published in revised form in Atmospheric Environment, 2004, 38/3 pp. 457-467

Introduction of data assimilation procedures in the meteorological pre-processor of atmospheric dispersion models used in emergency response systems

Ivan Kovalets[*a], Spyros Andronopoulos[b], John G. Bartzis[c], Nikos Gounaris[b], Anatoliy Kushchan[a]

[a] Institute of Mathematical Machine & System Problems, National Academy of Sciences of Ukraine, Department of Environmental Modelling, pr. Glushkova-42, 03187, Kiev, Ukraine

[b] National Centre for Scientific Research "Demokritos", Institute of Nuclear Technology and Radiation Protection, Environmental Research Laboratory, 15310 Aghia Paraskevi Attikis, Greece

[c] Aristotle University of Thessaloniki, Department of Energy Resources Management Engineering, Kastorias and Fleming Str., 50100 Kozani, Greece

Abstract - Data assimilation (DA) procedures were developed and implemented in the frames of the meteorological pre-processor (MPP) of an emergency response system (ERS) to enable simultaneous use of different meteorological measurements (wind velocity, cloud cover, net radiation, precipitation) with Numerical Weather Prediction (NWP) data. The DA procedures were based on the optimal interpolation algorithm and the method of iterations to optimal solution, combined with methods for scaling the weighting coefficient between fields obtained by the measurements and those obtained by the NWP data. For validation purposes, the calculated by the MPP meteorological fields were compared against measurements performed in two real-scale experiments (ETEX1 and 2). Data from ground-based synoptic weather stations were used for the improvement, through DA procedures, of the first-guess fields obtained from the NWP data, while measurements from surface stations, sonic anemometer and sodar were used for comparison with the results of the MPP. The performance of the two developed DA procedures was evaluated through statistical indices (root mean square and systematic deviation of wind speed and direction) and through graphical representations. Both DA procedures improved the agreement between computed and measured meteorological fields in both examined experiments.

Keywords: ETEX, RODOS, optimal interpolation, iterations to optimal solution

Introduction

Atmospheric Dispersion Models (ADMs) usually receive input from diagnostic wind models (meteorological pre-processors - MPPs), which act as interface between them and the incoming meteorological data. The meteorological data can be measurements from one or more stations in the area of interest or prognostic data from synoptic- or meso-

[*] Corresponding author.
E-mail address: ik@env.immsp.kiev.ua, Fax +380-44-2663615

scale Numerical Weather Prediction (NWP) models. The measurements are representative of the past and current local conditions, while the NWP data cover a wider range in space and time where no measurements exist. As it was stated in Seaman (2000) the optimal way of producing the input wind fields for ADMs is using the available measurements within the NWP models, employing four dimensional data assimilation procedures (4DDA).

ADMs play a key role in the sequence of model components of real-time emergency response systems (ERS) like RODOS (the **R**eal-time **O**n-line **D**ecisi**O**n **S**upport system for nuclear emergency management in Europe (Raskob and Ehrhardt, 1999). NWP models are not included in the existing ERSs and consequently cannot be rerun at arbitrary time moment. ERSs use either results of NWP models calculated externally or meteorological measurements from stations in the area of interest. The analysis time of the NWP data is usually several hours in the past. So in the cases that NWP data are used as input to ADM of ERS, the information from measurements available between the NWP analysis time and present time is lost. As a consequence, relatively large differences can be observed between results of the ADMs calculated with locally measured meteorological data and those obtained with the forecasts of the NWP models. Such deviations have actually been observed in practical applications of the RODOS system.

In literature several studies have appeared comparing the wind fields, calculated by MPPs with the use of only measurements or of only NWP data (Kumar and Russel, 1996, Lamprecht and Berlowitz, 1998). In works where wind fields are calculated by MPPs from measurements, variational divergence-minimizing procedures are adopted (comprehensive review of such kind of diagnostic models is given in Fisher et al., (1988)) to account for the influence of terrain on the wind flow. It is well known (Fisher et al., 1988) that performance of these methods crucially depends on the quality of the first-guess field, which is produced by interpolation of *only* the measurements (Fisher et al., 1988), neglecting NWP data.

Almost no studies have been performed for the case of wind fields calculated by the MPPs with the simultaneous use of both types of input data: NWP and measurements. Only in the MPP "CALMET" of the modelling system "CALPUFF" (Scire, 2000) an attempt was made to produce an optimal first guess field for divergence minimizing procedure, that used both NWP data and measurements. However, the basic assumption was that existing measurements were *already* used by the NWP model in its own DA procedure. That assumption is usually not valid for the operational use of real-time ERSs.

The simultaneous use of NWP data together with meteorological measurements within the diagnostic model is a problem of 3-dimensional data assimilation (3DDA). Previous 3DDA methods were developed and used for the calculation of initial conditions for synoptic- and meso-scale NWP models, but were never (except in wind model CALMET, mentioned above) used in the meteorological pre-processors for air-quality studies. Furthermore, meteorological pre-processors usually operate on smaller spatial scales than the NWP models. So, the main objective of the work presented in this paper is to introduce suitably adapted 3DDA techniques into a MPP used in the frames of the emergency response system RODOS. The aim is also to evaluate the effects of the introduced 3DDA procedures, by comparing calculated meteorological variables obtained with the use of NWP data only and with the use of both NWP data and meteorological measurements, with a real case experimental data.

The existing 3DDA methods, can be classified in the following two main categories (Daley, 1991):

1. Formal methods, sometimes called objective wind analysis methods, such as Cressman and Barnes methods.
2. Statistical methods, such as the well-known "Optimal Interpolation", first introduced by Gandin (1968).

Each of the abovementioned types of DA methods has its own advantages and weak sides: formal methods are the most robust and operationally inexpensive (i.e., more suitable for real-time ERSs), while statistical methods use information about the statistical structure of the meteorological fields and are good when the latter is well defined. It is also known (Gandin, 1968), that the performance of the formal methods is more sensitive to the density of the measuring network than the performance of the statistical methods. At the same time, for a very high density of the measuring network, results of both types of methods are identical.

An additional difficulty that usually arises when either 3DDA or 4DDA methods are implemented is their validation (Seaman, 2000). Usually it is difficult to validate the DA procedures against the meteorological measurements, as these were already used in the DA procedures (Seaman, 2000), and such a validation demands significant additional number of meteorological measurements that is usually rather expensive. Another, indirect, approach for the validation of the DA procedures in a wind model is comparison of concentrations calculated by the dispersion model, which used wind fields calculated by the wind field model as input (Seaman, 2000, Lamprecht and Berlowitz, 1998). Though, the number of concentrations measurements is usually enough for making statistics, this approach suffers from another drawback: the dispersion model has many sources of its own errors, such as different parameterisations. Therefore it is sometimes difficult to filter out the effect of errors of the dispersion model from the effect of the DA procedures.

In this paper the development of a 3DDA procedure based on the two types of DA methods is presented. Results of calculations are compared against the meteorological data set measured during the European Tracer Experiment (ETEX, S.E. Gryning., et. al., 1998).

Method of solution

The developed DA procedures in this work were introduced into the MPP of RODOS system. This MPP calculates all meteorological variables needed by ADMs, such as 3-dimensional fields of wind velocity, temperature, pressure, and diffusivity coefficients and 2-dimensional variables, such as precipitation, cloud cover, net radiation, sensible heat flux, stability category, friction velocity, Monin Obukhov length, convective velocity, mixing layer height. With the introduced DA procedures, calculation of the abovementioned meteorological variables is performed in the following main steps:

1. Calculation of the first guess estimation of the wind field, temperature and other meteorological variables on the computational grid of the MPP by $1/r^2$ interpolation of the corresponding values from the grid of the NWP model

2. Assimilation of the scalar variables measurements (such as surface temperature, cloud cover, net radiation, precipitation)
3. Assimilation of the wind velocity measurements
4. Final calculation of all remaining meteorological fields, such as stability category, Monin Obukhov length, friction velocity etc, based on the existing methodologies in the current version of the MPP of RODOS system (Andronopoulos, 1998).

Assimilation of the scalar fields measurements is performed using the variant of Cressman-type objective analysis procedure called "Iterations to optimal solution" (IOS) described by Daley (1991). Before describing it, let's note, that from statistics theory, if there are two one-point observations f_O and f_B of the same physical quantity f, and these observations are known to have root mean square errors E_O and E_B, then the "optimal" estimate f_A of the quantity f will be given by:

$$f_A = \frac{(E_O/E_B)^{-2} f_O + f_B}{(E_O/E_B)^{-2} + 1} \qquad (1)$$

For the vectors of observations $\mathbf{f}_O$ and $\mathbf{f}_B$ of quantity $\mathbf{f}$ measured at the same set of points $0 < k < K+1$, with $K \times K$ covariance matrices $\mathbf{O} = \left\langle \left(f_O^i - f^i\right) \cdot \left(f_O^j - f^j\right) \right\rangle$, $\mathbf{B} = \left\langle \left(f_B^i - f^i\right) \cdot \left(f_B^j - f^j\right) \right\rangle$, $0 < i, j < K$ the optimal estimate $\mathbf{f}_A$ of the vector $\mathbf{f}$ in the points k, $0 < k < K+1$ will be, according to Daley (1991):

$$\mathbf{f}_A = \mathbf{f}_B + \underline{\underline{\mathbf{B}}}\left[\underline{\underline{\mathbf{B}}} + \underline{\underline{\mathbf{O}}}\right]^{-1}\left[\mathbf{f}_O - \mathbf{f}_B\right] \quad (2)$$

Now, if we define the background (or first-guess) field of some meteorological variable as $\mathbf{f}_B$ with constant root mean square error E_B and the observations of the same variable as $\mathbf{f}_O$ with constant root mean square error E_O then, as it is proved by Daley (1991), the following iterative procedure converges at the points of observations to the value defined by relationships (1) or (2):

$$q_i = \sum_k E_B^2 \left| w(r_{ik}) \right| E_O^{-2}$$
$$f_A^{j+1}(r_i) - f_A^j(r_i) = (1+q_i)^{-1} \sum_k E_B^2 w(r_{ik}) E_O^{-2} \left[f_O(r_k) - f_A^j(r_k) \right] + (1+q_i)^{-1} \left[f_B(r_i) - f_A^j(r_i) \right] \quad (3)$$

if the elements of covariance matrices $\mathbf{B} = (b_{ik})$ and $\mathbf{O} = (o_{ik})$ introduced above, can be represented as $b_{ik} = w(r_{ik}) E_B^2$, $o_{ik} = E_O^2 \mathbf{I}$, where $\mathbf{I}$ is identity matrix. In (3) index "*i*" denotes the node of the pre-processor grid, index "*k*" the point of observation, $w(r_{ik})$ is the weight function, defined, for instance, by Daley (1991):

$$w(r_{ik}) = \exp(-r_{ik}^2 / R_0^2) \qquad (4),$$

where R_O is the radius of influence.

The IOS method (3)-(4) is used for the assimilation of measurements of the surface temperature, cloud cover, net radiation and precipitation, with parameters E_B^2 / E_O^2 and R_O given in Table 1. The "typical" values for relative errors and radii of influence for these meteorological variables were taken from Gandin (1978) where they were estimated from measurements. It should be noted here that values of radius of influence and relative errors given in Table 1 were estimated by Gandin (1978) for the measurements of the corresponding variables, averaged through 6 hours per measurement (this averaging time for a single measurement is not to be mixed with the averaging time through which correlation functions were defined). Usually, measurements used in an emergency response system, as the RODOS system, are averaged through shorter time periods, e.g., from 10 minutes to 3 hours. However, it is well known that for smaller averaging times the relative error E_B^2 / E_O^2 can increase and the radius of influence R_O can decrease, as it was observed by Gandin (1978). So, the values given here should be the object of further investigation.

Here it is worth to note that, for more physical consistency of the meteorological fields calculated by the MPP, assimilation of measurements of cloud cover and net radiation is not performed independently. At first at all observation points, where cloud cover is measured, net radiation is calculated using relationships from Hanna and Chang (1993). The same relationships are used at the points where net radiation is measured to calculate the cloud cover. After that, the assimilation of the *resulting* measurements of *either* cloud cover *or* net radiation is done depending on what field was delivered by the NWP model.

Assimilation of the wind velocity observations is done in the following two steps:

1. Extrapolation / interpolation of the wind velocities observed values from the observational levels to the vertical levels of the MPP (Figure 1).
2. Assimilation of the extrapolated / interpolated wind velocity values on each of the vertical levels of the MPP

Extrapolation is done only in the lower 200 m of the atmosphere, where Monin-Obukhov similarity theory usually can be applied. The values of friction velocity and Monin-Obukhov length required by the Monin-Obukhov similarity theory are calculated *at the points of observations* using the following iterative procedure (Fisher et al., 1998):

$$u_*^{j+1} = \kappa U(z_1) / \left(\ln(z_1 / z_0) - \psi(z_1 / L^{j+1}) + \psi(z_0 / L^{j+1}) \right)$$

$$L^{j+1} = -\rho c_p T \left(u_*^j\right)^3 / \kappa g Q_h \qquad (5)$$

Here ψ is stability function, defined, for instance, by Fisher et al. (1998), z_1 is the height of the first measurement level of velocity, z_0 is the roughness height, Q_h is the sensible heat flux at the measurement point. The latter is calculated from the measured cloud cover or net radiation using empirical relationships (Hanna and Chang, 1993). The first approximations to u_* and L in the iterative procedure are defined as for neutral stratification: $L = 10001\,\mathrm{m}$, $u_* = \kappa U(z_1)/\ln(z_1/z_0)$.

Wind direction is extrapolated according to the approach, proposed by van Ulden and Holtslag (1985) to account for the effect of the Coriolis force on it. In that approach the *deviation* $D(z)$ of the wind direction at height z from that at $z = 0$ is assumed to be:

$$D(z)/D(h) = d_1[1 - \exp(-d_2 z/h)] \qquad (6)$$

where $D(h)$ is the deviation of the wind direction at $z = h$ with respect to the wind direction at $z = 0$, h is a reference height (taken to be 200 m), and $d_1 = 1.568$, $d_2 = 1.0$ are constants. $D(h)$ depends upon the Monin-Obukhov length and that dependence is represented by the empirically defined table function given by van Ulden and Holtslag (1985).

Assimilation of the measured values of the wind velocity can be done in two ways: 1) using the already described IOS method and 2) using a multivariate optimal interpolation (OI) method.

In the first case the relative error, E_B^2/E_O^2 required by the IOS method is defined using the following considerations. In the meteorological pre-processor CALMET (Scire, 2000) the wind field $\mathbf{f}_A$ defined at the nodes of MPP grid is calculated as the weighted sum of $\mathbf{f}_B$ and $\mathbf{f}_O$:

$$\mathbf{f}_A = W_O \cdot \mathbf{f}_O + (1 - W_O) \cdot \mathbf{f}_B \qquad (7)$$

where $\mathbf{f}_B$, $\mathbf{f}_O$ are calculated at the nodes of the MPP by interpolation from the nodes of the NWP model and from observations locations respectively, and W_O is the weighting coefficient. Comparing (7) and (1) a relationship between the weighting coefficient W_O and the relative error E_B^2/E_O^2 can be easily established:

$$E_B^2/E_O^2 = W_O/(1 - W_O) \qquad (8)$$

After that, the relationships proposed by Scire (2000) for the calculation of W_O can be used for the calculation of relative error E_B^2/E_O^2 using (8). In the present work the latter were slightly modified to account for the fact, that observations were not already used in the NWP model in its own data assimilation procedure, as assumed in the CALMET model. So the following relationships are used here for the determination of the weighting coefficient W_O:

$$W_O = W_Z W_S \quad (9)$$

$$\begin{cases} W_{zi} = [MIN(\delta z_i / \Delta H_0, 1.0)] \ , \delta z_i > 0 \\ W_{zi} = 1, \quad \delta z_i < 0 \end{cases} \quad (10),$$

where, $W_S = 0.9$ is set to be constant, ΔH_0 is also constant, with default value 100 m, δz_i is the height difference between the i-th vertical level of MPP and the highest level of wind velocity observation at the given point of observation as it is shown on Figure 1. Thus, $W_O = W_O(r_k, z_i)$ is expressed as a function of the observation number *k* and the vertical level of MPP, where observed values of the wind velocities were interpolated / extrapolated. After calculating the value of W_O by the relationships (9)-(10), the parameter E_B^2 / E_O^2 is calculated using the relationship (7). Note that if $W_S = 0.9$ and $W_Z = 1$ then $E_B^2 / E_O^2 = 9$. This is a reasonable estimate of relative error for the ground level measurements of wind velocity (Gandin, 1978).

The radius of influence by default is defined from the root mean square (RMS) deviation of the terrain height above the sea level from the "mean" terrain height above the sea level (the height, averaged through all grid points). This dependence is given in Table 2 and it shows a decreasing radius of influence with increasing RMS, which is obvious from a physical point of view. The value R_0 = 150km (for the relatively smooth terrain) is taken from Gandin (1978).

The IOS scheme (3) converges to the "optimal" solution (2) when the variable f is homogeneously and isotropically distributed, and its correlation function corresponds to the weighting function used in (3). But, it is well known (Monin and Yaglom, 1975), that homogeneity and isotropy of the wind field *does not mean* that correlation functions $\mu_{uu}(r_i, r_j)$, $\mu_{vv}(r_i, r_j)$ of the U and V components of velocity are isotropic, since they *can be* dependent on the turnings of the coordinate system. At the same time, when IOS procedure (3) with the weight function (4) is applied, the isotropy of $\mu_{uu}(r_i, r_j)$ and $\mu_{vv}(r_i, r_j)$ is *implicitly assumed*. The error of this assumption grows with distance. An additional drawback of the IOS scheme is that it is impossible to use the increasing with distance bi-correlation function $\mu_{uv}(r_i, r_j)$ for the wind field. So the multivariate OI scheme was also considered as an alternative for the assimilation of the wind fields. In this case, the correlation functions of the isotropic 2D non-divergent velocity field, can be assumed to have the following form (Daley, 1991):

$$\mu_{uu}(r_i, r_j) = \exp(-r/R_0)\left[1 - \frac{r}{R_0}\left(1 - \frac{(x_i - x_j)^2}{r^2}\right)\right] \quad \text{(11-a)}$$

$$\mu_{vv}(r_i, r_j) = \exp(-r/R_0)\left[1 - \frac{r}{R_0}\left(1 - \frac{(y_i - y_j)^2}{r^2}\right)\right] \quad \text{(11-b)}$$

$$\mu_{uv}(r_i, r_j) = \exp(-r/R_0)\frac{r}{R_0}\frac{(x_i - x_j)(y_i - y_j)}{r^2} \quad \text{(11-c)}$$

The estimates $u_A(r_i)$ and $v_A(r_i)$ of the u and v components of the analysed velocity field at the point r_i are expressed in the following form:

$$\begin{aligned} u_A(r_i) - u_B(r_i) &= \underline{\mathbf{W}}_{uu}\left(\underline{\mathbf{u}}_O - \underline{\mathbf{u}}_B\right) + \underline{\mathbf{W}}_{uv}\left(\underline{\mathbf{v}}_O - \underline{\mathbf{v}}_B\right) \\ v_A(r_i) - v_B(r_i) &= \underline{\mathbf{W}}_{vu}\left(\underline{\mathbf{u}}_O - \underline{\mathbf{u}}_B\right) + \underline{\mathbf{W}}_{vv}\left(\underline{\mathbf{v}}_O - \underline{\mathbf{v}}_B\right) \end{aligned} \qquad (12)$$

where $u_B(r_i)$, $v_B(r_i)$ are background (first guess) values of components of velocity at the MPP grid, $\underline{\mathbf{u}}_O$ and $\underline{\mathbf{v}}_O$ are vectors of observed values of length K (total number of the observation points where observations of velocity are available), $\underline{\mathbf{u}}_B$ and $\underline{\mathbf{v}}_B$ are vectors of background values *at the points of observations* (calculated by interpolation from the nearest points of the MPP grid), and the weight vectors $\underline{\mathbf{W}}_{uu}, \underline{\mathbf{W}}_{uv}, \underline{\mathbf{W}}_{vu}, \underline{\mathbf{W}}_{vv}$ of length K are calculated by solving the following system of equations:

$$\begin{aligned} &\left[\underline{\underline{\boldsymbol{\eta}}}^B_{uu} + \mathbf{I}\right]\underline{\mathbf{W}}_{uu} + \underline{\underline{\boldsymbol{\eta}}}^B_{uv}\underline{\mathbf{W}}_{uv} = \underline{\boldsymbol{\eta}}^B_{uu}(r_i) \\ &\underline{\underline{\boldsymbol{\eta}}}^B_{uv}\underline{\mathbf{W}}_{uu} + \left[\underline{\underline{\boldsymbol{\eta}}}^B_{vv} + \mathbf{I}\right]\underline{\mathbf{W}}_{uv} = \underline{\boldsymbol{\eta}}^B_{uv}(r_i) \\ &\left[\underline{\underline{\boldsymbol{\eta}}}^B_{uu} + \mathbf{I}\right]\underline{\mathbf{W}}_{vu} + \underline{\underline{\boldsymbol{\eta}}}^B_{uv}\underline{\mathbf{W}}_{vv} = \underline{\boldsymbol{\eta}}^B_{uv}(r_i) \\ &\underline{\underline{\boldsymbol{\eta}}}^B_{uv}\underline{\mathbf{W}}_{vu} + \left[\underline{\underline{\boldsymbol{\eta}}}^B_{vv} + \mathbf{I}\right]\underline{\mathbf{W}}_{vv} = \underline{\boldsymbol{\eta}}^B_{vv}(r_i) \end{aligned} \qquad (13)$$

Matrices and vectors, included in (13) are defined by the following relationships:

$$\begin{aligned} &\left(\eta^B_{uu}\right)_{kl} = \mu^B_{uu}(r_k, r_l)\left(\sigma^2_B / \left(\sigma^2_O\right)_k\right),\ 1 \le k, l \le K \\ &\left(\eta^B_{uu}(r_i)\right)_k = \mu^B_{uu}(r_i, r_k)\left(\sigma^2_B / \left(\sigma^2_O\right)_k\right),\ 1 \le k \le K \end{aligned} \qquad (14)$$

where K is the number of observations, $\sigma_B(z_m), 1 \le m \le N$ is the root mean square error of the first guess velocity field for the given vertical level m, N is the number of the vertical levels of the MPP, $\sigma_O(r_k, z_m)$ is the root mean square error of the observations at the given observation point k and vertical level m. Definitions for the matrixes $\underline{\underline{\boldsymbol{\eta}}}^B_{uv}, \underline{\underline{\boldsymbol{\eta}}}^B_{vv}$ and vectors $\underline{\boldsymbol{\eta}}^B_{uv}, \underline{\boldsymbol{\eta}}^B_{vv}$ are the same as (14) with changed only indices.

The system of equations (14) was derived following Gandin (1968) in Kovalets (2003) using the assumptions that correlation functions of the errors of observations satisfy: $\mu^O_{uu}(r_i, r_k) = \mu^O_{vv}(r_i, r_k) = \delta(r_i, r_k)$, $\mu^O_{uv} = 0$. The root mean square errors of the observations (for the given vertical level) satisfy: $\sigma^O_u(r_k, z_m) = \sigma^O_v(r_k, z_m) = \sigma_O(r_k, z_m)$, the root mean square error of the background fields can be assumed to be constant (for the given vertical level, for which the optimal interpolations is performed), so that $\sigma_u^B(r_k, z_m) = \sigma_v^B(r_k, z_m) = \sigma_B(z_m)$.

Thus, the system of equations (13) contains besides correlation functions, defined by the relationships (11a-c) only the *relative* errors of the values of the background field and observations. Relative errors were already defined above by the relationships (8)-(10). So, the system of equations (13) is closed and can be solved for each node of the MPP. After that, correction of the wind field with the use of equations (12) is performed.

Finally, it should be noted that the following variables are subject of DA procedures: wind velocity, temperature, cloud cover, net radiation and precipitation. This is because routine meteorological measurements exist for these variables and are usually available for RODOS system. At the same time, other variables such as mixing layer height, sensible heat flux, stability category, friction velocity and Monin-Obukhov length, for which routine measurements are not usually available, are affected by the DA procedures indirectly, through their dependence on the wind velocity and net radiation.

Comparisons with experiments

Calculated meteorological variables were compared with the meteorological measurements, performed during the ETEX (S.E. Gryning et al., 1998). The ETEX database contains both ground and upper air observations collected from the time of the tracer releases (23 October and 14 November 1995) and three days ahead. The weather forecast data for the periods of both of the ETEX releases were obtained from the ECMWF data archive. The measurements performed during the ETEX covered a domain of almost 1500 x 2000 km^2, which is much more extended than the computational domain of the RODOS MPP. The latter is designed for calculations on the local to meso-scales (Raskob and Ehrhardt, 1991), i.e., for domain sizes of 60 to 400 km. So, calculations with the RODOS MPP were performed in a square domain covering approximately 400x400 km^2 around the point of tracer release in the ETEX experiments (Monterfil, see Figure 2). The computational domain was discretised by a 5x5 km^2 horizontal grid (solid lines in Figure 2).

Data from the 8 ground-based synoptic weather stations, shown by the triangles in Figure 2, were used for the improvement of the first-guess fields in the data assimilation procedure. This choice was made to produce better estimates of net radiation and stability category, because these stations contained, in addition to measurements of surface wind velocity and temperature, measurements of cloud cover, not available at the other ground stations, marked on Figure 2 by the circles. Data from the 71 observation stations marked by the circles were only used for the comparisons of the wind fields, calculated by the MPP in two cases: first using only the NWP data, and secondly using both the NWP data and the measurements.

Data from the sonic anemometer and the sodar located at the centre of the domain (Monterfil) were also used for comparisons of the calculated meteorological fields with the observations. The sonic anemometer data contained measurements of sensible heat flux and of momentum flux. The sodar data contained measurements of the wind velocity vertical profile.

Four basic parameters can characterize the level of agreement between modelled and observed wind fields. These are the root mean square deviations of wind velocity (*rmsu*) and of wind direction (*rmsd*) and the systematic deviations or bias of wind velocity (*biasu*) and of wind direction (*biasd*). They are defined by the following relationships:

$$rmsf = \left[\sum_{k}^{Nk} \sum_{i}^{Ni} \left(f_{ki}^{O} - f_{ki}^{C} \right)^2 \right]^{1/2} \Big/ \left(Nk \cdot Ni \right) \qquad (15)$$

$$biasf = \left[\sum_{k}^{Nk} \sum_{i}^{Ni} \left(f_{ki}^{O} - f_{ki}^{C} \right) \right] \Big/ \left(Nk \cdot Ni \right) \qquad (16)$$

f is either the wind velocity U, or the wind direction D, index "k" denotes the number of time steps of the NWP model in the ECMWF data base through which data were extracted for comparisons, index "i" denotes observation points used for comparisons. For the first ETEX release Nk=9, while for the second Nk=13. Ni = 71 for both ETEX 1 and 2 cases. To calculate *biasd*, at first differences of the wind direction were averaged through spatial locations, and after that, resulting values were averaged through the time steps.

The values of *rmsu*, *rmsd*, *biasu*, *biasd* calculated for the first guess field (with the use of NWP data only), and those calculated with the use of different data assimilation procedures (optimal interpolation, iteration to optimal solution) are presented for each of the ETEX releases in Table 3. The value for R_0 was taken from Gandin, (1976) and set equal to 150 km.

In both cases comparisons clearly show improvement of the wind fields with the use of DA procedures. For the case of the first ETEX experiment the values of the *rmsu* and *rmsd* are almost not affected by the DA procedures, while for the case of the second ETEX experiment the improvement of the *rmsu*, *rmsd* under the influence of the DA procedures is clearer. This can be explained by the fact that, according to Gryning, et.al. (1998) the first ETEX experiment is characterized by weather conditions better represented in parameterisations of the NWP models than the weather conditions of the second ETEX experiment. The values of *biasu* and *biasd* are strongly affected by the use of DA procedures in almost all cases. As it can be seen from the data presented in Table 3 the OI method generally performs better. This is expected, because, as it was discussed in the previous section, the OI method utilizes the information on the correlation functions of the wind fields to a greater extent than IOS. At the same time, the use of the OI method can be 5-10 times computationally more expensive than the use of the IOS method.

It is worth to compare results of 3DDA assimilating procedures, given in Table 3 with results of 4DDA from Seaman (2000) given in Table 4: it can be seen that the level of improvement, achieved by the use of 3DDA in the present work is in agreement with the effect of 4DDA when used in prognostic models.

Examples of the wind fields calculated by the MPP for the 00:00h of 25 of October are shown in Figure 3. As it can be seen from this picture, the background field calculated by the MPP using only the NWP data is much smoother than the one calculated using the optimal interpolation. This is expected, as small-scale features of the flow are filtered by the coarse grid of the NWP model (Figure 2). On the other hand, the fact that the wind field, calculated with the use of OI procedure is also smoother, than the wind field calculated with the IOS procedure, is mainly due to the properties of algorithm itself (Gandin, 1978). Furthermore, observed values of the wind velocities show rather big differences in both wind speed and direction between different locations. As it can be seen, the observed wind direction in the centre of the domain is mostly southern, and background values are corrected in right way by the OI procedure. However for more accurate modelling of the influence of terrain features on the wind field the statistical methods of data assimilation should be combined with the variational methods such as described in (Fisher et al., 1998).

Figure 4 shows comparisons between calculated by the MPP and measured values of friction velocity u_* and kinematical heat flux $\langle u'T' \rangle$ during the first ETEX experiment at the location of the sonic anemometer (Monterfil in the Figure 2). As it can be seen from Figure 4 the use of data assimilation procedure significantly improved the values of the friction velocity. At the same time, the values of the kinematical heat flux remained almost non-affected by the DA procedure, but in both cases they have reasonable values for both stable (negative values) and unstable (positive values) conditions. Thus, Figure 4 confirms the known fact that, when the first guess estimation of a certain meteorological variable is poor, then the DA procedure improves it; if the first guess estimation is good, then improvement cannot be expected.

At the same time, it is worth to note that the values of friction velocity and sensible heat flux are not affected directly by the DA procedures (as it was mentioned in the previous section), but only through their dependence on such variables as wind velocity, temperature and other that are directly affected by the DA procedures. Consequently improvement of these variables depends not only on the quality of the DA procedures, but also on accuracy of the parameterisations used for calculation of these variables from the "basic" variables (velocities, temperature and other).

Figure 5 shows comparisons of the vertical profiles of the wind fields, calculated by the MPP with those measured by the sodar. As it can be seen from that picture, the profiles of the wind velocity calculated by the MPP with the use of the observed surface wind velocities, are better than the profiles calculated with the use of the NWP data only. This is due to the extrapolation procedure performed before the assimilation of the wind velocities. As extrapolation (for the surface data) is performed only in the lower 200 m layer of the atmosphere, improvement (for that case) can be observed only in the lower 200 m layer as it is seen from Figure 5.

Using relationships (6) for the extrapolation of the wind direction also results in a generally good agreement of the dependence of the calculated wind direction with height with the observed data. The disagreement in wind direction that exists in some cases is due to disagreement between experimental data of ground level stations, used in DA procedure and the values provided by the sodar that sometimes could be up to 30º. This disagreement could be possibly attributed due to different averaging times (3 h for ground observation stations and 30 minutes for sodar).

In the current study sodar measurements were not used in the DA, because they were used for comparisons. In the case, when measurements of the wind velocity data are not vertically extrapolated, but interpolated (for instance, if sodar measurements were used for the data assimilation) improvement can be expected not only in the lower 200 m layer, but also at the higher levels.

Conclusions

The work presented in this paper concerned the development of a data assimilation methodology for the simultaneous use of both NWP data and meteorological measurements by the meteorological pre-processor of a real-time emergency response system. This methodology has been implemented in the MPP of RODOS. The methodological approach for solving the data assimilation problem developed in this work is based on the method of optimal interpolation (OI) and the variant of method of successive corrections called "Iteration to optimal solution" (IOS) (Daley, 1991). These methods were previously used for calculation of initial conditions in meteorological synoptic- and meso-scale prognostic models. By combining these methods with the approach used in the diagnostic wind model CALMET (Scire, 2000) for determination of the weighting coefficient, they were modified for use in the frames of the MPP that acts as local to meso-scale diagnostic model.

The developed methodologies of data assimilation were validated against the meteorological measurements performed during the ETEX. Comparisons were performed only against the independent measurements, i.e., those, which were not used in the DA procedure. Comparisons showed, that both of the developed procedures of data assimilation lead to improvement of the final calculated field of wind velocity, and better agreement with experimental data. The level of improvement was of the same order as of the 4DDA procedures used in the prognostic models (Seaman, 2000). Approaches presented in this work can be also used for the calculation of the first guess wind field used in variational divergence minimizing procedures and investigation of the effect of such combination of the two methods on the final wind field should be conducted.

Further validation of the MPP could include also comparisons of the concentrations predicted by the ADMs (which used calculated by the MPP wind field as input) with observed concentrations.

Acknowledgements

The present work has been fully supported by the European Commission through the grant RODOS Migration/grant-IK, contract № FIKR-CT-2002-50024 in connection to the European Project "RODOS Migration".

References

1. Andronopoulos S. et al., 1998, FILMAKER: a computer model fro pre-processing of the weather data. RODOS report WG2_TN98_08, http://www.rodos.fzk.de
2. Daley R., 1991, Atmospheric Data Analysis, Cambridge University Press
3. S.E. Gryning, et. al., 1998, Meteorological conditions at the release site during the two tracer experiments, Atmospheric Environment, 32, 4213-4137.
4. Gandin L., 1968, Objective Analyses of Meteorological Fields, English Translation, Jerusalem, Israel Program for Scientific Translation
5. Gandin L., 1978, Statistical Methods of Interpretation of the Meteorological Data, Leningrad, Gidrometeoizdat (in russian)
6. Fisher B.E.A., et.al (eds.), 1998, COST Action 710, Final report, Harmonisation of the pre-processing of meteorological data for atmospheric dispersion models, L-2985 European Commission, Luxembourg, EUR 18195 EN (ISBN 92-828-3302-X)
7. Hanna S., Chang J., 1993, Hybrid plume dispersion model improvements and testing at three field sites, Atmospheric Environment, **27A,** 1491-1508
8. Kovalets I., 2003, Introduction of data assimilation techniques in the meteorological pre-processor of the RODOS system, Final Report, EUROATOM grant, contract № FIKR-CT-2002-50024
9. Kumar N., Russel A., 1996, Comparing prognostic and diagnostic meteorological fields and their impacts on photochemical air quality modelling, Atmospheric Environment, 30, 1989-2010
10. Lamprecht R., Berlowitz D., 1998, Evaluation of diagnostic and prognostic flow fields over prealpine complex terrain by comparison of the lagrangian prediction of concentrations with tracer measurements, Atmospheric Environment, 32, 1283-1300.
11. Monin A., Yaglom A, 1975, Statistical Fluid Mechanics, Vol.2, Cambridge: MIT Press
12. Raskob W., Ehrhardt J. (eds.), 1999, The RODOS System: Decision Support For Nuclear Off-Site Emergency Management In Europe, RODOS report GEN_TN99_02, http://www.rodos.fzk.de
13. Scire J., 2000, A users guide for the CALMET meteorological model, Earth Tech, Inc., http://www.src.com/calpuff/calpuff1.htm
14. Seaman N., 2000, Meteorological modelling for air-quality assessments, Atmospheric Environment, **34,** pp.2231-2259
15. Straume A.G., et.al., 1997, Meteorological observations collected during the European Tracer Experiment (ETEX), JRC, Italy, http://rem.jrc.cec.eu.int/etex/
16. van Ulden A.P. and Holtslag A.A.M., 1985, Estimation of atmospheric boundary layer parameters for diffusion applications, Journal of Climate and Applied Meteorology, **24,** 1196-1207

List of Figures

Figure 1: On the determination of the weight parameter W_O

Figure 2: Computational domain for the MPP test case, with the points of meteorological observations from the ETEX database. Triangle points: measurements used for DA. Circle points: measurements used for comparisons. Cross points: nodes of the NWP model. Solid lines: MPP grid

Figure 3 Wind fields at 10 m height calculated by the MPP for the 25 October, 00:00UTC. a) Background wind field (calculated from NWP without DA); b) wind field calculated with the use of IOS procedure R_0 = 50 km; c) observed values of wind velocity; d) wind field, calculated with the use of OI procedure, R_0 = 150 km.

Figure 4 Dependence of the friction velocity (a) and kinematical heat flux (b) with time. Dots - measured data, solid line - calculated data with the use of DA procedures, dashed line - calculated with the use of the NWP data only.

Figure 5 Vertical profiles of the wind velocity (a1, b1) and of the wind direction (a2, b2) for different time moments: calculated by the MPP with the use of observations (■, solid line), with the use of the NWP data only (▲, dashed line), and measured by the sodar (♦).

Tables

Variable	R_0 (km)	E_B^2/E_O^2
Surface temperature T_S	150	9
Cloud cover	150	9
Net radiation	150	6
Precipitation	50	9

Table 1 Radius of influence and relative error used in the IOS procedure for different meteorological elements. Values were taken from Gandin (1978).

Terrain elevation RMS deviation (m)	R_0 (km)
0 < RMS < 100 (plane)	150
100 < RMS < 200 (hilly)	100
200 < RMS < 300 (small mountains)	70
300 < RMS (mountains)	50

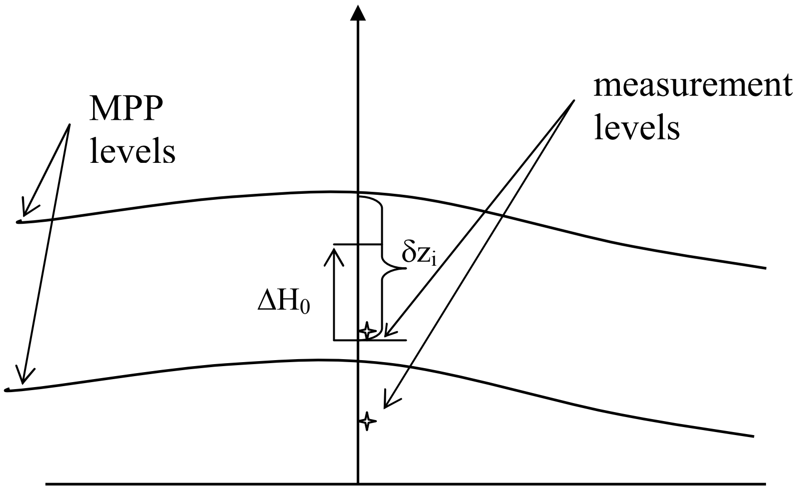
Table 2 Dependence of the radius of influence R_0 upon the RMS deviation of the terrain elevation

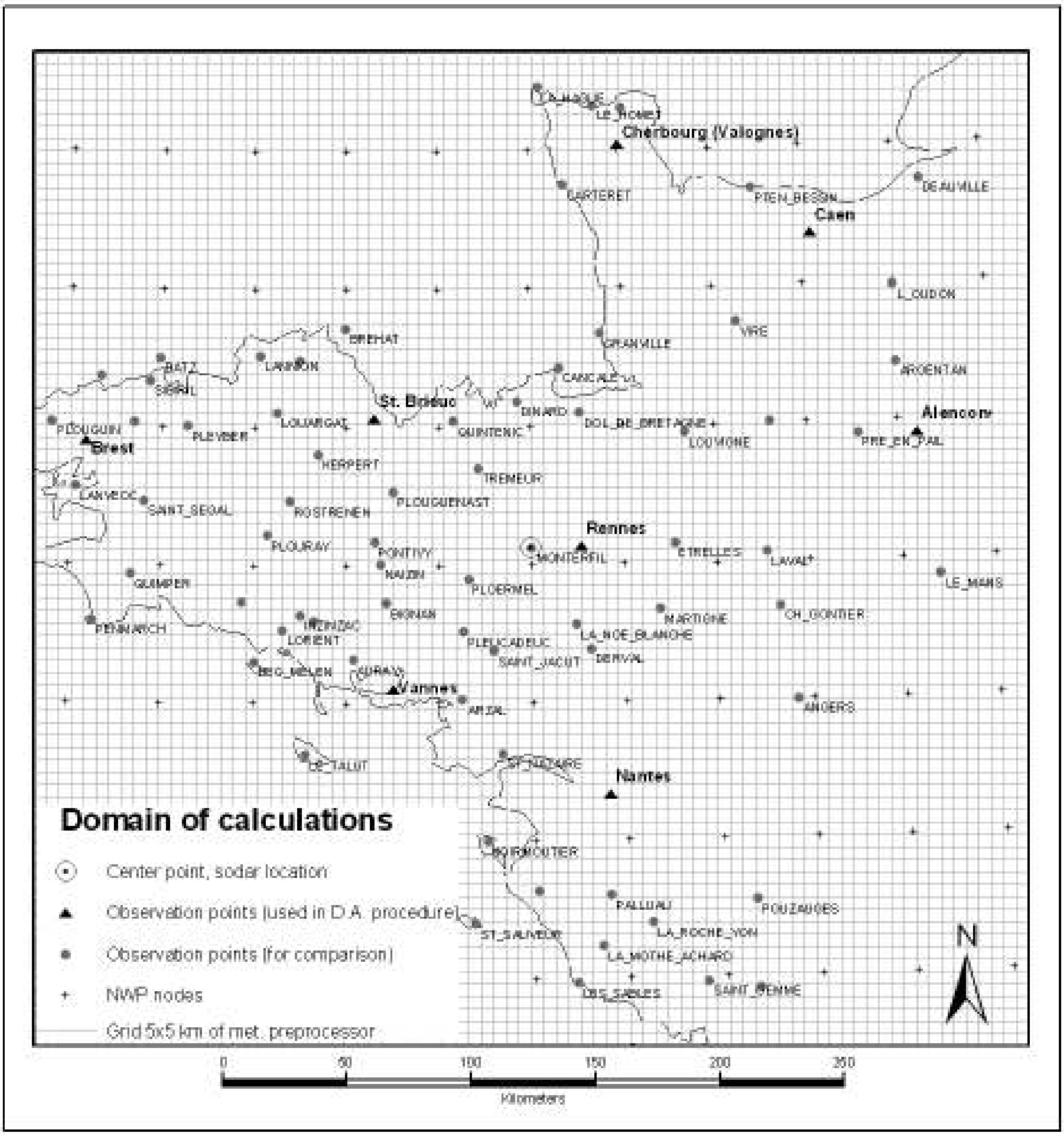
Variable	Background ETEX1	OI ETEX 1.	IOS ETEX 1.	Background ETEX 2	OI ETEX 2	IOS ETEX2
rmsu, m/s	2.57	2.44	2.51	2.21	1.94	2.0
biasu, m/s	0.67	-0.08	-0.39	0.5	-0.18	-0.37
rmsd, dec. degree	33	33	33.	56	48	42
biasd, dec. degree	10.3	5.5	7.23	18.7	5.9	-1.3

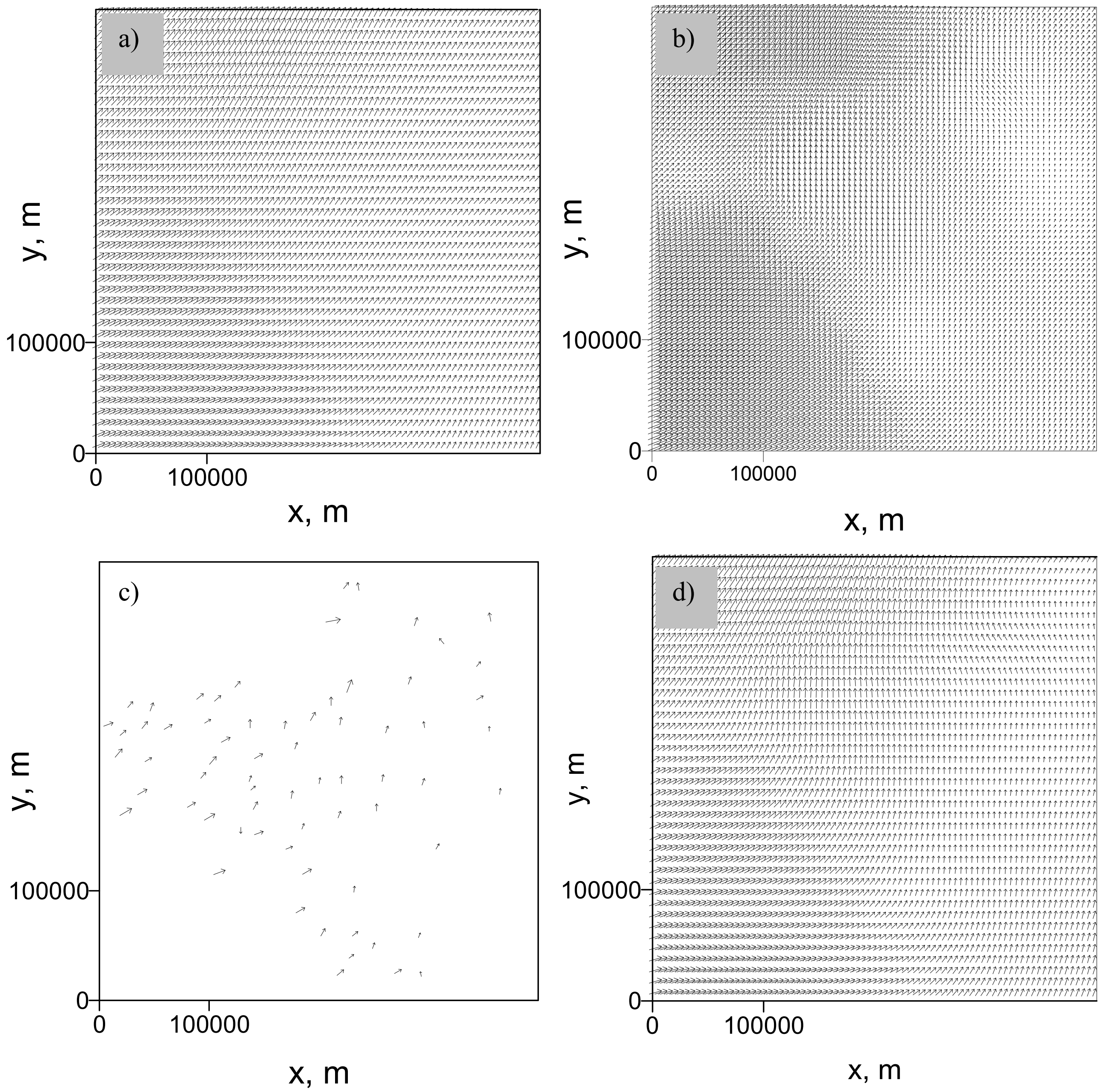
Table 3 Statistical characteristics of the calculated and observed wind fields

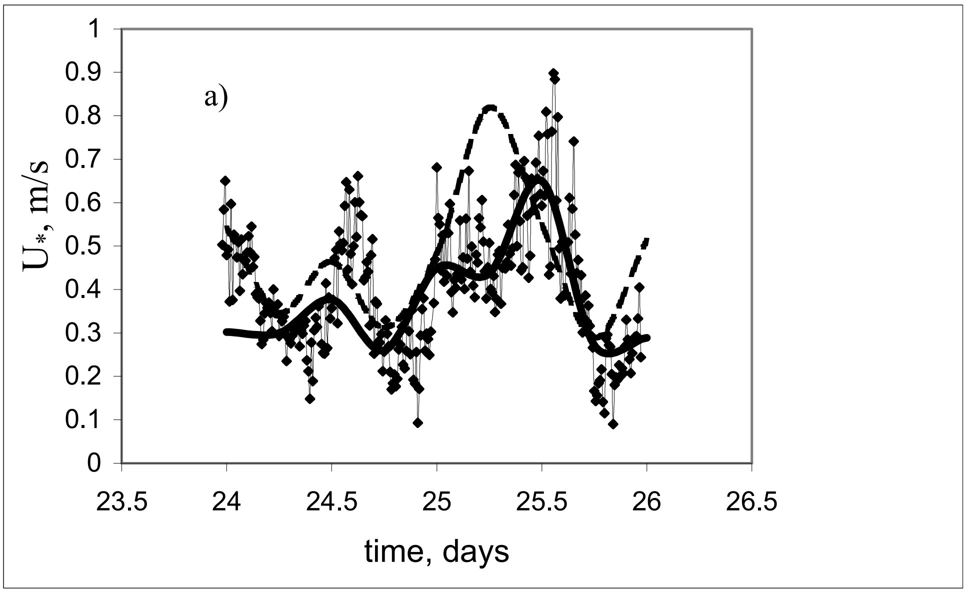
Model, scale of grid	Without data assimilation *rmsu* (m/s), *biasd* (dec. degree)	With data assimilation *rmsu* (m/s), *biasd* (dec. degree)
RAMS, dx = 1.32 km	3.63, -	0.93, -
RAMS, dx = 0.33 km	2.58, -	2.23, -
MM5, dx = 4 km	2.63, -8.4	1.72, -9.2

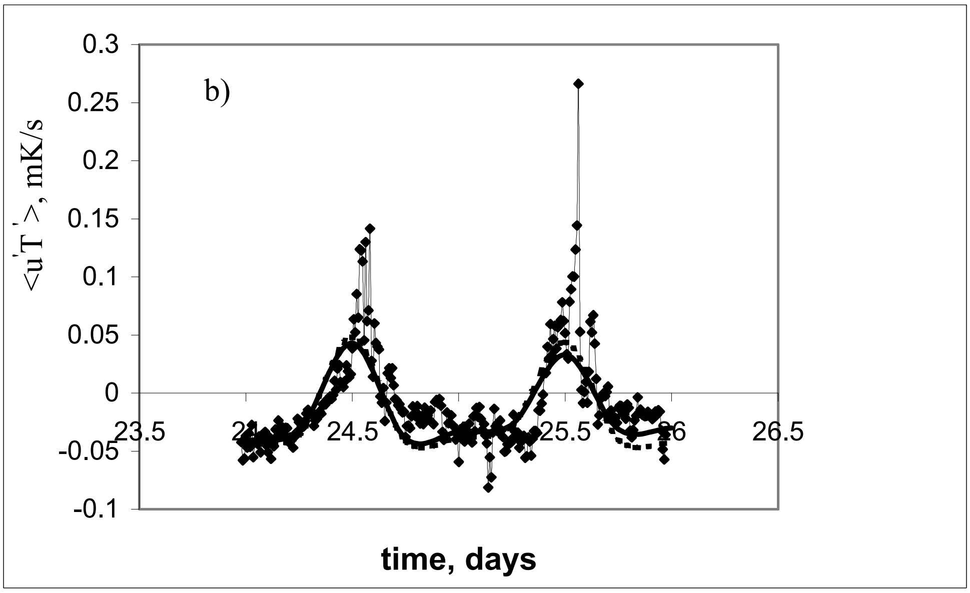
Table 4 Results of 4DDA used in different prognostic models far small-scale applications, results from review (Seaman, 2000)

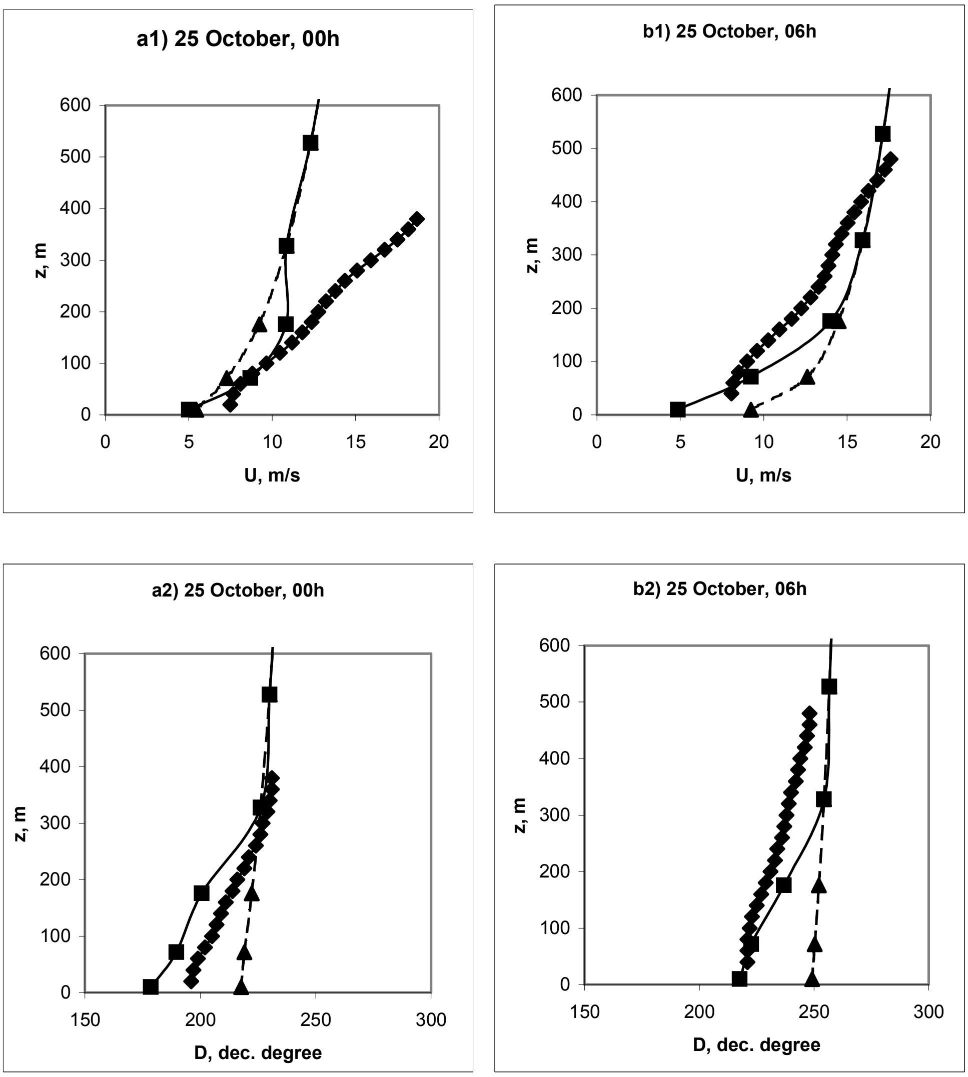

MPP
levels
measurement
levels
δz_i
ΔH_0


Domain of calculations
Center point, sodar location
Observation points (used in D.A. procedure)
Observation points (for comparison)
NWP nodes
Grid 5x5 km of met. preprocessor
Cherbourg (Valognes)
Caen
St. Brieuc
Brest
Rennes
Vannes
Nantes
Alencon
N
0
50
100
150
200
250
Kilometers


a)
y, m
100000
0
0
100000
x, m
b)
y, m
100000
0
0
100000
x, m
c)
y, m
100000
0
0
100000
x, m
d)
y, m
100000
0
0
100000
x, m


a)
U*, m/s
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
23.5
24
24.5
25
25.5
26
26.5
time, days


b)
<u'T'>, mK/s
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
23.5
24.5
25.5
26
26.5
time, days


a1) 25 October, 00h
z, m
U, m/s
b1) 25 October, 06h
z, m
U, m/s
a2) 25 October, 00h
z, m
D, dec. degree
b2) 25 October, 06h
z, m
D, dec. degree