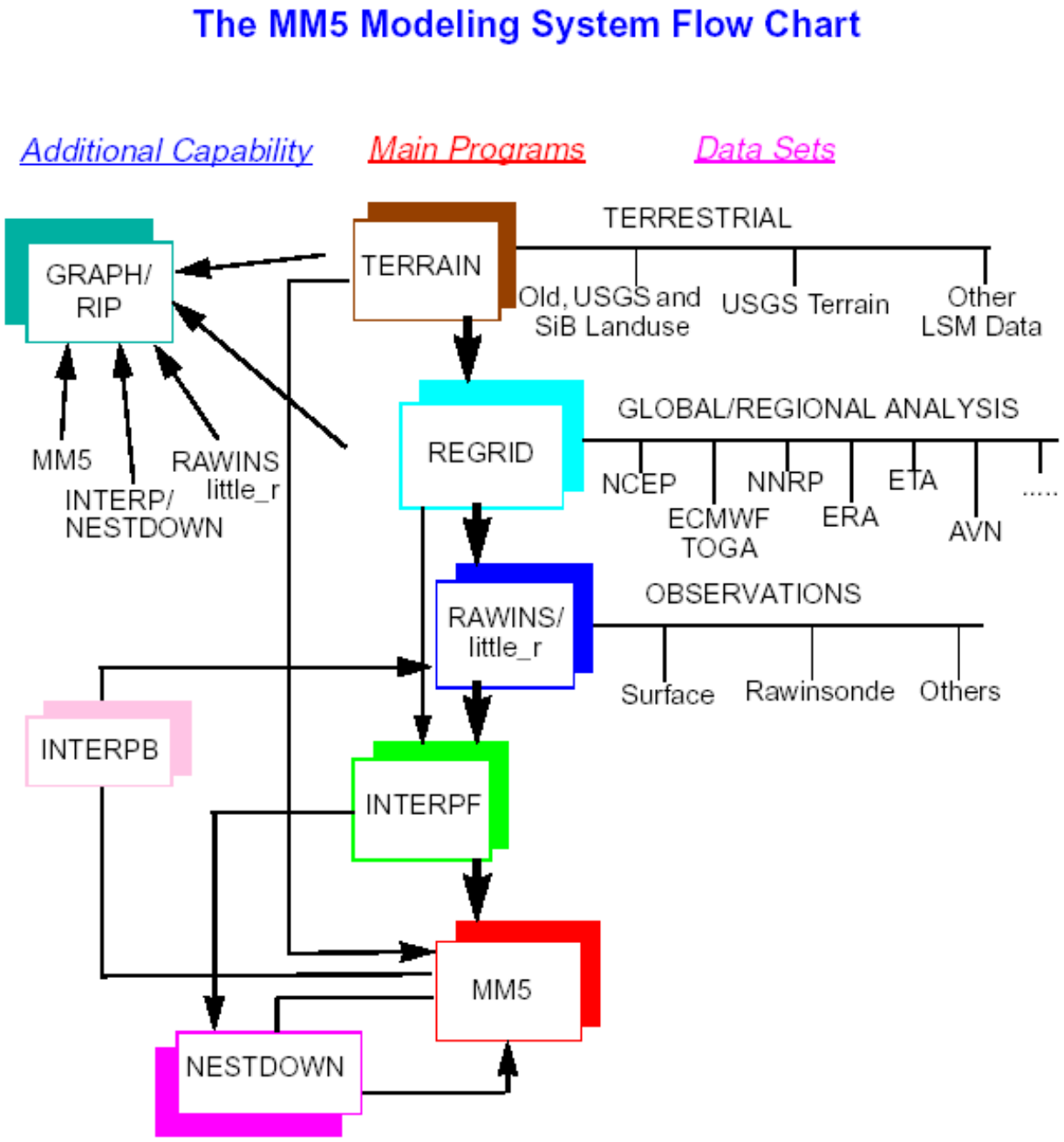


Figura 4.1.1.1.1 Schematic diagram of MM5

4.1.1.2 The CMAQ MODEL

The structure of the Models-3/CMAQ system is shown in Figure 1. Orchestrated through the Models-3 system framework, the Community Multiscale Air Quality (CMAQ) modeling system incorporates output fields from emissions and meteorological modeling systems and several other data source through special interface processors into the CMAQ Chemical Transport Model (CCTM). CCTM then performs chemical transport modeling for multiple pollutants on multiple scales. With this structure, CMAQ retains a flexibility to substitute other emissions processing systems and meteorological models. One of the main objectives of this project was to provide an air quality modeling system with a "one atmosphere" modeling capability based mainly on the "first principles" description of the atmospheric system. CMAQ contains state-of-science parameterizations of atmospheric processes affecting transport, transformation, and deposition of such pollutants as ozone, particulate matter, airborne toxics, and acidic and nutrient pollutant species. With science in a continuing state of advancement and review, the modeling structure of CMAQ is designed to integrate and to test future formulations in an efficient manner, without requiring the development of a completely new modeling system. Contents of the CMAQ in the June 1998 release version of Models-3 are summarized in Ching et al. (1998) and Byun et al. (1998b).

Currently, the Models-3 Emission Projection and Processing System (MEPPS) produces the emissions and the Fifth Generation Penn State University/ National Center for Atmospheric Research Mesoscale Model (MM5) provides the meteorological fields needed for the CCTM. They are considered to meet the present application needs for diverse air pollution problems in urban and regional scales. However, given the CMAQ paradigm, and other considerations, the emissions processing and meteorological modeling systems can be replaced with alternative processors.

Each of these three modeling systems are described briefly below, where associated chapters of this document are highlighted to provide directions to more in-depth discussions of these topics:

- The PSU/NCAR MM5 meteorological modeling system (Grell et al., 1994) generates the meteorological fields for CMAQ. MM5 is a complex, state-of-the-science community model, which is maintained by NCAR.
- The MEPPS emission modeling system is based on the Geocoded Emission Modeling and Projection System (GEMAP) (Wilkinson et al., 1994) now known as the Emission Modeling System-95 (EMS-95). MEPPS processes emission inventory data, performs future projections (including control scenarios), and pre-processes data for use in the CMAQ model. It provides speciated emissions consistent with CB-IV or RADM2 chemistry mechanisms.
- The CMAQ chemical transport modeling system (CCTM) is then used to perform model simulations for multiple pollutants and multiple scales with these input data.

The CMAQ modeling system also includes interface processors that process input data for the emission and meteorological modeling systems, and other processors that calculate photolysis rates, and develop initial and boundary conditions. CMAQ also has an internal program control processor.

Using the analysis routines provided in Models-3, the CMAQ output can be processed to provide process analysis information and/or analyzed further to provide aggregated statistical information.

An important design requirements for CMAQ is that it addresses multiple scales and pollutants, which requires that governing equations and computational algorithms among the different systems should be consistent and compatible across the multiple scales. However, modeling assumptions used in various modeling systems may not be valid across all scales. For example, the atmospheric dynamics description in a meteorological model may have been optimized for application of certain scale or limited range of scales (e.g., global vs mesoscale vs complex terrain to urban). It is incumbent upon the user community to ensure the model component formulations are applicable to the range of scales upon which CMAQ is applied. The current version of MM5 and the CCTM is designed for regional to urban scales. Furthermore, when using nesting procedures to scale down from regional to urban scales and for avoiding feedback between the scales, one way nesting is recommended. In addition to the challenges of creating a multiscale air quality model, CMAQ's multi-pollutant capability cannot be achieved if the emissions modeling system does not provide appropriate precursor or pollutant emissions to the chemical transport model (CTM). The development of Models-3 and CMAQ overcome these hurdles by providing the flexibility to modify specific requirements (e.g., chemical mechanisms, model inputs, etc.), a generic coordinate system that ensures consistency across spatial scales, and user interfaces that can integrate alternative emissions or meteorological modeling systems.

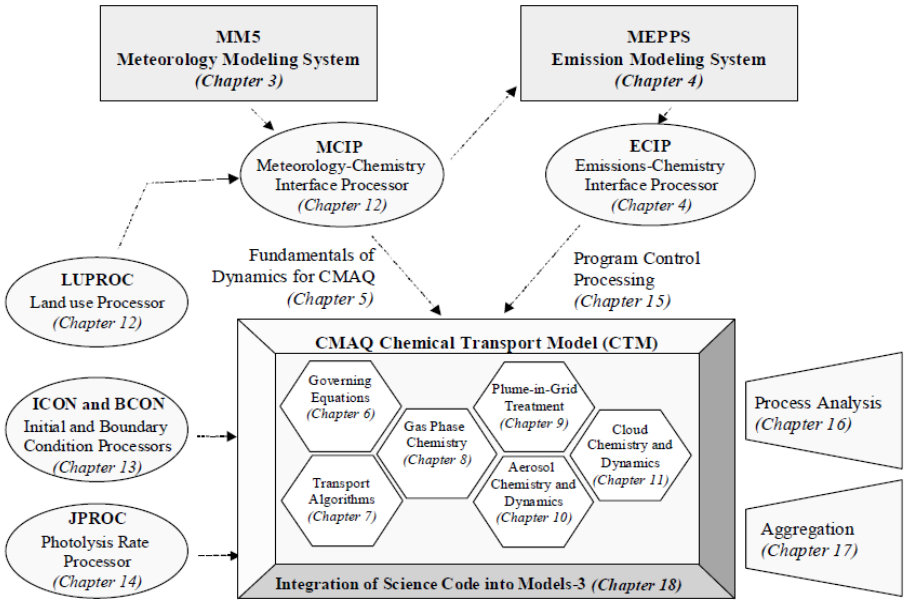


Figure 4.1.1.2.1.- Schematic scheme of the CMAQ modelling system

Due to this characteristics of this model, it should be run in OFF-LINE mode in BRIDGE.

4.1.2 The WRF/CHEM

WRF/CHEM. Is a mesoscale non-hydrostatic mesocale meteorological and chemical model. The chemistry and metrorology are embedded into one code. The advantages are that the climatic feedbacks for chemistry interactions with meteorological variables can be evaluated and estimated. All numerics are fully consistent since the transport used for the meteorological fluxes is the same than for the chemistry solver. As a first step towards the implementation of chemistry into WRF, "The Workshop on Modeling Chemistry in Cloud and Mesoscale Models" was held at NCAR on 6-8 March 2000 The goal of this workshop was produce a community assessment of approaches and methodologies used for chemistry modeling in cloud and mesoscale models.

In 2002, a first version of WRF/Chem was made available as an "online" (or "inline") model. In this form, the model is consistent, with all transport done by the meteorology model. The same vertical and horizontal coordinates are used (no horizontal or vertical interpolation), the same physics parameterization utilized for subgrid scale transport, and no interpolation in time is performed. This allows for easy handling from a data management standpoint, and is also the most efficient with regard to overall CPU costs. WRF grid-scale transport of all species is conducted, with subgrid-scale transport by turbulence and convection. Grid-scale advection in the mass coordinate WRF is mass and scalar conserving.

The last version of WRF/Chem 3.1.1.1 July, 31, 2009.

The Chemistry Package consists of the following components:

- Dry deposition, coupled with the soil/vegetation scheme.
- Aqueous phase chemistry coupled to some of the microphysics and aerosol schemes.
- Four choices for biogenic emissions:
  - No biogenic emissions.
  - Online calculation of biogenic emissions (as in Simpson, et al. 1995 and Guenther et al. 1994) includes emissions of isoprene, monoterpenes, and nitrogen emissions by soil.
  - Online modification of user specified biogenic emissions - such as the EPA Biogenic Emissions Inventory System (BEIS) version 3.13. The user must provide the emissions data for their own domain in the proper WRF data file format.
  - Online calculation of biogenic emissions using the MEGAN v2.04 biogenic emissions routine.
- Two choices for anthropogenic emissions:
  - No anthropogenic emissions.
  - User specified Anthropogenic emissions - such as those available from the EPA NEI-99 data inventory. The user must provide the emissions data for their own domain in the proper WRF data file format.
- Two choices for gas-phase chemical reaction calculations.
  - The RADM2 chemical mechanism.

- The CBM-Z mechanism.

- Several choices for gas-phase chemical reaction calculations through the use of the Kinetic Pre-Processor, or KPP. The equation files (using Rosenbrock type solvers) currently available are for:
  - The RADM2 chemical mechanism.
  - The RACM mechanism.
  - The RACM-MIM mechanism.
  - The CB4 mechanism (experimental).
  - The NMHC9 mechanism (experimental).
- Three choices for Photolysis schemes:
  - Madronich scheme coupled with hydrometeors, aerosols and convective parameterizations.
  - Fast-J Photolysis scheme coupled with hydrometeors, aerosols and convective parameterizations.
  - FTUV scheme scheme coupled with hydrometeors, aerosols and convective parameterizations.
- Two choices for aerosol schemes:
  - The Modal Aerosol Dynamics Model for Europe - MADE/SORGAM
  - The Model for Simulating Aerosol Interactions and Chemistry (MOSAIC - 4 or 8 bins) sectional model aerosol parameterization
  - The GOCART aerosol model (experimental). aerosol parameterization
- A tracer transport option in which the chemical mechanism, deposition, etc. has been turned off. The user must provide the emissions data for their own domain in the proper WRF data file format for this option.

In WRF version 3.0 chemistry the MOSAIC aerosol scheme is coupled to the NASA Goddard atmospheric radiation scheme.

Possible applications of the current modeling system:

- Prediction and simulation of weather, or regional or local climate
- Coupled weather prediction/dispersion model to simulate release and transport of constituents
- Coupled weather/dispersion/air quality model with full interaction of chemical species with prediction of O_3 and UV radiation, as well as PM

Due to this characteristics of this model, it should be run in OFF-LINE mode in BRIDGE.

4.1.3 The RCM3 Model

The regCM3 model is a climate version of the MM5 and/or WRF meteorological mesoscale models. It is a model which can be used to simulate regional climate periods provided global intial and boundary conditions which are also provided by the global climate models such as CCM3, MOZART and GIS models. The Sea Surface Temperature is a main driver for the climate simulations of the RegCM3 model and it can be provided by the ocean component of the CCM3 model (NCAR, US).

4.1.4 The MICROSYS (CFD) model

UPM will use also a CFD model called MICROSYS developed by UPM. MICROSYS is a microscale fluid dynamics model which includes chemical dispersion and transformation of species. MICROSYS received boundary conditions from the mesoscale models (MM5-CMAQ and/or WRF/CHEM) and runs over microscale domains (domains range between few km to meters). The atmospheric flow is also solved using numerical methods with higher spatial and temporal resolution (according to the Courant law) in a 4D environment. The MICROSYS model requires similar input information than the mesoscale models but, in addition, it requires information related to urban characteristics (soil type, asphalt, cement type, tree types, roof materials, etc.) in order to have a more detailed description on the heat flux exchange between surface and the atmosphere. In order to obtain a detailed emission dataset with a very high spatial resolution (meters) we usually apply a **traffic model** (for urban environments) based on a **cellular automata model** (developed in UPM) called CAMO. MICROSYS can then provide a detailed description of the heat flux exchange and can assimilated different types of observational datasets such as surface temperature, air temperature, etc.

Figure 4.1.4.1. Visual representation of outputs of MICROSYS and CAMO.

MICROSYS includes adaptations of RANS (Reynolds-averaged Navier-Stokes equations) CFD models such as MIMO and adaptation of EULAG (UCAR, US) LES (large eddy simulation) model. In case of EULAG, UPM has implemented the full energy balance module into the CFD EULAG system to produce detailed information on storage ground heat flux, sensible and latent heat fluxes and net radiation at every grid cell in dynamical and diagnostic modes.

4.1.5 The WRF/chem-UCM-MICROSYS model

The WRF/chem-UCM-MICROSYS model is an integration of mesoscale models and microscale (CFD) models. This model – with different versions – can be applied to scales up to 200 m of spatial resolution over urban areas in BRIDGE and also to microscales with MICROSYS with feedbacks to mesoscale domains. It is a combination of the models described before.

The amount of output variables of one of these models is quite large and could be larger than 400 variables. A summary of the variables can be seen as follows:

4.1.5.1 WRF INPUT DATA

To run the WRF meteorological mesoscale model we need the following input data for every grid point:

- 3-D meteorological data : pressure, u, v, temperature, relative humidity, geopotential height
- 3D soil data: soil temperature, soil moisture, soil liquid (optional, depending on physics choices in the model)
- 2D meteorological data sea level pressure, surface pressure, surface u and v, surface temperature, surface relative humidity, input elevation
- 2-D meteorological : sea surface temperature, physical snow depth, water equivalent snow depth (optional)
- 2D static data for the physical surface: terrain elevation, land use categories, soil texture categories, temporally interpolated monthly data, land sea mask, elevation of the input model's topography
- 2D static data for the projection: map factors, Coriolis, projection rotation, computational latitude
- constants: domain size, grid distances, date

These data can be generated by a preprocessing software package (WPS) which delivers data that is ready to be used in the model system. The data has already been horizontally interpolated to the correct grid-point staggering for each variable, and the winds are correctly rotated to the model map projection.

The preprocessing package needs the following input data to produce the final output data:

4.1.5.2 Static geographical data

- Topography or terrain height data for every grid point.
- Land use category according to USGS 24-category Land Use Categories**.**

Land Use Category	Land Use Description
1	Urban and Built-up Land
2	Dryland Cropland and Pasture
3	Irrigated Cropland and Pasture
4	Mixed Dryland/Irrigated Cropland and Pasture
5	Cropland/Grassland Mosaic
6	Cropland/Woodland Mosaic
7	Grassland
8	Shrubland
9	Mixed Shrubland/Grassland
10	Savanna
11	Deciduous Broadleaf Forest
12	Deciduous Needleleaf Forest
13	Evergreen Broadleaf
14	Evergreen Needleleaf
15	Mixed Forest
16	Water Bodies
17	Herbaceous Wetland
18	Wooden Wetland
19	Barren or Sparsely Vegetated
20	Herbaceous Tundra
21	Wooded Tundra
22	Mixed Tundra
23	Bare Ground Tundra
24	Snow or Ice

Each land use category is associated to the physical parameters: albedo, moisture, emissivity, roughnes length, thermal inertia.

- Soil categories according to **16-category Soil Categories**

Soil Category	Soil Description
1	Sand
2	Loamy Sand
3	Sandy Loam
4	Silt Loam
5	Silt
6	Loam
7	Sandy Clay Loam
8	Silty Clay Loam
9	Clay Loam
10	Sandy Clay
11	Silty Clay
12	Clay
13	Organic Material
14	Water
15	Bedrock
16	Other (land-ice)

Each soil category is associated to a physical parameter with the following default values:

Soil Category	**Max moisture content**	**Ref. soil moisture**	**Wilting point soil moisture**	**Air dry moist content limits**	**Sat. soil potential**	**Sat.Soil conductivity (10-6)**	**B paramet**	**Sat. soil diffusivity (10-6)**	**Soil diffu./ condu. coef.**
1	0.339	0.236	0.010	0.010	0.069	1.07	2.79	0.608	- 0.472
2	0.421	0.283	0.028	0.028	0.036	14.10	4.26	5.14	- 1.044
3	0.434	0.312	0.047	0.047	0.141	5.23	4.74	8.05	- 0.569
4	0.476	0.360	0.084	0.084	0.759	2.81	5.33	23.9	0.162
5	0.476	0.360	0.084	0.084	0.759	2.81	5.33	23.9	0.162
6	0.439	0.329	0.066	0.066	0.355	3.38	5.25	14.3	- 0.327
7	0.404	0.314	0.067	0.067	0.135	4.45	6.66	9.90	- 1.491
8	0.464	0.387	0.120	0.120	0.617	2.04	8.72	23.7	- 1.118
9	0.465	0.382	0.103	0.103	0.263	2.45	8.17	11.3	- 1.297
10	0.406	0.338	0.100	0.100	0.098	7.22	10.73	18.7	- 3.209
11	0.468	0.404	0.126	0.126	0.324	1.34	10.39	9.64	- 1.916
12	0.468	0.412	0.138	0.138	0.468	0.974	11.55	11.2	- 2.138
13	0.439	0.329	0.066	0.066	0.355	3.38	5.25	14.3	- 0.327
14	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15	0.200	0.108	0.006	0.006	0.069	141.0	2.79	136.0	- 1.111
16	0.421	0.283	0.028	0.028	0.036	14.10	4.26	5.14	- 1.044

- Annual mean deep soil temperature (Kelvin)
- Monthly surface albedo (%)
- Monthly green fraction (%)

By default we can use global data with the 30", 2', 5', and 10' spatial resolutions.

1. Global vegetation fraction data contained 12 percentage-values for 12 months at each of grid points
2. Global annual deep soil temperatura
3. Gridded global meteorological data, GRIB Edition 1, contained temperature, wind components, relative humidity, height of pressure levels, sea-level pressure, sea-surface temperature, and snow-cover data , Ground temperature, Soil moisture, sea ice. Time resolution 6 hours.
4. Information from observations from surface and radiosonde. The data must be included are: latitude, longitude and elevation of the observation point, date and time, Sea-level pressure (Pa), Reference pressure level (for thickness) (Pa), Ground Temperature (T), Sea-Surface Temperature (K), Surface pressure (Pa), Precipitation Accumulation, Daily maximum T (K), Daily minimum T (K), Overnight minimum T (K), 3-hour pressure change (Pa), 24-hour pressure change (Pa) Total cloud cover (oktas), Height (m) of cloud base.
5. Information from observations from surface and vertical. The data must be included are: latitude, longitude and elevation of the observation point, date and time, u wind - in m/sec, v wind - in m/sec, temperature - in Kelvin, water vapor mixing ratio - in kg/kg
6. Emission data from each simulated pollutant (g/s) at each of grid points and vertical level.

4.1.5.3 Gridded data

Initial and boundary conditions to the mesoscale model can be generated from GRIB model output files from different models like NAM, GFS, the NCEP/NCAR Reanalysis, RUC, AFWA's AGRMET, ECMWF.

These data included wind components, temperature, relative humidity at the standard pressure levels, plus sea-level pressure and ground temperature, sea-surface temperature, ,snow-cover data, soil moisture and soil temperature at 2 or 4 levels depending of the land surface model setup to the model run.

4.1.5.4 Data Assimilation

The modelling system can assimilate observational data using the "observational nudging" technique. Observational nudging uses relaxation terms based on the model error at observational stations, and the relaxation is done as to reduce this error. Each observation has a radius of influence, a time window, and a relaxation time scale determined by user-specified input.

The meteorological assimilated fields could be: u wind - in m/sec, v wind - in m/sec, temperature - in Kelvin, water vapour mixing ratio - in kg/kg for surface layer or sounding type data.

4.1.5.5 WRF OUTPUT DATA

WRF works with a large list of variables (annex I) and the main output fields are:

```
float LU_INDEX(Time, south_north, west_east) ;
        LU_INDEX:description = "LAND USE CATEGORY" ;
        LU_INDEX:units = "" ;
float ZNU(Time, bottom_top) ;
        ZNU:description = "eta values on half (mass) levels" ;
        ZNU:units = "" ;
float ZNW(Time, bottom_top_stag) ;
        ZNW:description = "eta values on full (w) levels" ;
        ZNW:units = "" ;
float ZS(Time, soil_layers_stag) ;
        ZS:description = "DEPTHS OF CENTERS OF SOIL LAYERS" ;
        ZS:units = "m" ;
float DZS(Time, soil_layers_stag) ;
        DZS:description = "THICKNESSES OF SOIL LAYERS" ;
        DZS:units = "m" ;
float U(Time, bottom_top, south_north, west_east_stag) ;
        U:description = "x-wind component" ;
        U:units = "m s-1" ;
float V(Time, bottom_top, south_north_stag, west_east) ;
        V:description = "y-wind component" ;
        V:units = "m s-1" ;
float W(Time, bottom_top_stag, south_north, west_east) ;
        W:description = "z-wind component" ;
        W:units = "m s-1" ;
float PH(Time, bottom_top_stag, south_north, west_east) ;
        PH:description = "perturbation geopotential" ;
        PH:units = "m2 s-2" ;
float PHB(Time, bottom_top_stag, south_north, west_east) ;
        PHB:description = "base-- state geopotential" ;
        PHB:units = "m2 s-2" ;
float T(Time, bottom_top, south_north, west_east) ;
        T:description = "perturbation potential temperature (theta-t0)"
;
        T:units = "K" ;
float MU(Time, south_north, west_east) ;
        MU:description = "perturbation dry air mass in column" ;
        MU:units = "Pa" ;
float MUB(Time, south_north, west_east) ;
        MUB:description = "base - state dry air mass in column" ;
        MUB:units = "Pa" ;
float NEST_POS(Time, south_north, west_east) ;
        NEST_POS:description = "-" ;
        NEST_POS:units = "-" ;
float P(Time, bottom_top, south_north, west_east) ;
        P:description = "perturbation pressure" ;
        P:units = "Pa" ;
```

```
float PB(Time, bottom_top, south_north, west_east) ;
        PB:description = "BASE - STATE PRESSURE" ;
        PB:units = "Pa" ;
float SR(Time, south_north, west_east) ;
        SR:description = "fraction of frozen precipitation" ;
        SR:units = "-" ;
float POTEVP(Time, south_north, west_east) ;
        POTEVP:description = "accumulated potential evaporation" ;
        POTEVP:units = "W m-2" ;
float SNOPCX(Time, south_north, west_east) ;
        SNOPCX:description = "snow phase change heat flux" ;
        SNOPCX:units = "W m-2" ;
float SOILTB(Time, south_north, west_east) ;
        SOILTB:description = "bottom soil temperature" ;
        SOILTB:units = "K" ;
float FNM(Time, bottom_top) ;
        FNM:description = "upper weight for vertical stretching" ;
        FNM:units = "" ;
float FNP(Time, bottom_top) ;
        FNP:description = "lower weight for vertical stretching" ;
        FNP:units = "" ;
float RDNW(Time, bottom_top) ;
         RDNW:description = "inverse d(eta) values between full (w)
levels" ;
        RDNW:units = "" ;
float RDN(Time, bottom_top) ;
         RDN:description = "inverse d(eta) values between half (mass)
levels" ;
        RDN:units = "" ;
float DNW(Time, bottom_top) ;
        DNW:description = "d(eta) values between full (w) levels" ;
        DNW:units = "" ;
float DN(Time, bottom_top) ;
        DN:description = "d(eta) values between half (mass) levels" ;
        DN:units = "" ;
float CFN(Time) ;
        CFN:description = "extrapolation constant" ;
        CFN:units = "" ;
float CFN1(Time) ;
        CFN1:description = "extrapolation constant" ;
        CFN1:units = "" ;
float Q2(Time, south_north, west_east) ;
        Q2:description = "QV at 2 M" ;
        Q2:units = "kg kg-1" ;
float T2(Time, south_north, west_east) ;
        T2:description = "TEMP at 2 M" ;
        T2:units = "K" ;
float TH2(Time, south_north, west_east) ;
        TH2:description = "POT TEMP at 2 M" ;
        TH2:units = "K" ;
float PSFC(Time, south_north, west_east) ;
```

```
        PSFC:description = "SFC PRESSURE" ;
        PSFC:units = "Pa" ;
float U10(Time, south_north, west_east) ;
        U10:description = "U at 10 M" ;
        U10:units = "m s-1" ;
float V10(Time, south_north, west_east) ;
        V10:description = "V at 10 M" ;
        V10:units = "m s-1" ;
float RDX(Time) ;
        RDX:description = "INVERSE X GRID LENGTH" ;
        RDX:units = "" ;
float RDY(Time) ;
        RDY:description = "INVERSE Y GRID LENGTH" ;
        RDY:units = "" ;
float RESM(Time) ;
        RESM:description = "TIME WEIGHT CONSTANT FOR SMALL STEPS" ;
        RESM:units = "" ;
float ZETATOP(Time) ;
        ZETATOP:description = "ZETA AT MODEL TOP" ;
        ZETATOP:units = "" ;
float CF1(Time) ;
        CF1:description = "2nd order extrapolation constant" ;
        CF1:units = "" ;
float CF2(Time) ;
        CF2:description = "2nd order extrapolation constant" ;
        CF2:units = "" ;
float CF3(Time) ;
        CF3:description = "2nd order extrapolation constant" ;
        CF3:units = "" ;
int ITIMESTEP(Time) ;
        ITIMESTEP:description = "" ;
        ITIMESTEP:units = "" ;
float XTIME(Time) ;
        XTIME:description = "minutes since simulation start" ;
        XTIME:units = "" ;
float QVAPOR(Time, bottom_top, south_north, west_east) ;
        QVAPOR:description = "Water vapor mixing ratio" ;
        QVAPOR:units = "kg kg-1" ;
float QCLOUD(Time, bottom_top, south_north, west_east) ;
        QCLOUD:description = "Cloud water mixing ratio" ;
        QCLOUD:units = "kg kg-1" ;
float QRAIN(Time, bottom_top, south_north, west_east) ;
        QRAIN:description = "Rain water mixing ratio" ;
        QRAIN:units = "kg kg-1" ;
float LANDMASK(Time, south_north, west_east) ;
        LANDMASK:description = "LAND MASK (1 FOR LAND, 0 FOR WATER)" ;
        LANDMASK:units = "" ;
float TSLB(Time, soil_layers_stag, south_north, west_east) ;
        TSLB:description = "SOIL TEMPERATURE" ;
        TSLB:units = "K" ;
float SMOIS(Time, soil_layers_stag, south_north, west_east) ;
```

```
        SMOIS:description = "SOIL MOISTURE" ;
        SMOIS:units = "m3 m-3" ;
float SH2O(Time, soil_layers_stag, south_north, west_east) ;
        SH2O:description = "SOIL LIQUID WATER" ;
        SH2O:units = "m3 m-3" ;
float SEAICE(Time, south_north, west_east) ;
        SEAICE:description = "SEA ICE FLAG" ;
        SEAICE:units = "" ;
float XICEM(Time, south_north, west_east) ;
        XICEM:description = "SEA ICE FLAG (PREVIOUS STEP)" ;
        XICEM:units = "" ;
float SFROFF(Time, south_north, west_east) ;
        SFROFF:description = "SURFACE RUNOFF" ;
        SFROFF:units = "mm" ;
float UDROFF(Time, south_north, west_east) ;
        UDROFF:description = "UNDERGROUND RUNOFF" ;
        UDROFF:units = "mm" ;
int IVGTYP(Time, south_north, west_east) ;
        IVGTYP:description = "DOMINANT VEGETATION CATEGORY" ;
        IVGTYP:units = "" ;
int ISLTYP(Time, south_north, west_east) ;
        ISLTYP:description = "DOMINANT SOIL CATEGORY" ;
        ISLTYP:units = "" ;
float VEGFRA(Time, south_north, west_east) ;
        VEGFRA:description = "VEGETATION FRACTION" ;
        VEGFRA:units = "" ;
float GRDFLX(Time, south_north, west_east) ;
        GRDFLX:description = "GROUND HEAT FLUX" ;
        GRDFLX:units = "W m-2" ;
float SNOW(Time, south_north, west_east) ;
        SNOW:description = "SNOW WATER EQUIVALENT" ;
        SNOW:units = "kg m-2" ;
float SNOWH(Time, south_north, west_east) ;
        SNOWH:description = "PHYSICAL SNOW DEPTH" ;
        SNOWH:units = "m" ;
float RHOSN(Time, south_north, west_east) ;
        RHOSN:description = " SNOW DENSITY" ;
        RHOSN:units = "kg m-3" ;
float CANWAT(Time, south_north, west_east) ;
        CANWAT:description = "CANOPY WATER" ;
        CANWAT:units = "kg m-2" ;
float SST(Time, south_north, west_east) ;
        SST:description = "SEA SURFACE TEMPERATURE" ;
        SST:units = "K" ;
float QNDROPSOURCE(Time, bottom_top, south_north, west_east) ;
        QNDROPSOURCE:description = "Droplet number source" ;
        QNDROPSOURCE:units = " /kg/s" ;
float MAPFAC_M(Time, south_north, west_east) ;
        MAPFAC_M:description = "Map scale factor on mass grid" ;
        MAPFAC_M:units = "" ;
float MAPFAC_U(Time, south_north, west_east_stag) ;
```

```
        MAPFAC_U:description = "Map scale factor on u-grid" ;
        MAPFAC_U:units = "" ;
float MAPFAC_V(Time, south_north_stag, west_east) ;
        MAPFAC_V:description = "Map scale factor on v-grid" ;
        MAPFAC_V:units = "" ;
float MAPFAC_MX(Time, south_north, west_east) ;
         MAPFAC_MX:description = "Map scale factor on mass grid, x
direction" ;
        MAPFAC_MX:units = "" ;
float MAPFAC_MY(Time, south_north, west_east) ;
         MAPFAC_MY:description = "Map scale factor on mass grid, y
direction" ;
        MAPFAC_MY:units = "" ;
float MAPFAC_UX(Time, south_north, west_east_stag) ;
         MAPFAC_UX:description = "Map scale factor on u-grid, x
direction" ;
        MAPFAC_UX:units = "" ;
float MAPFAC_UY(Time, south_north, west_east_stag) ;
         MAPFAC_UY:description = "Map scale factor on u-grid, y
direction" ;
        MAPFAC_UY:units = "" ;
float MAPFAC_VX(Time, south_north_stag, west_east) ;
         MAPFAC_VX:description = "Map scale factor on v-grid, x
direction" ;
        MAPFAC_VX:units = "" ;
float MF_VX_INV(Time, south_north_stag, west_east) ;
         MF_VX_INV:description = "Inverse map scale factor on v-grid, x
direction" ;
        MF_VX_INV:units = "" ;
float MAPFAC_VY(Time, south_north_stag, west_east) ;
         MAPFAC_VY:description = "Map scale factor on v-grid, y
direction" ;
        MAPFAC_VY:units = "" ;
float F(Time, south_north, west_east) ;
        F:description = "Coriolis sine latitude term" ;
        F:units = "s-1" ;
float E(Time, south_north, west_east) ;
        E:description = "Coriolis cosine latitude term" ;
        E:units = "s-1" ;
float SINALPHA(Time, south_north, west_east) ;
        SINALPHA:description = "Local sine of map rotation" ;
        SINALPHA:units = "" ;
float COSALPHA(Time, south_north, west_east) ;
        COSALPHA:description = "Local cosine of map rotation" ;
        COSALPHA:units = "" ;
float HGT(Time, south_north, west_east) ;
        HGT:description = "Terrain Height" ;
        HGT:units = "m" ;
float HGT_SHAD(Time, south_north, west_east) ;
        HGT_SHAD:description = "Height of orographic shadow" ;
        HGT_SHAD:units = "m" ;
```

```
float TSK(Time, south_north, west_east) ;
        TSK:description = "SURFACE SKIN TEMPERATURE" ;
        TSK:units = "K" ;
float P_TOP(Time) ;
        P_TOP:description = "PRESSURE TOP OF THE MODEL" ;
        P_TOP:units = "Pa" ;
float MAX_MSTFX(Time) ;
        MAX_MSTFX:description = "Max map factor in domain" ;
        MAX_MSTFX:units = "" ;
float MAX_MSTFY(Time) ;
        MAX_MSTFY:description = "Max map factor in domain" ;
        MAX_MSTFY:units = "" ;
float RAINC(Time, south_north, west_east) ;
        RAINC:description = "ACCUMULATED TOTAL CUMULUS PRECIPITATION" ;
        RAINC:units = "mm" ;
float RAINNC(Time, south_north, west_east) ;
          RAINNC:description   =   "ACCUMULATED   TOTAL   GRID   SCALE
PRECIPITATION" ;
        RAINNC:units = "mm" ;
float PRATEC(Time, south_north, west_east) ;
        PRATEC:description = "PRECIP RATE FROM CUMULUS SCHEME" ;
        PRATEC:units = "mm s-1" ;
float RAINCV(Time, south_north, west_east) ;
        RAINCV:description = "TIME-STEP CUMULUS PRECIPITATION" ;
        RAINCV:units = "mm" ;
float SNOWNC(Time, south_north, west_east) ;
        SNOWNC:description = "ACCUMULATED TOTAL GRID SCALE SNOW AND ICE"
;
        SNOWNC:units = "mm" ;
float GRAUPELNC(Time, south_north, west_east) ;
        GRAUPELNC:description = "ACCUMULATED TOTAL GRID SCALE GRAUPEL" ;
        GRAUPELNC:units = "mm" ;
float EDT_OUT(Time, south_north, west_east) ;
        EDT_OUT:description = "EDT FROM GD SCHEME" ;
       EDT_OUT:units = "" ;
float SWDOWN(Time, south_north, west_east) ;
         SWDOWN:description  =  "DOWNWARD  SHORT  WAVE  FLUX  AT  GROUND
SURFACE" ;
        SWDOWN:units = "W m-2" ;
float GLW(Time, south_north, west_east) ;
        GLW:description = "DOWNWARD LONG WAVE FLUX AT GROUND SURFACE" ;
        GLW:units = "W m-2" ;
float OLR(Time, south_north, west_east) ;
        OLR:description = "TOA OUTGOING LONG WAVE" ;
        OLR:units = "W m-2" ;
float XLAT(Time, south_north, west_east) ;
        XLAT:description = "LATITUDE, SOUTH IS NEGATIVE" ;
        XLAT:units = "degree_north" ;
float XLONG(Time, south_north, west_east) ;
        XLONG:description = "LONGITUDE, WEST IS NEGATIVE" ;
        XLONG:units = "degree_east" ;
```

```
float XLAT_U(Time, south_north, west_east_stag) ;
        XLAT_U:description = "LATITUDE, SOUTH IS NEGATIVE" ;
        XLAT_U:units = "degree_north" ;
float XLONG_U(Time, south_north, west_east_stag) ;
        XLONG_U:description = "LONGITUDE, WEST IS NEGATIVE" ;
        XLONG_U:units = "degree_east" ;
float XLAT_V(Time, south_north_stag, west_east) ;
        XLAT_V:description = "LATITUDE, SOUTH IS NEGATIVE" ;
        XLAT_V:units = "degree_north" ;
float XLONG_V(Time, south_north_stag, west_east) ;
        XLONG_V:description = "LONGITUDE, WEST IS NEGATIVE" ;
        XLONG_V:units = "degree_east" ;
float ALBEDO(Time, south_north, west_east) ;
        ALBEDO:description = "ALBEDO" ;
        ALBEDO:units = "-" ;
float ALBBCK(Time, south_north, west_east) ;
        ALBBCK:description = "BACKGROUND ALBEDO" ;
        ALBBCK:units = "" ;
float EMISS(Time, south_north, west_east) ;
        EMISS:description = "SURFACE EMISSIVITY" ;
        EMISS:units = "" ;
float TMN(Time, south_north, west_east) ;
        TMN:description = "SOIL TEMPERATURE AT LOWER BOUNDARY" ;
        TMN:units = "K" ;
float XLAND(Time, south_north, west_east) ;
        XLAND:description = "LAND MASK (1 FOR LAND, 2 FOR WATER)" ;
        XLAND:units = "" ;
float UST(Time, south_north, west_east) ;
        UST:description = "U* IN SIMILARITY THEORY" ;
        UST:units = "m s-1" ;
float PBLH(Time, south_north, west_east) ;
        PBLH:description = "PBL HEIGHT" ;
        PBLH:units = "m" ;
float HFX(Time, south_north, west_east) ;
        HFX:description = "UPWARD HEAT FLUX AT THE SURFACE" ;
        HFX:units = "W m-2" ;
float QFX(Time, south_north, west_east) ;
        QFX:description = "UPWARD MOISTURE FLUX AT THE SURFACE" ;
        QFX:units = "kg m-2 s-1" ;
float LH(Time, south_north, west_east) ;
        LH:description = "LATENT HEAT FLUX AT THE SURFACE" ;
        LH:units = "W m-2" ;
float SNOWC(Time, south_north, west_east) ;
        SNOWC:description = "FLAG INDICATING SNOW COVERAGE (1 FOR SNOW
COVER)" ;
      SNOWC:units = "" ;
```

4.1.5.6 WRF - UCM (URBAN CANOPY MODEL)

4.1.5.6.1 INPUTS

- Urban land use map: This information has to be provided directly or indirectly by the user. Every grid point have to be classified into some one of 3 urban categories:

    - Low Intensity residential: Includes areas with a mixture of constructed materials and vegetation. Constructed materials account for 30-80 percent of the cover. Vegetation may account 20 to 70 percent of the cover. These areas most commonly include single-family housing units. Population densities will be lower than in high intensity residential areas.

    - High Intensity residential: Includes highly developed areas where people reside in high numbers. Vegetation accounts for less than 20 percent of the cover. Constructed material account for 80 to 100 percent of the cover

    - Commercial/Industrial/Transportation: Includes infrastructure and al highly developed areas not classified as High Intercity residential.

Every urban category or grid point has the following urban parameter, which could be supply by the users as input data or the modeler will use the default values:

URBAN PARAMENTER	UNITS
Building Height	m
Roughness length above canyon for momentum	m
Roughness length above canyon for heat	m
Zero plane displacement height	m
Building coverage ratio	-
Normalized building height	-
Drag coefficient by buildings	-
Building volumetric parameter	1/m
Anthropogenic heat	W/m/m
Moisture availability on roof	-
Moisture availability on building wall	-
Moisture availability on road	-
Urban Fraction	-
Heat capacity of roof	Cal/cm/cm/cm/degC
Heat capacity of building wall	Cal/cm/cm/cm/degC
Heat capacity of road	Cal/cm/cm/cm/degC
Thermal conductivity of roof	Cal/cm/sec/degC
Thermal conductivity of building wall	Cal/cm/sec/degC
Thermal conductivity of road	Cal/cm/sec/degC
Surface albedo of roof	-
Surface albedo of building wall	-
Surface albedo of ground	-
Surface emissivity of roof	-
Surface emissivity of building wall	-
Surface emissivity of ground	-
Roughness length for momentum of roof	m
Roughness length for momentum of building wall	m
Roughness length for momentum of ground	m
Roughness length for heat of roof	m
Roughness length for heat of building wall	m
Roughness length for heat of ground	m
Number of roof layers	-
Number of wall layers	-
Number of road layers	-
Thickness of each roof layer	cm
Thickness of each building wall layer	cm
Thickness of each ground layer	cm

- Atmospheric variables from meteorological model: wind speed, air temperature, humidity, downward short wave radiation, downward long wave radiation, air density, cosine of solar zenith angle, solar declination, height of the first atmospheric level.

- Atmospheric variables from meteorological model or others sources like measurements : roof surface temperature, wall surface temperature, road surface temperature, roof layer temperature, wall layer temperature, road layer temperature, Monin-Obukhov stability length above roof, wall, and road.

4.1.5.6.2 OUTPUTS

"URBAN ROOF SKIN TEMPERATURE"	"K"
"URBAN WALL SKIN TEMPERATURE"	"K"
"URBAN ROAD SKIN TEMPERATURE"	"K"
"URBAN CANOPY TEMPERATURE"	"K"
"URBAN CANOPY HUMIDITY"	"kg kg{-1}"
"URBAN CANOPY WIND"	"m s{-1}"
"M-O LENGTH ABOVE URBAN ROOF"	"dimensionless"
"M-O LENGTH ABOVE URBAN WALL"	"dimensionless"
"M-O LENGTH ABOVE URBAN ROAD"	"dimensionless"
"M-O LENGTH ABOVE URBAN CANOPY"	"dimensionless"
"ROOF LAYER TEMPERATURE"	"K"
"WALL LAYER TEMPERATURE"	"K"
"ROAD LAYER TEMPERATURE"	"K"
"SENSIBLE HEAT FLUX FROM URBAN SFC"	"W m{-2}"
"LATENT HEAT FLUX FROM URBAN SFC"	"W m{-2}"
"GROUND HEAT FLUX INTO URBAN"	"W m{-2}"
"NET RADIATION ON URBAN SFC"	"W m{-2}"
"SKIN TEMPERATURE"	"K"

NOTE.- In WRF and WRF-UCM, no all variables can be output in one run. Sometimes is necessary to make several runs to obtain “all” variables.

4.1.5.7 MICROSYS CFD MODEL

4.1.5.7.1 INPUT DATA

MICROSY is a CFD code which can estimate the meteorological variables and derive heat fluxes with a high spatial resolution (1 m – 10 m). MICROSYS is typically applied in urabn environments where the buildings make the 3D environment extremely complex. MICROSYS requires extremely detailed data on buildings geometry and heights, roads geometry, structure (number of lanes and direction), speed limits, traffic lights, traffic flows (vehicles/second) and type of vehicles. This information could be stored in geographic information system (GIS) files, typically tied to regional or global coordinate systems (e.g. latitude-longitude, - state plane or Universal Transverse Mercator, UTM). This information should be provided by the user in a specific location an domain. MICROSYS demands intense computational power.

4.1.5.7.2 OUTPUT DATA

List of main outputs:

' u component	' [m/s]
' v component	' [m/s]
' w component	' [m/s]
' potential temperature	' [øC]
' turbulent kinetic energy	' [m^2/s^2]
' dissipation of turbulent kinetic energy	' [m^2/s^3]
' exchange coefficient	' [m^2/s]
' pollutants concentration	' [kg/kg]

The MICROSYS output data are: A) air pollutants concentration for the simulated pollutants (depend of the chemical mechanism). The main outputs are **ozone, nitrogen dioxide, nitrogen oxide, sulphur dioxide, carbon monoxide, methane, formaldehyde, acetaldehyde, primary particulate matter, and secondary organic aerosol, sulphur acid, nitric acid, ammonia.**

There are two main input data sets: meteorological data and emission data. Meteorological data could come from a meteorological driver like WRF or MM5. A very important process in air quality modeling is to prepare detailed emission data sets. This means that we have to obtain emission data from every simulated primary pollutant (g/s) at every grid point (at surface and eventually at vertical levels).

We can use the EMIMO model to produce the needed emission data. EMIMO is a software developed by UPM which estimates emissions in high spatial and temporal resolution environment based on global, European and national annual emission inventory data sets.

4.1.5.8 EMIMO MODEL

EMIMO is an Emission Model which is capable to estimate in a combined bottom-up and top-down approach, the emissions of primary pollutants at 1 km spatial resolution and 1 hour temporal resolution. A special version of EMIMO is called MICRO-EMIMO which can estimate emissions at 1 m resolution. EMIMO is currently based on GIS local data and global and European emission inventories such as EMEP, EDGAR, GEIA, etc.

EMIMO model requires the following data list:

- Annual emission for all domain including the following pollutant: SOx,NOx,CO,VOC,NH3,PM10,PM25
- Time splitting factors, monthly, daily and hourly.
- VOC, NOx,SOx ,PM splitting factor to the chemical mechanism (CB4,CB05,CBMZ)
- Population at every grid point (high spatial resolution)
- Roads line (vector files) and type of road. (GIS information)

4.1.5.9 EMISSION MODELLING INPUT DATA

1. Annual emission for all domain including the following pollutant: SOx, NOx, CO, VOC, NH3, PM10, PM2.5
2. Time splitting factors, monthly, daily and hourly.
3. VOC, NOx, SOx, PM splitting factor to the chemical mechanism (CB4,CB05,CBMZ)
4. Population at each of grid points
5. Roads line (vector) and type of road.

4.1.5.10 MICROSCALE MODELLING INPUT DATA

1. Buildings polylines.
2. Buildings heights
3. Street lines (vector)
4. Vehicle traffic flow (vehicles/s) at each of grid points and Type of vehicles.
5. Initital data at each of grid points including: temperature, u wind component, v wind componet and all simulated pollutants.

4.1.5.11 The CAMO Model

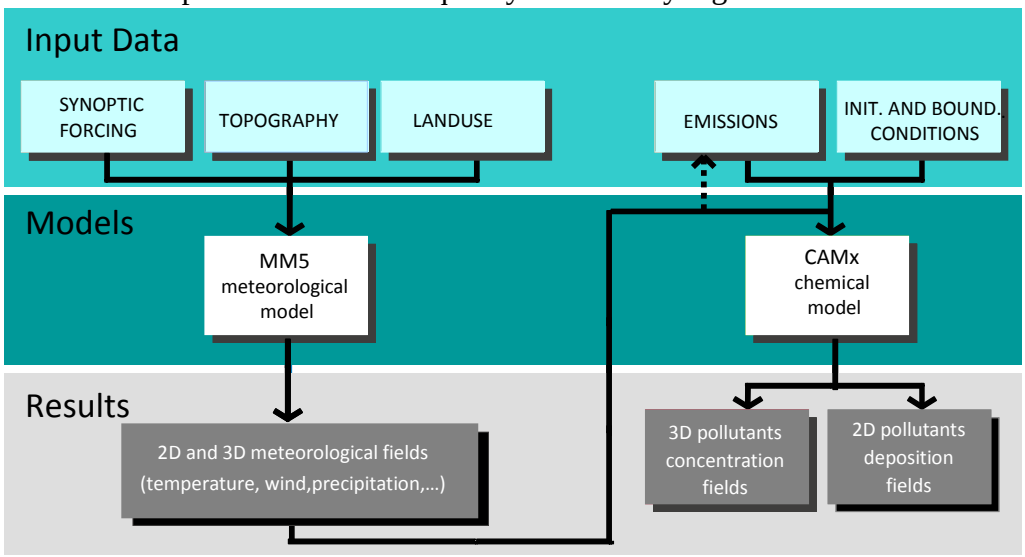
The CAMO Model is a Cellular Automata Traffic Model which is based on rules and algorithms which are simulating the vehicular traffic flow based on one pixel= one car. The system allow to include several rules such as traffic lights, waiting times, “give way”, different lanes, parking options, elevated street ways, etc. It requires a substantial computer power particularly in large cities. The system is normally used to provide traffic emissions in MICROSYS when enough detailed information is available and it is an OFF-LINE model due to the complexity and computer power required.

4.2 UAVR Models

4.2.1 MM5/CAMx model

The MM5/CAMx air quality modelling system is composed by the chemistry-transport model CAMx, forced by the MM5 meteorological fields. This system has been used in several research applications (Borrego et al., 2008; Ferreira et al., 2003, 2005). This modelling system uses the meteorological fields driven by the MM5 model and CAMx computes the atmospheric concentrations of various gaseous and aerosols.

The Figure presents a simplified scheme of the MM5-CAMx modelling system applied to the simulation of the atmospheric flow and air quality in the study region.



Simplified scheme of the MM5-CAMx modelling system (Martins, 2009)

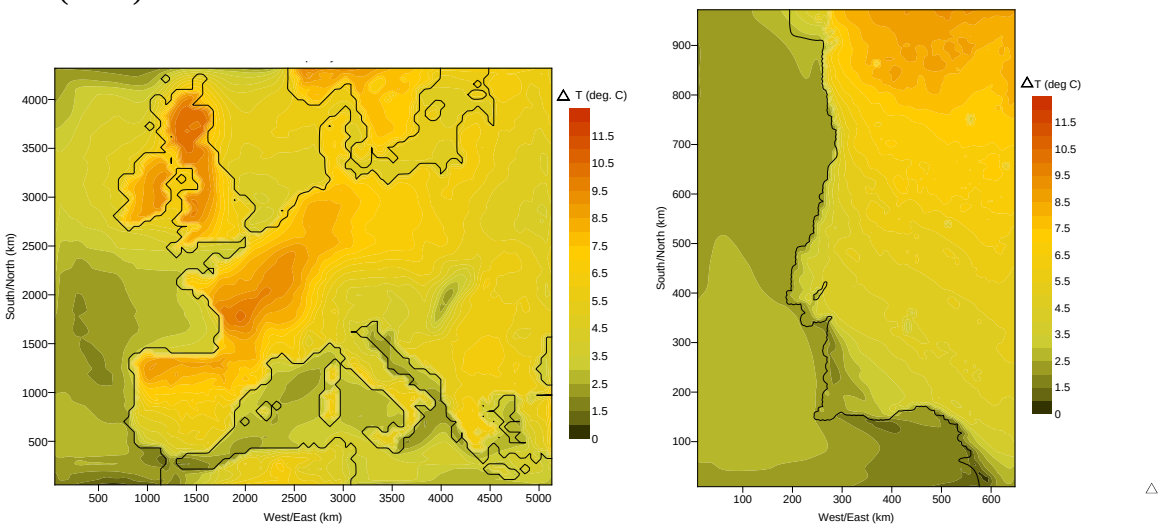
Figure 4.2.1.1 Within BRIDGE and due to the time consuming simulations this numerical system has the characteristics of an off-line model.

4.2.1.1 MM5 model

The Fifth-Generation Penn State University/National Center for Atmospheric Research (PNU/NCAR) Mesoscale Model, known as the MM5 (Grell et al., 1994), is a powerful meteorological model that contains comprehensive descriptions of atmospheric motions; pressure, moisture, and temperature fields; momentum, moisture, and heat fluxes; turbulence, cloud formation, precipitation, and atmospheric radiative characteristics.

MM5 is a nonhydrostatic, vertical sigma-coordinate model designed to simulate mesoscale atmospheric circulations. MM5 has multiple nesting capabilities, availability of four-dimensional data assimilation (FDDA), and a large variety of physics options. The most interesting features in MM5 are related with its different physics parameterisations that can be selected by the user and being capable of running in different computational platforms. Since MM5 is a regional model, it requires an initial condition as well as lateral boundary conditions to run. To produce lateral boundary conditions for a model run, one needs gridded data to cover the entire time period that

the model is integrated. The MM5 model has been successfully applied worldwide for different purposes namely weather prediction, air quality analysis and forecast, climate change assessments and impact assessment studies.As an example of the MM5 application over Europe and over Portugal, Figure 5 presents the changes in surface temperature from future (2100) to reference climate (1990).



a) b)

Figure 4.2.1.1.1 - Monthly mean surface temperature differences for July simulated a) over Europe and b) over Portugal with MM5 model between 2100 climate and 1990 climate.

4.2.1.2 INPUT DATA

Model	temporal resolution	spatial resolution	inputs	units	comments
MM5 meteorological model	hourly or 6 hourly	depending on the input database (2.5º, 1º or higher)	relative humidity	(%)	at surface and at mandatory pressure levels (1000, 850, 700, 500, 400, 300, 250, 200, 150, 100 mb)
			temperature	K	
			u wind component	$m.s^{-1}$	
			v wind component	$m.s^{-1}$	
			geopotencial height	m	
			sea level pressure (SLP)	hPa	
			sea surface temperature (SST)	K	
			topography (included in the MM5 databases)	m	
		The highest possible (250m)	land-use (included in the MM5 databases)	-	With as many land use categories as possible

4.2.1.3 OUTPUT DATA

Model	temporal resolution	spatial resolution	outputs	Units	comments
MM5 meteorological model	hourly	50km, 10km, 5km or higher	2D wind components (U, V)	m.s-1	3D forecast fields (some variables are dependent on the selected physic options)
			Temperature	K	
			Water vapour mixing ratio (if IMPHYS .ge. 2)	kg.kg-1	
			Cloud water mixing ratio (if IMPHYS .ge. 3)	kg.kg-1	
			Rain water mixing ratio (if IMPHYS .ge. 3)	kg.kg-1	
			Ice cloud mixing ratio (if IMPHYS .ge. 5)	kg.kg-1	
			Snow mixing ratio (if IMPHYS .ge. 5)	kg.kg-1	
			Graupel (if IMPHYS .ge. 6)	kg.kg-1	
			Number concentration of ice (if IMPHYS = 7)	-	
			Turbulent k.e. (if IBLTYP = 3,4,6)	J.kg-1	
			Atmospheric radiation tendency (if FRAD .ge. 2)	K.day-1	
			Vertical velocity (on full s - levels)	m.s-1	
			Perturbation pressure	Pa	
			Pstar	mb	2D forecast fields (some variables are dependent on the selected physic options)
			Ground temperature	K	
			Accum. convective rainfall	cm	
			Accum. nonconv. rainfall	cm	
			PBL height	m	
			PBL regime (category, 1-4)		
			Surface sensible heat flux	W.m-2	
			Surface latent heat flux	W.m-2	
			UST: Frictional velocity	m.s-1	
			Surface downward shortwave radiation and many other variables.	W.m-2	

4.2.1.4 CAMx model

The Comprehensive Air quality Model with extensions (CAMx) was developed by ENVIRON International Cooperation, from California, United States of America. CAMx [Morris et al., 2004] is an Eulerian photochemical dispersion model that allows the integrated "one-atmosphere" assessment of gaseous and particulate air pollution over many scales ranging from sub-urban to continental. It simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant continuity equation for each chemical species on a system of nested three-dimensional grids.

Meteorological fields are supplied to the model to quantify the state of the atmosphere in each grid cell for the purposes of calculating transport and chemistry. CAMx incorporates two-way grid nesting, which means that pollutant concentration information propagates into and out of all grid nests during model integration. Any number of grid nests can be specified in a single run, while grid spacing and vertical layer structures can vary from one grid nest to another. The nested grid capability of CAMx allows cost-effective application to large regions in which regional transport occurs, yet at the same time providing fine resolution to address small-scale impacts in selected areas [ENVIRON, 2008].

The CAMx chemical mechanisms are based on Carbon Bond version 4 (CB4) [Gery et al., 1989] and SAPRC99 [Carter, 2001].

As an example of the CAMx application over a Portuguese urban region (Porto), the next figure presents the changes in PM10 concentrations resulting from different urban development scenarios (SPRAWL and COMPACT), due to changes in land use and pollutants emissions.

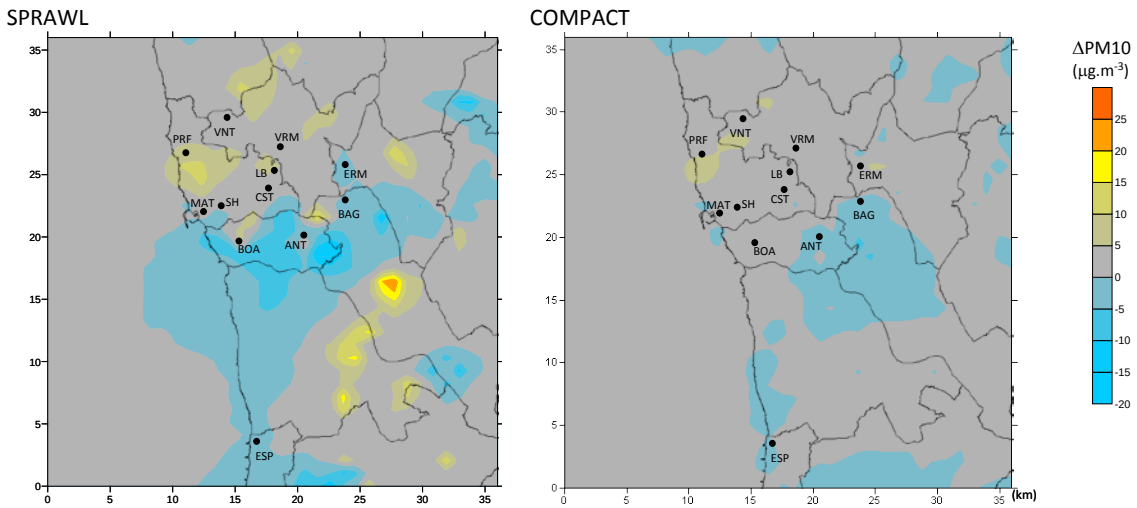


Figure. 4.2.1.2.1 PM10 annual average differences between SPRAWL and reference, and between COMPACT and reference (Martins, 2009)

4.2.1.5 INPUT DATA

CAMx requires input files that configure each simulation, define the chemical mechanism, and describe the photochemical conditions, surface characteristics, initial/boundary conditions, emission rates, and various meteorological fields over the entire modelling domain. The following table summarizes the input data requirements of CAMx.

Model	temporal resolution	spatial resolution	inputs	units	comments
CAMx	hourly	Depending on the MM5 spatial resolution (50km or 10km or 5km or higher)	specific humidity	g.kg-1	Available from MM5 outputs
			temperature	K	
			u wind component	m.s-1	
			v wind component	m.s-1	
			cloud liquid water content	kg.kg-1	
			surface pressure	hPa	
			heat fluxes	W.m-2	
			2 m temperature	K	
			cloud cover	-	
	annual	As high as possible (1km)	annual emissions of NOx, VOCs, CH4, CO, SO2, PM10, PM2.5) for area and point sources.	ton.km-2	For area and point sources (include point sources location)
	Monthly, daily, hourly	-	Emissions time splitting factors	-	For area and point sources.
	-	-	Species (VOCs, NOx and PM) splitting factors	-	For CB-IV mechanism
	-	As high as possible	Population data	-	Emissions spatial disaggregation
	As high as possible	50km or 10km or 5km or higher	Biogenic emissions	ton.km-2	-
			Land use		Available from MM5 outputs

4.2.1.6 OUTPUT DATA

CAMx post-processors allow the extraction of time series simulated concentrations for predefined locations, and bi-dimensional concentration fields for a given pollutant, respectively. These tools permit the comparison between simulated and observed data and also the evaluation of concentrations all over the study area. Next, the table presents a summary of the model outputs.

Model	temporal resolution	spatial resolution	outputs	Units	comments
CAMx air quality model	hourly	50km, 10km, 5km or higher	Air pollutants concentration (Ozone, nitrogen dioxide, nitrogen oxide, particulate matter with equivalent aerodynamic diameter < 10 µm, particulate matter with equivalent aerodynamic diameter < 2.5 µm and other pollutants)	$\mu g.m^{-3}$	

4.2.2 VADIS model

The CFD model VADIS was developed in 1998 at the Department of Environment and Planning of the University of Aveiro (UAVR), Portugal, and has been in continuous improvement and validation since then (Martins, 1998; Borrego et al., 2003 and 2006; Costa, 2008). Its structure is based on two modules, FLOW and DISPER. The first is a Reynolds Averaged Navier-Stokes (RANS) prognostic model with a standard k-ε turbulence closure that calculates the wind components, the turbulent viscosity, the pressure, the turbulent kinetic energy (k), the energy dissipation (ε) and the temperature three-dimensional (3D) fields through the finite volume method. A structured meshing scheme is used in the spatial discretisation of the domain. The second module, DISPER, applies the lagrangian approach to the computation of the 3D concentration field of inert pollutants using the wind field estimated by FLOW.

The model requires information that allows characterising the simulation domain, the meteorological conditions at the entrance of the domain, and the emissions for the considered period of time. It uses as meteorological initial conditions the air temperature and the wind speed and direction, at the entrance of the domain, and at a specified reference height. Specific initial vertical profiles are used by the model to describe the variation with height of the mean wind speed, k and ε at the entrance of the domain. Road traffic emissions are estimated by the Transport

Emission Model for Line Sources (TREM), also developed in the UAVR, using detailed data on vehicles counting.

The output data is constituted by the three wind velocity components, turbulent viscosity, k, ε, pressure, temperature, and pollutant concentration in each grid cell. Figure 7 shows an example of a simulated dispersion field.

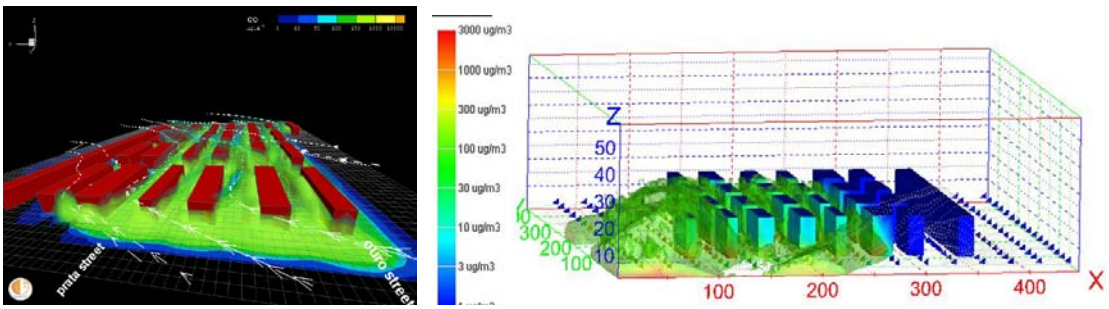


Figure 4.2.2.1 - Examples of carbon monoxide dispersion fields within an urban area.

With the purpose of allowing a friendly user access, a graphical interface has been developed that allows the configuration of the input parameters, as also the graphical representation of the input and output data.

Under development is the capability of VADIS to simulate the effect of urban vegetative canopies on the 3D flow and temperature fields, as a methodology for the evaluation of the effect of trees on air quality (outdoor/indoor) and human comfort.

Due to the highly spatially-detailed simulations, this CFD model requires a significant computational time to run the required air quality simulations in complex urban environments. This advanced computational tool will be applied to all case-studies, depending on the availability and characteristics of the input data.

4.2.2.1 INPUT DATA

Model	temporal resolution	spatial resolution	inputs	units	comments
VADIS microscale air quality model	-	-	Simulation domain: dimensions and grid resolution	m	
	-	-	Buildings volumetry: 3D coordinates	m	
	-	-	Windows size and location in each building	-	
	-	-	Roads location: 3D coordinates	m	
	Hourly	For each road	Road traffic emission rate (for each air pollutant considered)	$kg.s^{-1}$	Estimated by the road traffic emission model TREM
	Hourly	-	Indoor emissions	$\mu g.h^{-1}$	
	Hourly	At a specific measuring point	Boundary meteorological conditions: wind velocity, wind direction and temperature at a given reference height	$m.s^{-1}$ o ^oC	
	Hourly	At a specific measuring point	Background concentrations of the air pollutants	$\mu g.m^{-3}$	
	-	-	Trees definition: location and Leaf Area Density – LAD (or Leaf Area Index – LAI)	$m^2.m^{-3}$ (or $m^2.m^{-2}$)	
	Hourly	dimensions and grid resolution o the simulation domain	Population or individual time-activity patterns (3D matrices)	-	For the estimation of human exposure
	-	dimensions and grid resolution o the simulation domain	3D micro-environment matrices (ex.: outdoor, transport, residence, school, office)	-	For the estimation of human exposure

4.2.2.2 OUTPUT DATA

Model	temporal resolution	spatial resolution	outputs	Units	comments
VADIS microscale air quality model	hourly	value given for each grid cell (3D field)	wind velocity components (u, v, w)	$m.s^{-1}$	
	hourly	value given for each grid cell (3D field)	turbulent kinematic viscosity (ν_t)	$m^{-2}.s^{-1}$	
	hourly	value given for each grid cell (3D field)	turbulent kinetic energy (k)	$m^2.s^{-2}$	
	hourly	value given for each grid cell (3D field)	rate of dissipation of k (ε)	$m^2.s^{-3}$	
	hourly	value given for each grid cell (3D field)	pressure	$kg.m^{-1}.s^{-2}$	
	hourly	value given for each grid cell (3D field)	temperature	ºC	
	hourly	value given for each grid cell (3D field)	air pollutants concentration	$\mu g.m^{-3}$	Only passive air pollutants are considered (no chemistry included)
	hourly	-	population/individual exposure to air pollutants	$\mu g.m^{-3}.h^{-1}$	
	hourly	-	building's natural ventilation rate	h^{-1}	
	hourly	-	indoor air pollutants concentration	$\mu g.m^{-3}$	

4.2.3 URBAIR model

The URBAIR urban air quality model is a second generation Gaussian plume model intended to be used for distances up to about 10 km from the source. URBAIR is a steady state atmospheric dispersion model, based on boundary layer scaling parameters, instead of relying on Pasquill stability classification. The model was developed for simulating passive or buoyant gas dispersion and deposition at local and urban scales. It is designed to allow consideration of dispersion in rural or urban areas, including the treatment of building effects.

To characterize the meteorological conditions within the simulation domain, the model requires meteorological information driven by mesoscale meteorological models or by surface measurements and upper air soundings databases. URBAIR requires also the characterization of topography, land-use and the emissions of anthropogenic sources, which can be provided by inventories or by the Transport Emission Model for Line Sources (TREM), using vehicles counting data. Emission and meteorology information is defined on an hourly or daily basis.

The output data is constituted by the meteorological parameters and pollutant concentration at user-specified receptor points or spatially distributed over a regular grid.

This is a second generation Gaussian model with all the requirements to be integrated into BRIDGE's DSS as an on-line model.

This operational computational tool will be applied to all case-studies, depending on the availability and characteristics of the input data.

4.2.3.1 INPUT DATA

Model	Temporal resolution	Spatial resolution	Inputs	Units	Comments
URBAIR urban air quality model	Hourly or daily	Depending on meteorological input database	Relative humidity	(%)	From surface observations and upper air soundings or alternatively from mesoscale meteorological models
			Temperature	K	
			Wind velocity	m/s	
			Wind direction	º	
			Atmospheric pressure	hPa	
			Surface roughness	m	
			Cloud cover	(-)	
			Net radiation	W/m^2	
			Albedo and Bowen ration	(-)	

Model	Temporal resolution	Spatial resolution	Inputs	Units	Comments
			Solar radiation	W/m2	
			Solar angle elevation	o	
	-	-	Simulation domain and grid resolution	m	
	-	-	Land-use	-	Depending on simulation domain
	-	-	Topography	m	
	-		Buildings volumetry 3D: coordinates	m	
	-	-	Emission sources coordinates	m	
	Hourly or daily	For each emission source	Emission rate (for each air pollutant considered)	$kg.s^{-1}$	

1.4.1.1 OUTPUT DATA

Model	temporal resolution	spatial resolution	inputs	units	comments
URBAIR urban air quality model	Hourly or daily		Vertical profiles of wind velocity	m/s	
			Vertical profiles of potential temperature	K	
			Mixing Layer Height	m	
			Surface sensible heat flux	W/m2	
			Friction velocity	m/s	
			Atmospheric stability class	(-)	
			Monin-Obukhov length	m	
			Roughness length	m	
	Hourly or daily	Depending on simulation domain and grid	Air pollutants concentration	$\mu g.m^{-3}$	

4.3 KCL MODELS

4.3.1 LUMPS v5: LUMPS - UWB - SUES - NARP - OHM

4.3.1.1 Model Overview

The Local-scale Urban Meteorological Parameterization Scheme (LUMPS)3 is a surface flux model that utilises standard meteorological observations and land cover characteristics. It can model the variability in fluxes both spatially and temporally.

The sub-models utilised within LUMPS (Figure 1) are used to calculate:

a) the net all-wave radiation, Q^*, using NARP4 (Net All-wave Radiation Parameterization);

b) the storage heat flux, ΔQS, using the OHM3 (Objective Hysteresis Model);

c) the latent heat flux, *QE*, using LUMPS3 and SUES2 (Single-source Urban Evapotranspiration - interception Scheme);

d) the turbulent sensible heat flux, *QH*, using LUMPS3 and the residual method (using the surface energy balance). In addition the Urban Water Balance (UWB)1 is currently being added to LUMPS to simulate the urban hydrologic cycle which impacts directly on *QE* and therefore *QH*.

Our objectives are:

1) to evaluate the model, which has not been tested in the UK;

2) to improve the parameterization of processes; including reduced data inputs, producing feedback between model subroutines etc. The addition of the UWB1 model will allow us to study the effects of the urban environment on the water cycle and the effectiveness of urban water management techniques using a combination of meteorological measurement and model output.

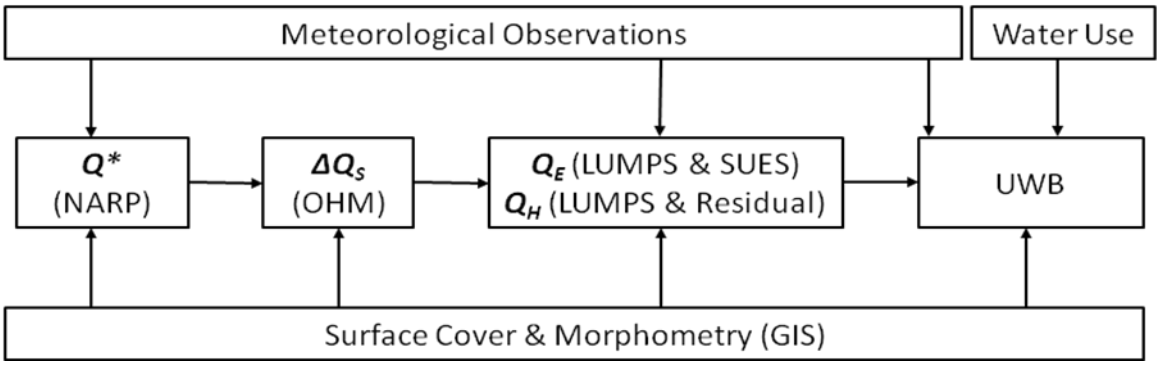


Figure 4.3.1.1.1: Structure of the LUMPS - UWB - SUES - NARP - OHM Model (based on Grimmond and Oke (2003)).

For more details see http://geography.kcl.ac.uk/micromet/index.htm - select LUMPS

4.3.1.2 Input and Output Files

Table 4.3.2.1: Input and output files used and generated by the LUMPS v5 Model. Required files have a bold file name while user defined names are in italics.

File Name	Description	Input/ Output	Tables with contents
HeaderInput.NML	Namelist called by the mode	Input	Table 2 – alphabetical listing
SUESInput.NML	Namelist called by the mode	Input	Table 2 – alphabetical listing
SSYY.ohm	File of parameters to run th Objective Hysteresis Mod (OHM).	Input	Table 2 - via the setup comman FileOHM
Smith1966.grd	Grid used in the calculatic of longwave radiation.	Input	Table 2 – via the setup comman smithFile
User specified filename ar format (e.g. *SSYY*_all60.txt)	Meteorological ar hydrological input data.	Input	Table 3 – alphabetical listin Filename and format specified Table 2 by commands FileMet InputMetFormat
User specified filename ar format (e.g. *SSYY*_all60.txt)	GIS input data	Input	Table 4 – alphabetical listin Filename and format specified Table 2 by commands FileGIS GISInputType.
User specified filename (e.g. *SSYY*_all60.txt)	Combined meteorologica hydrological and GIS inp data	Input	Tables 3 & 4 alphabetical listin Filename and format specified Table 2 by commands FileMe FileGIS, InputMetFormat GISInputType.
daily_out.txt	Daily radiation and wat balance output.	Output	Table 5 – Listed by file structure
MonthlySeason_out.txt	Monthly, seasonal and annu radiation and water balanc output.	Output	Table 5 – Listed by file structure
SSYYYY_mm.txt	Specified time perio radiation and water balanc output	Output	Table 6 – Listed by file structure

Inputs

Table 4.3.2.2: Alphabetical listing of contents of (1) HeaderInput.nml and (2) SUESInput.nml files. Param. –indicates parameter values that need to be specified for a site. (or all grid locations). Setup - indicates a decision needs to be made in the model runs options. Var. Indicates a variable

Name	Units	File	Type	Description
AerodynamicResistanceMethod	-	1	Setup	Decides which aerodynamic resistance method

Name	Units	File	Type	Description
				used.
ALB		1	Param.	Surface albedo
ALB_SNOW		1	Param.	Surface albedo for snow
BaseT(1)	°C	1	Param.	Base temp for vegetation growth (coniferous).
BaseT(2)	°C	1	Param.	Base temp for vegetation growth (deciduous).
BaseT(3)	°C	1	Param.	Base temp for vegetation growth (grass irrig.).
BaseT(4)	°C	1	Param.	Base temp for vegetation growth (grass unirrig.).
BaseTe(1)	°C	1	Param.	Base senescence temp for vegetation growth (conif).
BaseTe(2)	°C	1	Param.	Base senescence temp for vegetation growth (decid).
BaseTe(3)	°C	1	Param.	Base senescence temp for vegetation growth (gra irrig.).
BaseTe(4)	°C	1	Param.	Base senescence temp for vegetation growth (gra unirrig.).
BldgDrainCoef1	mm	2	Param.	Building surface storage coefficient
BldgDrainCoef2	mm	2	Param.	Building surface storage coefficient
BldgDrainEq	-	2	Setup	Determines buildings drainage equation
BldgState	mm	2	Param.	Initial condition of Building surfaces
BldgStorCap	mm	2	Param.	Building surface storage capacity
CommonChoiceAllSites	-	1	Setup	Determines which OHM is called.
ConifDrainCoef1	mm	2	Param.	Coniferous storage coefficient
ConifDrainCoef2	mm	2	Param.	Coniferous storage coefficient
ConifDrainEq	-	2	Setup	Determines coniferous drainage equation
ConifState	mm	2	Param.	Initial condition of Coniferous surfaces
ConifStorCap	mm	2	Param.	Coniferous storage capacity
DecidDrainCoef1	mm	2	Param.	Deciduous storage coefficient
DecidDrainCoef2	mm	2	Param.	Deciduous storage coefficient
DecidDrainEq	-	2	Setup	Determines deciduous drainage equation
DecidState	mm	2	Param.	Initial condition of Deciduous surfaces
DecidStorCap	mm	2	Param.	Deciduous storage capacity
defaultPres	Pa	1	Param.	Default pressure
defaultRH	%	1	Param.	Default relative humidity
defaultT	°C	1	Param.	Default air temperature
EMIS		1	Param.	Surface emissivity

Name	Units	File	Type	Description
EMIS_SNOW	-	1	Param.	Surface emissivity for snow
FileChoices	-	1	Setup	Name of LUMPS params output file
FileGIS	-	1	Setup	Full location (including directory) for GIS data.
FileMet	-	1	Setup	Full location (including directory) for Meteorologic data.
FileOHM	-	1	Setup	Name of file containing setup information for th Objective Hysteresis Model.
FileOut15	-	1	Setup	15 minute output data file name
FileOut30	-	1	Setup	30 minute output data file name
FileOut60	-	1	Setup	60 minute output data file name
G1	mm s^{-1}	2	Param.	Surface conductance parameter
G2	W m^{-2}	2	Param.	Surface conductance parameter
G3	kg g^{-1}	2	Param.	Surface conductance parameter
G4	g kg^{-1}	2	Param.	Surface conductance parameter
G5	°C	2	Param.	Surface conductance parameter
G6	mm^{-1}	2	Param.	Surface conductance parameter
GDDFull(1)	-	1	Param.	Canopy growth param (coniferous)
GDDFull(2)	-	1	Param.	Canopy growth param (deciduous)
GDDFull(3)	-	1	Param.	Canopy growth param (grass irrig.)
GDDFull(4)	-	1	Param.	Canopy growth param (grass unirrig.)
GISInputType	-	1	Setup	Declares the file structure of the GIS data.
GrassFractionIrrigated	-	1	Param.	Fraction of irrigated grass
GrassIDrainCoef1	mm	2	Param.	Grass irrigated storage coefficient
GrassIDrainCoef2	mm	2	Param.	Grass irrigated storage coefficient
GrassIDrainEq	-	2	Setup	Determines grass irrigated drainage equation
GrassIState	mm	2	Param.	Initial condition of Grass irrigated surfaces
GrassIStorCap	mm	2	Param.	Grass irrigated storage capacity
GrassUDrainCoef1	mm	2	Param.	Grass un-irrigated storage coefficient
GrassUDrainCoef2	mm	2	Param.	Grass un-irrigated storage coefficient
GrassUDrainEq	-	2	Setup	Determines grass un-irrigated drainage equation
GrassUState	mm	2	Param.	Initial condition of Grass un-irrigated surfaces
GrassUStorCap	mm	2	Param.	Grass un-irrigated storage capacity
Name	**Units**	**File**	**Type**	**Description**

Name	Units	File	Type	Description
InputMetFormat	-	1	Setup	Declares the file structure of the met. data.
internalwaterUse	mm da[1]		Param.	Daily water usage
INTERVAL	-	1	Setup	Model time interval
Irig	-	2	Setup	Determines if the surface is irrigated
ITY	-	2	Setup	Determines evapotranspiration method is used
LAICalcYes	-	1	Setup	Are Leaf Area Indexes calculated?
LAImax(1)	-	1	Param.	Maximum LAI value (coniferous)
LAImax(2)	-	1	Param.	Maximum LAI value (deciduous)
LAImax(3)	-	1	Param.	Maximum LAI value (grass irrig.)
LAImax(4)	-	1	Param.	Maximum LAI value (grass unirrig.)
LAImin(1)	-	1	Param.	Minimum LAI value (coniferous)
LAImin(2)	-	1	Param.	Minimum LAI value (deciduous)
LAImin(3)	-	1	Param.	Minimum LAI value (grass irrig.)
LAImin(4)	-	1	Param.	Minimum LAI value (grass unirrig.)
lat	°	1	Param	Latitude
Lm	-	2	Param.	Surface conductance parameter
lng	°	1	Param	Longitude
NetRadiationChoice	-	1	Setup	Determines net-radiation scheme
OhmFileType	-	1	Setup	Determines OHM method
PavDrainCoef1	mm	2	Param.	Pavement surface storage coefficient
PavDrainCoef2	mm	2	Param.	Pavement surface storage coefficient
PavDrainEq	-	2	Setup	Determines pavement drainage equation
PavedFractionIrrigated	-	1	Param.	Fraction of irrigated paved areas
PavState	mm	2	Param.	Initial condition of paved surfaces
PavStorCap	mm	2	Param.	Pavement surface storage capacity
Qmax	W m^{-2}	2	Param.	Max hourly net radiation (Surface conductanc param.)
QSChoice	-	1	Setup	Identifier to determine surface heat flu method/measured
qe	W m^{-2}	3	Param.	Latent heat flux (optional)
qh	W m^{-2}	3	Param.	Sensible heat flux (optional)
qn1	W m^{-2}	3	Param.	Net all-wave radiation (optional)

Name	Units	File	Type	Description
qs	W m^{-2}	3	Param.	Storage heat flux (optional)
S1	mm	2	Param.	Fitted soil moisture (Surface conductance param.)
S2	mm	2	Param.	Fitted soil moisture (Surface conductance param.)
SDDFull(1)	-	1	Param.	Vegetation parameter (coniferous)
SDDFull(2)	-	1	Param.	Vegetation parameter (deciduous)
SDDFull(3)	-	1	Param.	Vegetation parameter (grass irr)
SDDFull(4)	-	1	Param.	Vegetation parameter (grass unirr)
SDEC1	-	2	Param.	Vegetation parameter (coniferous)
SDEC2	-	2	Param.	Vegetation parameter (deciduous)
SDEC3	-	2	Param.	Vegetation parameter (grass irrig.)
SDEC4	-	2	Param.	Vegetation parameter (grass unirr)
SDECstor	-	2	Param.	Vegetation parameter
SkipHeaderGIS	-	1	Setup	Number of lines to skip in GIS input file
SkipHeadersMet	-	1	Setup	Number of lines to skip in meteorology input file
smithFile	-	1	Setup	Full location of Smith1966.grd
Name	**Units**	**File**	**Type**	**Description**
soilstoreBldg	mm	2	Param.	Soil storage (building)
soilstoreBldgState	mm	2	Param.	Initial soil storage condition (building)
soilstoreConif	mm	2	Param.	Soil storage (coniferous)
soilstoreConifstate	mm	2	Param.	Initial soil storage condition (coniferous)
soilstoreDec	mm	2	Param.	Soil storage (deciduous)
soilstoreDecState	mm	2	Param.	Initial soil storage condition (deciduous)
soilstoreGrassIrr	mm	2	Param.	Soil storage (grass irrigated)
soilstoreGrassIrrState	mm	2	Param.	Initial soil storage condition (grass irrigated)
soilstoreGrassUnir	mm	2	Param.	Soil storage (grass un-irrigated)
soilstoreGrassUnirState	mm	2	Param.	Initial soil storage condition (grass un-irrigated)
soilstorePav	mm	2	Param.	Soil storage (pavement)
soilstorePavstate	mm	2	Param.	Initial soil storage condition (pavement)
StabilityMethod	-	1	Setup	Determines stability method used
TH	°C	2	Param.	Max temperature (Surface conductance param.)
TIMEZONE	-	1	Param.	Time zone location
TL	°C	2	Param.	Min temperature (Surface conductance param.)

Name	Units	File	Type	Description
TRANS_SITE	-	1	Setup	
TreeFractionIrrigated	-	1	Param.	Fraction of irrigated tree areas
Tstep	-	2	Param.	Timestep (seconds)
Veg_type	-	1	Setup	Determines if area is irrigated or un-irrigated
WaterUseArea	ha	1	Param.	Area of water use in hectares.
year	-	1	Var.	Year of study
z	m	1	Param.	Measurement height
z0_method	-	1	Setup	Method used to calculate roughness length
z0m	m	1	Param.	Aerodynamic roughness length
zdm	m	1	Param.	Displacement height

Table 4.3.2. 3: Meteorological and hydrological input variables (Var.). These are presented in alphabetical order.

Name	Units	Type	Description
avkdn	W m^{-2}	Var.	Average incoming shortwave radiation
AvLup	W m^{-2}	Var.	Average upwelling longwave radiation
avrh	%	Var.	Average relative humidity
avu1	m s^{-1}	Var.	Average wind speed
dectime	-	Var.	Decimal time
ph	mm hr^{-1}	Var.	Hourly Precipitation
Press_hPa	hPa	Var.	Atmospheric pressure
snow	-	Var.	Snow cover fraction
Temp_C	°C	Var.	Air Temperature
wuh	mm hr^{-1}	Var.	Hourly water use
xsmd	mm	Var.	Soil water deficit
z0m	m	Var.	Surface roughness
zdm	m	Var.	Zero-plane displacement height

Table 4.3.2.4: GIS input variables (VAR)/parameters. The GIS input can be treated as either parameters (defined at the start of the model) or variables depending on dataset used. There are two classification

methods for surface cover fraction each with 6 categories. Either can be used dependent on how surface fraction cover was determined (marked by either a [1] or [2]). These are presented in alphabetical order.

Name	Units	Type	Description
build [1]	-	Var./ Param.	Surface cover fraction – buildings
cany3d	-	Var./ Param	Surafce cover fraction of street canyons
gras [1]	-	Var./ Param	Surface cover fraction – grass
lai_hr	-	Var./ Param	Hourly leaf Area Index (optional)
ROOF3D	-	Var./ Param	Surface cover fraction of 3-dimensional roofs
sfr(1) [2]	-	Var./ Param	Surface cover fraction – pavement
sfr(2) [2]	-	Var./ Param	Surface cover fraction – buildings
sfr(3) [2]	-	Var./ Param	Surface cover fraction – coniferous
sfr(4) [2]	-	Var./ Param	Surface cover fraction – deciduous
sfr(5) [2]	-	Var./ Param	Surface cover fraction – grass un-irrigated
sfr(6) [2]	-	Var./ Param	Surface cover fraction – grass irrigated
tree_sh [1]	-	Var./ Param	Surface cover fraction – trees
unman [1]	-	Var./ Param	Surface cover fraction – unmanaged
watr [1]	-	Var./ Param	Surface cover fraction – water
ximper [1]	-	Var./ Param	Surface cover fraction – impervious

Outputs

Table 4.3.2.5: Output included in daily_out.txt; MonthlySeason_out.txt.

Name	Units	Description
day/season/year	-	Time period (dependent on output period)
Counter	-	Output counter (number of cases in each period)
qn	W m-2	Net all-wave radiation
qs	W m-2	Storage heat flux
QE_S	W m-2	Latent heat flux (SUES)
QE_L	W m-2	Latent heat flux (LUMPS)
Precip	mm	Precipitation
extWU	mm	External Water Usage
int_WU	mm	Internal Water Usage
Evap_S	mm	Evapotranspiration
Drain	mm	Drainage
SoilSt	mm	Soil Storage
Ch	mm	Change in storage
Runoff	mm	Runoff

Table 4.3.2.6: Output included in *SSYYYY_mm*.txt – *SS* is the two letter site identification and *mm* is the number of minutes used for the averaging period. Within the table, i represents the file time period (e.g. P/15 minutes is precipitation per 15 minutes).

Variable	Units	Description
dectime	-	Decimal time
Kdown	W m^{-2}	Incoming shortwave radiation
Kup	W m^{-2}	Reflected shortwave radiation
Ldown	W m^{-2}	Downwelling longwave radiation
Lup	W m^{-2}	Upwelling longwave radiation
Tsurf	°C	Surface temperature
qn	W m^{-2}	Net all-wave radiation
h_mod	W m^{-2}	LUMPS sensible heat flux
e_mod	W m^{-2}	LUMPS latent heat flux
qs	W m^{-2}	Storage heat flux
QF	W m^{-2}	Anthropogenic heat flux
QE	W m^{-2}	Latent heat flux
QH	W m^{-2}	Sensible heat flux
P/i	mm i^{-1}	Precipitation per unit time
WU/i	mm i^{-1}	Water use per unit time
EV/i	mm i^{-1}	Evapotranspiration per unit time
DR/i	mm i^{-1}	Drainage per unit time
ST/i	mm i^{-1}	Soil storage per unit time
CH/i	mm i^{-1}	Change in storage per unit time
RA	s m^{-1}	Aerodynamic resistance
RS	s m^{-1}	Surface resistance
ustar	m s^{-1}	Friction velocity
L_mod	m	Modified Obukhov length
State	mm	Surface state
pav	mm	Surface state paved
bldg	mm	Surface state buildings
conf	mm	Surface state coniferous
decid	mm	Surface state deciduous
grassU	mm	Surface state un-irrigated grass
grassI	mm	Surface state irrigated grass
FCLD	tenths	Fraction cloud cover

4.4 CNRM MODELS (CNRM Météo France)

4.4.1 SURFEX overview

SURFEX is an externalised surface scheme that can be run either in a coupled mode in which case the atmospheric forcing is provided by the host atmospheric model, or in a standalone mode where the atmospheric drivers are derived from observations. SURFEX contains various modules allowing to describe the exchanges of water, momentum, and energy on **4 tiles of surface**: sea, lake, vegetation, and the city, a grid value is then simply an area averaged value of the different tiles present in the grid cell (Figure 1). Over vegetated areas, SURFEX includes the Interactions between Soil, Biosphere, and Atmosphere (ISBA) scheme[4]. ISBA solves simultaneously the energy and water budget of the soil and vegetation. Water budget is forced by precipitation (rain and snow), and takes into account evaporation of the soil, transpiration from the vegetation, interception and evaporation of water on the leaves, runoff and drainage. The energy budget is forced by incoming radiation (both solar and infrared), and computes outgoing radiation (reflected solar and emitted/reflected thermal infrared radiation), heat flux towards/from the ground, and turbulent fluxes (sensible heat and latent heat from the water vapor flux). Vegetation parameters should be prescribed, for example from the ECOCLIMAP database[2]. Over urban surfaces, SURFEX includes the Town Energy Balance (TEB) single layer urban canopy module[1]. Urban canopy is assumed to be an isotropic array of street canyons (Figure 2). The advantage over more comprehensive urban surface schemes, which include parameterizations for the canyon orientation and heterogeneous buildings morphology is that relatively few individual surface energy balance evaluations need to be resolved, radiation interactions are simplified, and therefore computational time is kept low. TEB simulates heat and water exchanges and climate of three generic surfaces (roof, wall, and road), where heat transfers are computed through several layers of materials. Anthropogenic heat and vapor releases from buildings, vehicles and chimneys can also be added. TEB utilises standard surface thermal parameters and observed or simulated atmospheric and radiation data from above roof level and returns at the neighborhood scale the fluxes and urban canyon climate characteristics (air temperature, humidity, wind). Despite the simplification hypotheses, offline simulations of TEB have been shown to accurately reproduce surface energy balance, canyon air temperature, energy consumption and surface temperatures observed in dense urban areas for various seasons. SURFEX also includes a surface boundary layer (SBL) scheme[3]. With this version, several prognostic air layers are added from the ground up to the forcing level and the surface boundary layer is, thus, resolved prognostically, taking into account large scale forcing, turbulence and, if any, drag and canopy forces. The interest of this approach is to improve the restitution of the climate near the surface.

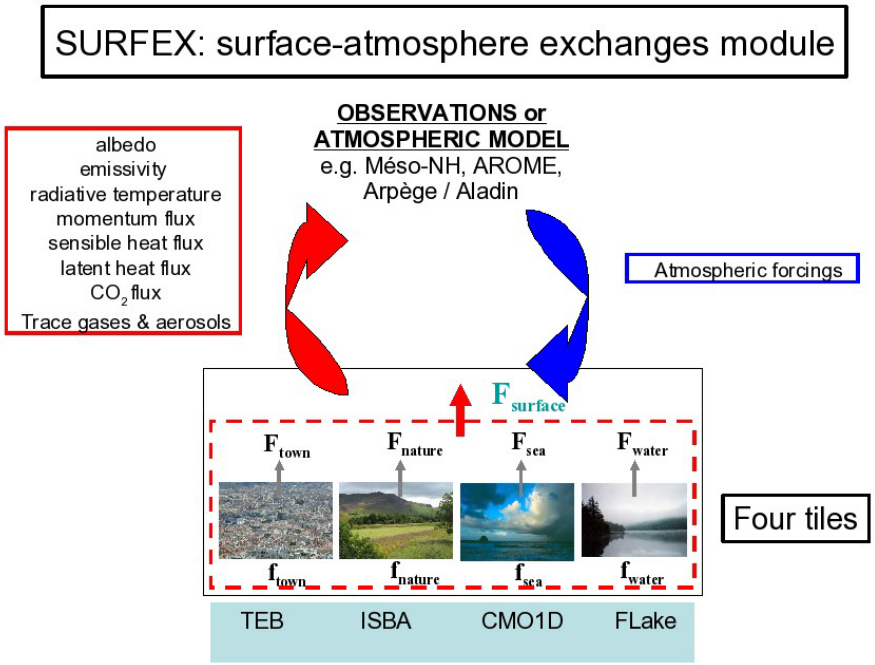


Figure 4.4.1.1: Structure of SURFEX

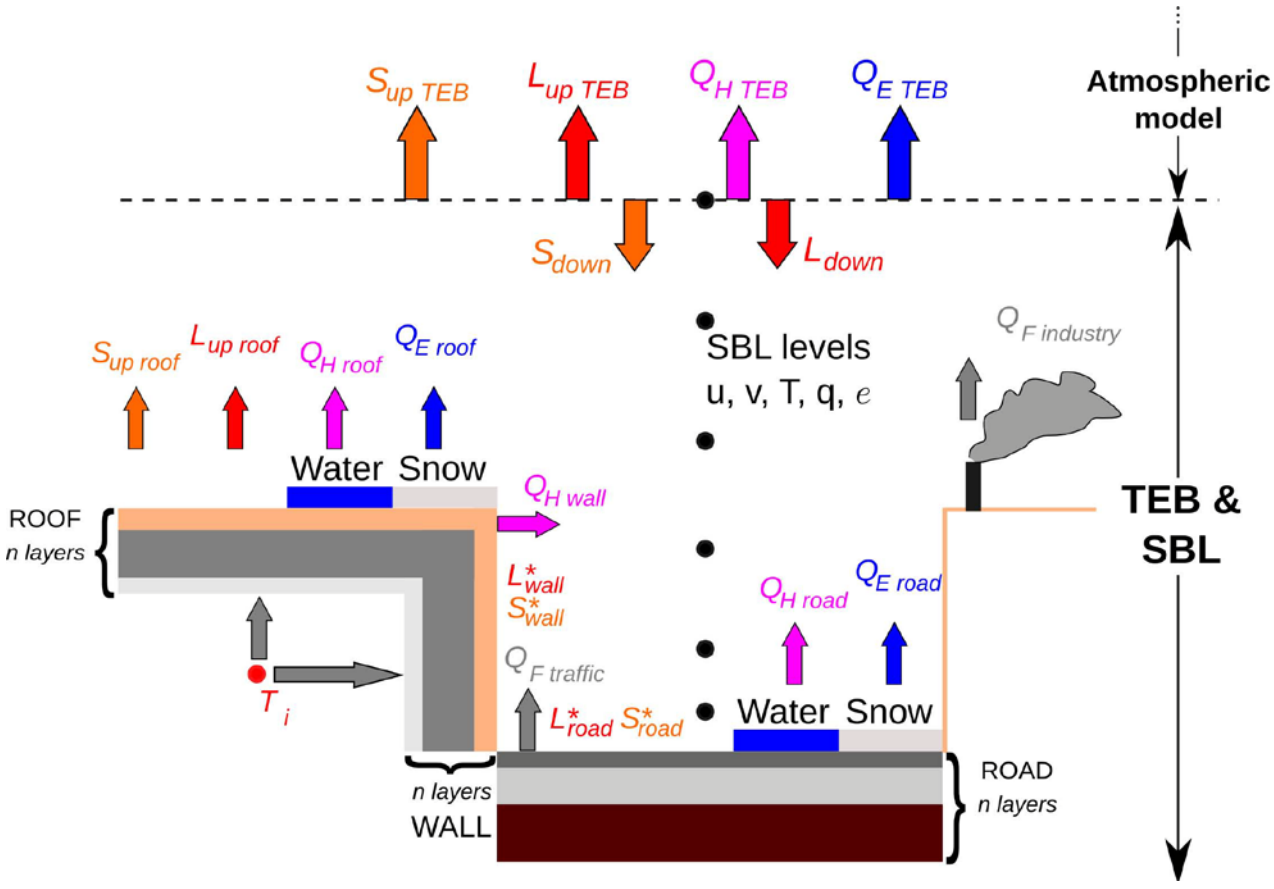


Figure 4.4.1.2: Schematic representation of the generic urban canyon used in TEB

4.4.2 INPUT DATA

INPUTS	Units	Spatial resolution	Time resolution
Air temperature above canopy	K or °C	1 rural and 1 urban point	30 minutes to 3 hours
Specific humidity above canopy	kg/kg	1 rural and 1 urban point	30 minutes to 3 hours
Incoming solar radiation	W m^{-2}	1 rural and 1 urban point	30 minutes to 3 hours
Infrared solar radiation	W m^{-2}	1 rural and 1 urban point	30 minutes to 3 hours
Air pressure	Pa	1 point	30 minutes to 3 hours
Rain rate	Kg m^{-2} s^{-1} (or mm/s)	1 rural and 1 urban point	30 minutes to 3 hours
Wind speed	m s^{-1}	1 rural and 1 urban point	30 minutes to 3 hours
Wind direction	°/N	1 rural and 1 urban point	30 minutes to 3 hours
Building plan area density	- (m^2/m^2)	Local scale (10^2 to 10^3m)	For each urban planning scenario
Road plan area density	- (m^2/m^2)	Local scale (10^2 to 10^3m)	For each urban planning scenario
Vegetation plan area density (possibility to separate between types)	- (m^2/m^2)	Local scale (10^2 to 10^3m)	For each urban planning scenario
Water plan area density	- (m^2/m^2)	Local scale (10^2 to 10^3m)	For each urban planning scenario
Wall surface/horizontal surface	- (m^2/m^2)	Local scale (10^2 to 10^3m)	For each urban planning scenario
Building height	m	Local scale (10^2 to 10^3m)	For each urban planning scenario
Wall layer depths	m	Local scale (10^2 to 10^3m)	For each urban planning scenario
Roof layer depths	m	Local scale (10^2 to 10^3m)	For each urban planning scenario
Road layer depths	m	Local scale (10^2 to 10^3m)	For each urban planning scenario
Wall layer specific heat	J m^{-3} K^{-1}	Local scale (10^2 to 10^3m)	For each urban planning scenario

Roof layer specific heat	J m^{-3} K^{-1}	Local scale (10^2 to 10^3m)	For each urban planning scenario
Road layer specific heat	J m^{-3} K^{-1}	Local scale (10^2 to 10^3m)	For each urban planning scenario
Wall layer thermal conductivity	W m^{-1} K^{-1}	Local scale (10^2 to 10^3m)	For each urban planning scenario
Roof layer thermal conductivity	W m^{-1} K^{-1}	Local scale (10^2 to 10^3m)	For each urban planning scenario
Road layer thermal conductivity	W m^{-1} K^{-1}	Local scale (10^2 to 10^3m)	For each urban planning scenario
Anthropogenic heat flux associated with traffic	W m^{-2} or number of vehicles / hour	Local scale (10^2 to 10^3m)	For each urban planning scenario

4.4.3 OUTPUT DATA

LIST OF SURFEX (TEB, ISBA etc...) OUTPUTS/ POSSIBLE INDICATORS

OUTPUTS	POSSIBLE INDICATORS
Upward solar radiation (W/m²)	
Upward longwave radiation (W/m²)	
Sensible heat flux (W/m²)	
Latent heat flux (W/m²)	
Storage heat flux (W/m²)	
Anthropogenic heat flux associated with heating/cooling (W/m²)	Energy demand ; Heat releases
Air temperature profile in Canopy (K, or °C)	Outdoor Thermal Comfort index
Wind speed profile in Canopy (ms^{-1})	
Moisture profile in Canopy (kg/kg or %)	
Wall outdoor surface temperature (K or °C)	
Road surface temperature (K or °C)	
Roof outdoor surface temperature (K or °C)	
Wall indoor surface temperature (K or °C)	Indoor Thermal Comfort index
Roof indoor surface temperature (K or °C)	
Floor indoor surface temperature (K or °C)	
Indoor air temperature (K or °C)	
CO_2 net exchange with vegetation (µmol m^{-2} s^{-1})	Carbon dioxide budget

- Spatial resolution, coverage and time resolution :
  - typical spatial resolution : local or neighborhood scale (10^2 to 10^3 m)
  - typical coverage of the domain : mesoscale (up to 10^5 m)
  - typical time resolution : 30 minutes

4.5 UHEL MODELS

4.5.1 An Overview of the SCADIS Footprint Calculator

The SCADIS model solves the wind and turbulence fields over a heterogeneous scene. The scene-specific terrain topography and forest canopy height and leaf area density (or possible a corresponding description for an urban canopy) can be described in detail, to provide a realistic description of the scene (see the figures below). SCADIS then computes the footprint, for an eddy flux tower or other such measurement instrument, based on the wind and turbulence fields.

The SCADIS Footprint Calculator operates in a 2D mode (x-horizontal, z-vertical). The horizontal resolution can be adjusted by the user, in vertical the domain is up to 3 km, so that all of the atmospheric boundary layer is contained. The SCADIS Footprint Calculator assumes neutral atmospheric stratification.

This description applies to the SCADIS Footprint Calculator, as is available for end users on the SCADIS website. There are also other versions of SCADIS, e.g. 3D-versions, and versions for nonneutral stratification, in development and in research use.

SCADIS website: http://www.necc.nu/NECC/Activities/Scadis/

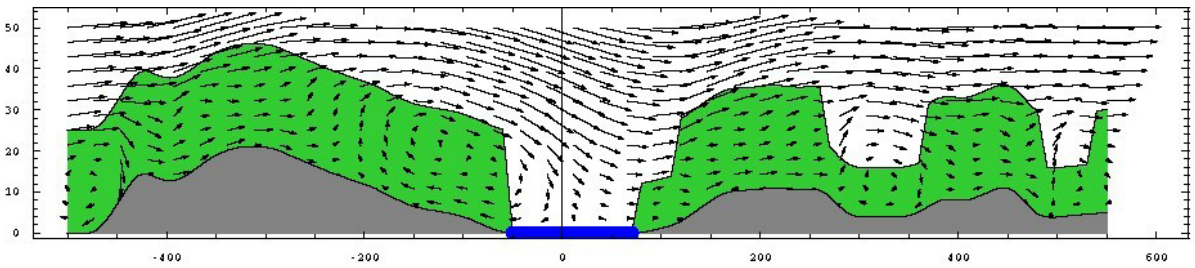


Figure 4.5.1. Wind vector field, topography, forest canopy and a lake.

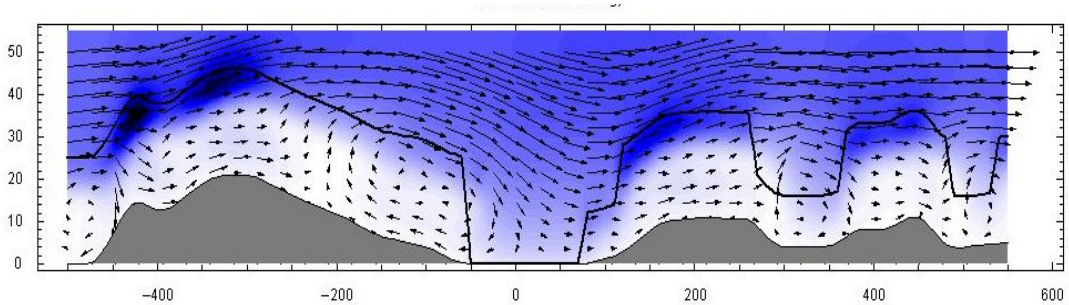


Figure 4.5.2. Wind vector field, and Turbulence Kinetic Energy (TKE), in blue density plot.

SCADIS Footprint Calculator is a 2-dimensional footprint model based on solving the turbulent wind flow inside and above the canopy in a 50 (x) by 75 (z) computational grid. SCADIS uses a 1.5-order turbulence closure. The conditions of neutral atmospheric statification are assumed.

SCADIS Footprint Calculator consists of 3 programs: (1) A graphical user interface program to prepare the input data into files, (2) a program to calculate the wind and turbulence fields, based on the input files, and (3) a program to calculate the footprint, based on the wind and turbulence fields.

The software, with a manual accompanying, is available as Windows executables at: http://www.necc.nu/NECC/Activities/Scadis/

4.5.1.1 Input Parameters

Latitute (Recommended to limit between 10 N and 80 N)

Geostrophic Wind

Horizontal grid incement (The dx stepsize for the computational grid)

Location of measurement point Specified as the number of the grid cell where it is located, and height.

SCADIS Footprint Calculator uses 50 grid cells in the horizontal direction. Each grid cell is assigned a surface class. Surface parameters are defined for each surface class. By using 50 classes and assigning each grid cell to a different surface class, one can define different vegetation properties for each grid cell. Alternatively, using only few surface classes makes the input simpler.

For each surface class one assigns:

Roughness This is ground surface roughness, it does not include the overstorey vegetation.

Canopy Height

Leaf Area Index

Canopy Shape Parameter The vertical distribution of leaf area index is described by beta distribution, and this is the alpha-parameter. For example, a value of 1 produces a canopy with most leaf area in the bottom, a value 3 gives a symmetrical distribution with a maximum in the middle, and 18 concentrates most of the leaf area at the very top of the canopy. See figure on p. 6 in SCADIS Footprint Calculator manual (available from the above website).

Other Versions

There are other versions of models in the SCADIS family, including 1-dimensional and 3-dimensional models, and some models including radiation, canopy photosynthesis, CO_2-flux, water vapour flux, heat flux, and time dependency and the diurnal cycle. For more information, contact the author of SCADIS:

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Here is a list of output variables for the SCADIS model:

4.5.1.2 Primary output:

Footprint intensity (dimensionless) for 3 cases:

- sources inside vegetation canopy
- sources on soil surface
- for joint distribution of the two

Auxiliary (but potentially very useful) outputs:

1. wind velocity, vector (m s-1)
2. turbulent kinetic energy - TKE (m2 s-2)
3. dissipation rate of TKE (m2 s-3)
4. vertical eddy diffusivity (m2 s-1)
5. mixing length (m)
6. pressure perturbation (pa)
7. local velocity scale uL (m s-1)
8. (just above the canopy this is the friction velocity)
9. CO2 concentration caused by all present sources (mmol mol-3).
10. CO2 concentration caused by sources located on soil surface only (mmol
11. mol-3)
12. CO2 concentration caused by sources located inside the vegetation
13. canopy only (mmol mol-3)
14. CO2 vertical fluxes caused by all present sources (umol m-2 s-1).
15. CO2 vertical fluxes caused by sources located on soil surface
16. only (umol m-2 s-1)
17. CO2 vertical fluxes caused by sources located inside the vegetation
18. canopy only (umol m-2 s-1).

The SCADIS model is a 2-dimensional (x,z) model, and solves for the equilibrium in neutral stratification conditions, so there is no time dimension. The spatial dimension is in 50 m steps. The is also an experimental 3-dimensional version of the model, and an experimental time-dependent model for non-neutral situations.

4.6 ALTERRA MODELS

For the hydrological modeling we use our modeling code SIMGRO and more specific the module SIMGRO-urban. The code is relatively simple (compared to most of the climate models), and does not require much computer power. SIMGRO-urban describes the rainfall runoff process of urban areas, including paved and unpaved areas, the unsaturated zone, plant-atmosphere relations and the sewerage system. Modules for groundwater flow and surface water flow can be included, depending on relevance and data availability. Typical model outcomes are: sewerage outflow, (reduction of) evapotranspiration, groundwater recharge. With SIMGRO-urban the hydrological impact of measures (like green roofs), land use change (urbanisation) and climate change can be assessed.

SIMGRO is a mechanistic distributed hydrologic model. The schematisations can be constructed as shown in Figure 5.6.1.1. At the bottom layer there are the combined land-use and soil units (which can be obtained from an overlay procedure of land-use and soil maps). Then follows the layer with the cells of the groundwater model. The third layer is formed by the sub-catchments of the urban water model. Surface water is modelled as a network of watercourse trajectories that connect to these sub-catchments. Depending on the way the model has been implemented, this can involve even the smallest of watercourses. But in most applications a certain degree of lumping is done in the headwaters. In the top layer of Figure 5.6.1.1., the schematisations are combined. These are the so-called SVAT-units (Soil Vegetation Atmosphere Transfer) which are used for the top-system modelling. The atmosphere itself is not described as a separate entity.

The used solutions of fundamental underlying differential equations inevitably involve a certain degree of simplification. Essential for the practical relevance of the model is that it has remained possible to make long simulation runs within acceptable computation times. During the model development this has been a guiding principle of the utmost consideration.

The model is dynamic, with separate time steps for the ‘fast’ processes (Δt_s) and for the ‘slow’ ones (Δt_g). The ‘fast’ processes include plant/atmosphere interactions, flow over the soil surface, urban sewage flow, drainage with surface water feedback, and channel flow.

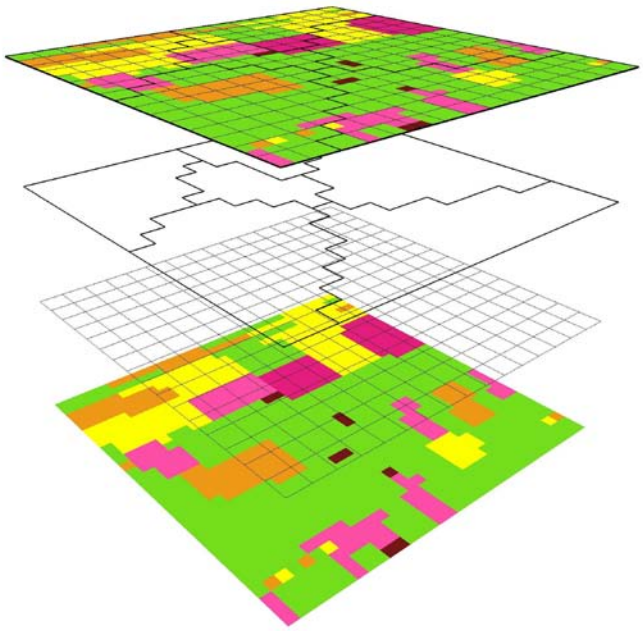

Figure 4.6.1.1. Example of how the spatial schematisations of the integrated model can be constructed. The bottom layer involves the units obtained from an overlay of the land use and soil maps. The next layer represents the cells of the groundwater model, followed by the sub-catchments of the urban water model in the next layer. The top layer shows how the schematisations have been combined.

Soil water and groundwater flow are modelled as 'slow' processes. Typical time steps used in the current modelling practice of integrated regional modelling with SIMGRO are Δt_s=1 hour and Δt_g =1 day. Model output includes all calculated states and fluxes for each time step. An overview of the processes in SIMGRO-urban is offered below.

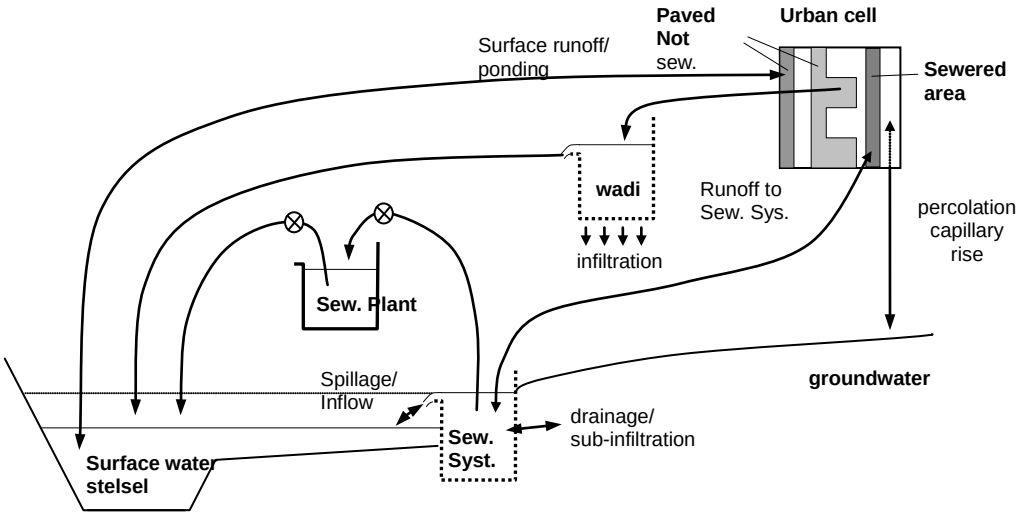

Figure 4.6.1.2. The SIMGRO-urban runoff process

The SIMGRO model can be integrated on-line into the DSS, provided enough input data is available. The complexity, size and computer demands are limited. We will build the SIMGRO model for 2 case studies: Helsinki and Firenze, for the part of the cities the CoP's are focusing on. It is our idea to present the results of the model during one the CoP-meetings and to try to use the model during the CoP-meeting as a hydrological DSS. In other words: we would like to use the model more or less interactively to evaluate measures or changes during the meeting. This could be a valuable learning lesson on how to bring together models/DSS's and CoP's.

4.6.1 Input

The GIS data needed for the implementation of the SIMGRO model include: Topography (DEM), Land Use/Land Cover data (Roads & Buildings, Surface water, Vegetation), Soil, Sewage and Drainage. Time dependend input includes: precipitation and (parameters to calculate) evapotranspiration. Below you find the most important input files along with a comprehensive list of the input variables/parameters and model setup information for SIMGRO-urban. Each SVAT-unit is to be specified in de input file area_svat.inp.

Input file	Description
AREA_SVAT.INP	area, soil surface elevation , soil unit, land use, thickness root zone meteo station
LUSE_SVAT.INP	set of land use options and their characteristics
FACT_SVAT.INP	values of vegetation factors, interception characteristics
UNSA_SVAT.BDA	database with steady states of soil moisture profiles
METE_SVAT.INP	precipitation and evapotranspiration

AREA_SVAT.INP

The file AREA_SVAT.INP contains the main parameters of the SVAT units.

Variable format and description

col	Format	name	unit	description
1-10	I10	svat	-	SVAT unit
11-20	F10.0	ark	m2	area
21-28	F8.0	glk	m+MSL	soil surface elevation
29-36	F8.0	vxmu	m	micro storage capacity
37-42	I6	slk	-	soil physical unit number
43-50	F8.0	qinfmaxik	m/d	infiltration capacity of soil surface
51-58	8x	-	-	blank
59-64	I6	luk	-	land use type
65-72	F8.0	dprzk	m	root zone thickness
73-82	I10	nmmend	-	meteorological region code number
83-90	F8.0	calprec	-	local calibration factor for precipitation
91-98	F8.0	caletref	-	local calibration factor for potential evapotranspiraiton c reference crop

LUSE_SVAT.INP

The file LUSE_SVAT.INP contains the set of land use options and their characteristics.

Variable format and description

col	format	name	unit	Description
1-6	I6	lu	-	index of land use type
7-26	A20	luna	-	name of land use type
27-32	I6	vglu	-	index of vegetation type
39-46	F8.0	p1fd	m	p1 Feddes function
47-54	F8.0	p2fd	m	p2 Feddes function
55-62	F8.0	p3hfd	m	p3h Feddes function
63-70	F8.0	p3lfd	m	p3l Feddes function
71-78	F8.0	p4fd	m	p4 Feddes function
79-86	F8.0	t3hfd	mm d^{-1}	t3 Feddes function
87-94	F8.0	t3lfd	mm d^{-1}	t3 Feddes function
95-102	F8.0	pbgsplu	m	pressure head begin sprinkling
103-110	F8.0	frevsplu	-	fraction evaporated sprinkling water
111-118	F8.0	gisplu	mm	gift in rotational period
119-126	F8.0	tigisplu	d	duration gift
127-132	F6.0	rpsplu	d	rotational period
133-138	F6.0	tdbgsplu	d	beginning of sprinkling period, in days from beginnin of year at 00:00:00
139-144	F6.0	tdedsplu	d	end of sprinkling period

FACT_SVAT.INP

The file FACT_SVAT.INP contains values of vegetation factors and interception characteristics.

Variable format and description

col	format	Name	unit	description
1-6	I6	vg	-	vegetation type
7-12	I6	dy	-	day number
13-20	F8.0	csvg	m2/m2	soil cover
21-28	X8	empty		-
29-36	F8.0	vxicvg	m3/m2	interception capacity
36-44	F8.0	faevvg	-	crop factor
45-53	F8.0	faeivg	-	factor for interception evaporation

UNSA_SVAT.BDA

The file UNSA_SVAT.BDA contains the database with steady states of soil moisture profiles.

Variable format and description

col	format	name	unit	description
bin	-	sl	-	soil number
bin	-	rz	-	rootzone number
bin	-	dprztb	-	thickness rootzone
bin	-	ig	-	index groundwater level
bin	-	ip	-	index percolation
bin	-	srtb	-	storage rootzone (table)
bin	-	s2tb	-	storage box 2 (table)
bin	-	qmrtb	-	flux bottom rootzone (table)
bin	-	p2tb	-	pressure head box 2 (table)
bin	-	prztb	-	pressure head rootzone (table)

METE_SVAT.INP

The file METE_SVAT.INP contains the precipitation and evapotranspiration data per meteo station. The time step is not fixed.

Variable format and description

Col	format	name	unit	description
1-15	F15	td	d	time from beginning of year at 00:00:00
16-20	I5	iy	-	year number
21-30	F10	prec	mm/d	precipitation intensity
31-40	F10	etref	mm/d	reference evapotranspiration intensity
41-50	I10	nmme	-	meteorological station number
51-60	F10	rad	kJ/m2/d	radiation intensity
61-70	F10	temp	ºC	temperature
71-80	F10	hum	kPa	humidity
81-90	F10	wind	m/s	wind speed at altw(nmme) m (see METE_STAT.INP)

4.6.2 Output

Output can be generated for:

- Sewerage and surface water units: state and balance variables;
- SVAT-units: state and balance variables.

Below a detailed list of output variables of the SIMGRO-model is presented.

Sewerage and surface water system

Vusw	m3	Upstream inflow from surface water	≥0.
Vdsw	m3	Outflow to surface water	≤0.
Vsurv	m3	supply from reservoir	≥0.
Vexrv	m3	abstraction by reservoir	≤0.
Vexsp	m3	abstraction for sprinkling	≤0.
Vru	m3	runoff/runon	+=off
Vdr	m3	drainage	≥0.
Vif	m3	Sub infiltration	≤0.
decSsw	m3	decrease of storage	+/-
Ssw	m3	storage	≥0.
Hsw	m+MSL	water level	+/-
Hwr	m+MSL	weir level	+/-
Hta	m+MSL	target level	+/-

Soil Water / Groundwater

key	unit	item	sign
decSic	m3/m2	decrease of interception storage	+/-
decSpd	m3/m2	decrease of ponding storage	+/-
decS1	m3/m2	decrease of water storage in rootzone, box 1	+/-
decS2	m3/m2	decrease of water storage in subsoil	+/-
Pm	m3/m2	measured precipitation	≥0.
Ps	m3/m2	sprinkling precipitation	≥0.
Eic	m3/m2	evaporation interception water	≤0.
Epd	m3/m2	evaporation ponding water	≤0.

key	unit	item	sign
Ebs	m3/m2	evaporation bare soil	≤0.
Tact	m3/m2	actual transpiration vegetation	≤0.
qrun	m3/m2	runon	+/-
qdr	m3/m2	net infltration of surface water	- =drn
qspgw	m3/m2	groundwater extraction for sprinkling	≤0.
Ebspot	m3/m2	potential evaporation bare soil	≤0.
Tpot	m3/m2	potential transpiration vegetation	≤0.
Trel	m3/m3	relative transpiration	≥0.
ETact	m3/m2	total actual transpiration	≤0.
qinf	m3/m2	infiltration on soil surface	+=down
qmr	m3/m2	flow through bottom of root zone	+=up
Sic	m3/m2	interception storage	≥0.
Spd	m3/m2	ponding storage	≥0.
S1	m3/m2	soil water storage in rootzone, box 1	≥0.
S1sd	m3/m2	soil water saturation deficit of box 1	≥0.
S2sd	m3/m2	soil water saturation deficit of subsoil	≥0.
phrz1	m3/m2	mean root zone pressure head	+/-
Hpd	m+MSL	MetaSWAP ponding water level	+/-
Hgw	m+MSL	MetaSWAP groundwater level	+/-
dHgw	m	MetaSWAP groundwater level change	+=rise
sc1	-	groundwater storage coefficient	0.< ≤1
Hgwmodf	m+MSL	MODFLOW groundwater head	+/-
Hsw	m+MSL	surface water level	+/-

4.7 NKUA MODELS

4.7.1 Model description

The proposed model is developed by the National Kapodestrian University of Athens for the estimation and prediction of the urban heat island intensity in various locations of a large urban area. The specific model is based on neural networks technology. Neural networks are a computational technique that simulates the operation of the human brain's neurons. To some extent, the NN approach is a non-algorithmic, black box strategy, which is trainable. The purpose is to train the neural black-box to learn the correct response or output (e.g. classification) for each of the training samples. This strategy is attractive to the system designer, since the required amount of a priori knowledge and detailed knowledge of the internal system operation is minimal. After training the internal (neural) structure of the artificial implementation the NN is self-

organized to enable extrapolation when faced with new, yet similar, patterns, on the basis of experience with the training set.

4.7.2 Measurements

The application of NN model to the urban structure requires the following measurements for various urban positions:

- **Hourly ambient air temperature (°C)**
- **Hourly humidity values (%)**

Moreover the NN model requires a series of urban stations and a reference station which is placed in a rural area.

4.7.3 List of input and output variables for NKUA NN model

4.7.3.1 Model the nightime heat island intensity

The input parameters of the neural network model are the following:

Maximum daily values of the ambient air temperature (Tmax in °C), measured at each urban station: Maximum diurnal air temperature depends on various climatic factors such as the short-wave solar radiation, sunshine duration, vegetation and grounds' thermal properties, altitude and precipitation. Maximum daily air temperature is regarded as the representative urban parameter to the model, taking into account that it is the result of various major physical processes produced in the urban environment.

Nighttime values of the ambient air temperature (Tref in °C), measured at the reference station, at the time when ΔTmax,n is observed: Night time air temperature at the reference station is an important parameter contributing significantly to the heat island intensity estimation. The reference temperature is usually lower than the corresponding urban temperature, especially during calm and clear nights. This is mainly caused by the stronger rural cooling rates if compared with those of the urban environments.

$$\Delta T_{\max,n} = \left(T_{URBAN-}T_{REFERENCE}\right)_{\max,n}$$

The outputs of the neural network model are **the night time heat island intensity** values for each of the remaining twenty-two stations. Heat island intensity can be regarded as a measure of the numerous physical processes that produce the difference between rural and urban areas.

4.7.3.2 Model the daytime heat island intensity

The input parameters of the neural network model are the following:

Daytime values of the ambient air temperature (Tmax in °C) measured at each urban station at the time where $\Delta T_{\max,d} = \left(T_{URBAN} - T_{REFERENCE}\right)_{\max,d}$ is observed.

Maximum daily values of global solar radiation, (*Ig*, in MJ/m^2)

Daytime values of reference air temperature, (Tref, in _C), measured at the reference station at the time when the ΔTmax,d is observed.

The outputs of the neural network model are **the daytime time heat island intensity** values for each of the remaining twenty-two stations.

The NKUA model can operate either on-line or off-line depending on the length of data provided. In case there are no data available or the monitoring period is short (less than 1 year) then the UHI intensity prediction should be based on historical data that should be continuously updated. In this case the model should be operated in on-line mode. If the monitoring period is long (higher than 3 years) then the prediction can be based in off line operation of the model.

4.7.4 Requirements for On- line System

4.7.4.1 Solution No.1

Each station

- Intel Pentium 4 and above RAM 512 MB (At least 1024 MB recommended)
- Windows XP or Vista 32bit (not Linux)
- Data Acquisition Card (see supported cards at http://www.mathworks.com/products/daq/supportedio.html)
- Internet connection (wired or wireless)

For this option a central computer is necessary to collect and analyze the data from all station. Using Matlab compiler we can transform our Matlab code into components witch can be used from Java, C# or .Net. Then a specially design program (in Java, C# or .Net with a Matlab module) must be written in order to acquire the measurement using the data acquisition card, prepare and transmit the data from each station to the central computer. The central computer must receive and verify the data from all station and store them. Then the data must be feed into the neural network , witch will generate the desired output like a plot.

4.7.4.2 Solution No.2

Each station

- Data Acquisition Card with TCP/IP support (see supported cards

at http://www.mathworks.com/products/daq/supportedio.html , like http://www.ueidaq.com/data-acquisition-chassis/ethernet-daq)
- Internet connection (wired or wireless)

For this option a central computer will communicate via TCP/IP with the data acquisition card's and collect the measurement. A program entire written in Matlab will make the necessary data manipulation and feed the data into neural network , witch will generate the desired output like a plot.

Considering the difficulties to apply the specific model to other cities we propose the following:

1. Applying the model in on line mode for **Athens Case Study** using the configuration described in section 3
2. Predict the UHI on-line for Athens using the data collected by the system.
3. Predict the UHI in the other cities in off line mode as a validation procedure.

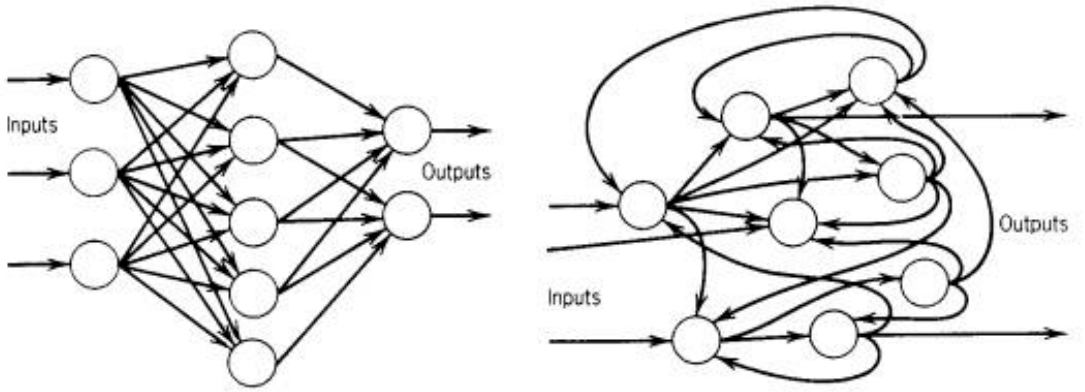

Fig.4.7.4.2.1. The neural network topology

4.8 CMCC MODELS

4.8.1 Description of models

The **Advanced Canopy-Atmosphere-Soil Algorithm** (**ACASA**) model (Pyels et al., 2000; 2003), developed by University of California, Davis (UCD), is one of the most sophisticated models for estimating energy and mass fluxes between surface and the atmosphere. It treats the surface and associated fluxes as an interconnected system, and the atmosphere, the urban surface, and the soil are represented as a multilayer system. The ACASA domain extends maximally to 100m above the city and plant canopy elements to ensure applicability of the turbulence assumptions.

ACASA incorporates higher-order closure principles for turbulent statistics to predict effects that higher-order turbulent kinetic and thermodynamic processes have on the surface microenvironment and associated fluxes of heat, moisture, and momentum. These processes include turbulent production and dissipation to turbulence kinetic energy, turbulent vertical

transport of heat, mass, and momentum fluxes. Using a set of governing equations, ACASA creates vertical profiles of temperature, humidity, mean wind, and CO_2 concentration. ACASA has several additional features including (1) radiative transfer within the surface layers, (2) surface heat storage processes.

ACASA is an OFF-LINE model. In the BRIDGE project, it will be used for Firenze case study. In addition, simulations from the London case study will be produced if input data will be available. As input the model requires meteorological information deriving from surface measurements or by mesoscale meteorological models, as well as morphological parameters to describe the surface.

ACASA is being coupled with the newest version of mesoscale model WRF (the Weather Research & Forecasting Model) developed by NCAR and several other agencies. The ACASA model will be coupled to the WRF model as a surface-layer scheme to replace WRF's pre-existing ones due to ACASA's more complex and realistic representations in physical and physiological parameters. The WRF model, driven by North American Regional Reanalysis data (NCAR-NCEP), is run down to its planetary boundary layer, where ACASA is called.

The WRF-ACASA coupling will be able to identify how multiple environmental factors, in particularly climate variability, population density, and species distribution, impact future carbon cycle prediction across a wide geographical range. A scheme of ACASA-WRF coupling is reported below.

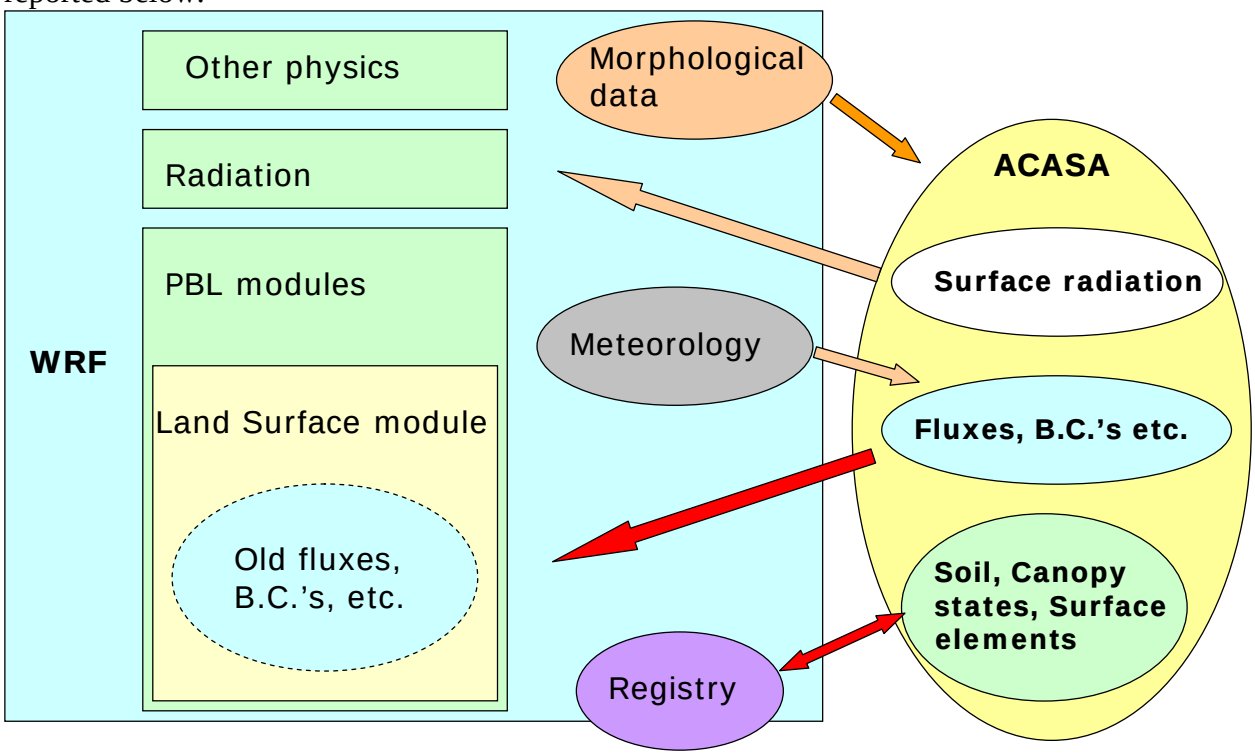

Figure 4.8.1.1. Scheme of ACASA-WRF coupling

4.8.2 Input

The ACASA model requires certain input variables and parameters in order to run meaningfully. Some of these quantities can be set to estimated values whenever measurements or literature guidance do not exist. These are listed in several groups according to context. Required units fit the SI convention.

4.8.2.1 Inputs – initialization only

Soil temperature (K) and soil moisture content (fraction of unity) as functions of depth beneath the surface; also snowpack water content, height, and temperature (if snow is present initially). Soil levels are at 10 cm intervals from the surface to 1.5m, with the lowest layer at 3m (lower boundary condition). Snowpack layers are 5cm thick and change in number as the snowpack grows and decays. As measurement depths often differ from the model soil & snow domains, initialization profiles using observed values may require interpolation to match the ACASA domain.

4.8.2.2 Inputs that vary with each time step

These are modelled (WRF) or measured meteorological quantities representing averages (or cumulants), ideally covering intervals of 15 to 120 minutes: time step length (30 minutes is best), mean wind speed, mean air temperature, mean specific humidity, mean carbon dioxide concentration, liquid and/or frozen precipitation rates, mean air pressure, and mean downwelling solar (shortwave) and thermal-infrared radiation flux densities, and solar zenith angle (often calculated from latitude & time of day).

4.8.2.3 Surface morphology

The second main group of input parameters describe the structure of the surface & canopy elements that vary with plant species, human population density, and building architectural design, but often vary so slowly with time as to require only one set of values for the total model simulation time interval. These represent the vertically-variable presence of leaves, stems, buildings, as fluxing obstacles averaged over a one km2 or so footprint scale. These include vertical canopy element area index profiles, element light reflectivity and transmissivity (visible-PAR and near-IR bands), basal respiration rate and Arrhenius-type q-10 values for leaves, stems, roots, & soil microbes, human population density, mean diameter of individual canopy elements, mean canopy element drag coefficient, maximum ideal carboxylization rate for plants, and an analoge of water use efficiency. Plant root distribution as a function of soil depth, currently assumed to be 1:1 with total canopy element area, can also be adjusted to account for local conditions. ACASA internally allows for all of these parameters to vary with height. Most often for practical purposes all aforementioned morphological parameters, except the element area indices, are considered the same at each canopy layer. Soil type (USDA 16-type classification) is also required.

4.8.2.4 WRF-ACASA coupling

At each WRF gridpoint, WRF drives ACASA using the aforementioned meteorological inputs corresponding to the WRF sigma-level at a height aboveground that is at least twice the maximum height of canopy elements. The ACASA domain for the WRF coupling is the region that exists between this sigma-level and three meters belowground. WRF also provides ACASA with cross-compatible surface morphological parameters at each WRF horizontal grid point, used also by existing land surface models in the WRF suite. These are: total leaf area index, soil type, and maximum canopy height. Values are keyed in by a 'vegetation type index'. These parameters for roughly two dozen land-surface types are given by WRF; more are possible given the availability of gridded data. Other ACASA morphological parameters are not in the original WRF suite, but which are being developed currently at UC Davis and will be provided in the WRF-ACASA version planned for the BRIDGE project. These include 'maximum ideal carboxylization velocity and the 'water use efficiency analogue'. Taken together both are somewhat analogous in function to the existing WRF vegetation parameter ‘minimum stomatal resistance’. Other ACASA morphological parameters in this vein include the canopy architecture (WRF gives total LAI, but not LAI(z)), and leaf-scale optical properties (WRF provides bulk surface albedos only), leaf-scale drag coefficient, and mean leaf & canopy element diameters. Again, these are keyed in by using the WRF-provided vegetation type index for each grid point call from WRF to ACASA. Surface state variables (soil, snow thermal and hydrological variables) are retained in the WRF registry between each ACASA-calling WRF time step interval. WRF timesteps are often a few seconds for fine mesh simulations. Generally, calls to ACASA are best when kept simultaneous with calls to the WRF radiation modules, which usually range from ten to thirty minutes.

When coupled with the mesoscale model WRF, the initial conditions for the WRF-ARW real-data cases are pre-processed through a separate package called the WRF Preprocessing System (WPS). The input to the WRF-ARW real-data processor from WPS contains:

- The 2-dimensional static terrestrial fields such as:

- albedo*
- Coriolis parameters,
- terrain elevation*
- vegetation/land-use type*
- land/water mask*
- map scale factors
- map rotation angle
- soil texture category*
- vegetation greenness fraction*
- annual mean temperature*

- latitude/longitude

* indicate static data requirements to WPS.

- The 3-dimensional fields from the external model [Reanalysis data] (including the surface):

- temperature (K),
- relative humidity (RH),
- horizontal components of momentum (m/s, already rotated to the model projection).

The 2-dimensional time-dependent fields from the external model [Reanalysis data], after processing by WPS, include (not all these required):

- surface pressure and sea-level pressure (Pa),
- layers of soil temperature (K) and soil moisture (kg/kg, either total moisture, or binned into total and liquid content),
- snow depth (m),
- skin temperature (K),
- sea surface temperature (K),
- sea ice flag.

4.8.3 Output

ACASA calculates, each independently, the following output quantities (and associated vertical gradients) often used for output comparisons (at each model layer throughout the air, soil, or snowpack domains):

Mean microenvironmental stare quantities *(used also in successive runs of ACASA involving multiple time steps)*

These include wind speed (with streamwise and crosswise components), air temperature, specific humidity, carbon dioxide concentration. Soil (and snowpack) temperature, total snowpack water equivalent and height, and canopy element temperatures.

4.8.3.1 Turbulent moments – 2nd- and 3rd- order correlations

These include vertical flux densities of heat, water, CO_2, as well as sreamwise and crosswise momentum. The abovecanopy values of the scalar set of these flux densities, converted to W/m^2, represent the main elements of the total surface energy balance (Rn=H+LE+G+S). Output carbon dioxide flux density includes both the total and fractional contributions of photosynthesis and/or respiration fluxing from different canopy element types. Also included are canopy element resistances to water and heat (microlayer) transports, turbulence kinetic energy components (3D) and diabatic scalar correlations, and a number of turbulence triple-moments that are often rarely measured and thus have not been tested extensively.

4.8.3.2 Other

Diagnostic variables representing aspects or combinations of the above quantities, such as those required for WRF coupling or offline model intercomparison efforts such as PILPS and SNowMIP2, are also calculated.

4.8.4 Specifics of WRF-ACASA coupling

WRF uses only a subset of the total retinue of microenvironmental conditions and exchanges that are simulated by ACASA. Specifically, WRF requires all surface-layer schemes to provide turbulent exchange coefficients that are used to calculate tendencies that drive the PBL schemes and turbulent dynamics above the surface-layer domain. ACASA values of these exchange coefficients are provided by taking total heat and moisture fluxes in kinematic form, and dividing them each by the corresponding gradients of temperature and humidity near the canopy top. CO_2 exchange between ACASA and WRF domains is also represented in a similar fashion. The total ACASA momentum flux is given to WRF in the form of its positive square root (friction velocity). WRF also needs a surface-layer bulk Richardson number, which is obtained from a combination of ACASA output kinematic and scalar turbulent fluxes. Lastly, WRF requires a surface (skin) temperature, which is estimated by ACASA as the near-blackbody temperature corresponding to output total upward thermal infrared radiation flux density.

ACASA also feeds total TKE to WRF, at a level also near the canopy top, as half the sum of the three component wind velocity variances. However, such is only used with a fraction of the WRF turbulence schemes (PBL+, above the SL). It is probably best to run WRF-ACASA using these more elaborate PBL modules to include the greatest amount of ACASA surface forcing information in the WRF simulations."

5. OFF and ON-LINE models in BRIDGE

In this section we will declare which models will be used in ON-LINE mode and OFF-LINE mode. The models called as “off-line” are those models that due to its size and high computer demands are needed to be run in clusters and/or surpercomputer and in any case, due to the long duration of the simulation, are needed to be run “in-house” instead to be implemented into the DSS tool. However the quality of the simulations and the large amount of data used for the “off-line” simulations have to be taken into account. The results of the “off-line” simulations produced by these validated and recognized large computer models are stored in the DSS database according to a format to be requested by DSS developers. The “on-line” models are those models which due to the simplicity and limited computer resources are to be installed in the DSS tool and are prepared to be run by the BRDGE DSS tool.

5.1 OFF-LINE Models

WRF-UCM model (run by UPM)
MICROSYS (CFD) model (run by UPM)
MM5-CAMx model (run by UAVR)
VADIS (CFD) model (run by UAVR)
NKUA Models (Neural Network) (run by NKUA)
ACASA model (run by CMCC)

5.2 ON-LINE MODELS

LUMPS V.5 model (produced by KCL)
SURFEX model (produced by CNRM)
SCADIS model (UHEL)
URBAIR model (UAVR)
SIMGRO model (ALTERRA)

6. APPLICATION OF DIFFERENT MODELS: CASE STUDIES

6.1 CITY OF FIRENZE

Models to be applied and mode

1. ACASA MODEL (CMCC) (OFF-LINE)
2. ALTERRA models (SIMGRO Hydrological Model), ON-LINE
3. SCADIS MODEL (UHEL), ON-LINE
4. SURFEX MODEL (CNRM). ON-LINE
5. LUMPS MODEL (KCL), ON-LINE
6. MM5-CAMx, (UAVR), OFF-LINE
7. VADIS MODEL, (UAVR), OFF-LINE
8. URBAIR MODEL, (UAVR), ON-LINE
9. MM5-CMAQ, (UPM), OFF-LINE
10. WRF-UCM/CHEM, (UPM), OFF-LINE
11. MICROSYS, (UPM), OFF-LINE.

6.2 CITY OF ATHENS

Models to be applied and mode

1. NKUA models (Neural Networks), OFF-LINE and ON-LINE modes.
2. SCADIS MODEL (UHEL), ON-LINE
3. SURFEX MODEL (CNRM), ON-LINE
4. LUMPS MODEL (KCL), ON-LINE
5. MM5-CAMx, (UAVR), OFF-LINE
6. VADIS MODEL, (UAVR), OFF-LINE
7. URBAIR MODEL, (UAVR), ON-LINE
8. MM5-CMAQ, (UPM), OFF-LINE
9. WRF-UCM/CHEM, (UPM), OFF-LINE
10. MICROSYS, (UPM), OFF-LINE

6.3 CITY OF HELSINKI

Models to be applied and mode

1. ALTERRA models (SIMGRO Hydrological Model), ON-LINE.
2. SCADIS MODEL (UHEL), ON-LINE
3. SURFEX MODEL (CNRM), ON-LINE
4. LUMPS MODEL (KCL), ON-LINE
5. MM5-CAMx, (UAVR), OFF-LINE
6. VADIS MODEL, (UAVR), OFF-LINE
7. URBAIR MODEL, (UAVR), ON-LINE
8. MM5-CMAQ, (UPM), OFF-LINE
9. WRF-UCM/CHEM, (UPM), OFF-LINE
10. MICROSYS, (UPM), OFF-LINE

6.4 GREATER LONDON

Models to be applied and mode

1. MM5-CMAQ, (UPM), OFF-LINE
2. WRF-UCM/CHEM, (UPM), OFF-LINE
3. MICROSYS, (UPM), OFF-LINE
4. MM5-CAMx, (UAVR), OFF-LINE
5. VADIS MODEL, (UAVR), OFF-LINE.
6. URBAIR MODEL, (UAVR), ON-LINE.
7. WRF (KCL) with NOAH/UCM option –offline.
8. Noah/UCM (KCL) – offline.
9. LUMPS (KCL) offline or online
10. KCL RS (KCL) model – offline – this is being developed (based on Voogt and Grimmond 2000; Xu et al. 2008).
11. ACASA MODEL (CMCC), OFF-LINE

6.5 CITY OF GLIWICE

Models to be applied and mode

1. MM5-CMAQ, (UPM), OFF-LINE
2. WRF-UCM/CHEM, (UPM), OFF-LINE
3. MICROSYS, (UPM), OFF-LINE
4. MM5-CAMx, (UAVR), OFF-LINE
5. VADIS MODEL, (UAVR), OFF-LINE
6. URBAIR MODEL, (UAVR), ON-LINE