Applicability of Minimisation Techniques for Improvement of Reliability of Environmental Pollution Model Predictions Based on Assimilation with Measured Data.

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Abstract: Improvement of mathematical model predictions of environmental pollution based on assimilation with real observations incoming from terrain represents great challenge and commitment for modellers. The authors are engaged in the grant project dealing with development of advanced statistical assimilation techniques and their implementation into corresponding software tool for support of decision making during emergency situations. In this article we pay attention to one simple method based on least square approach which, according to our opinion, has its own specific role among wide palette of assimilation techniques. Output background fields of resulting potentially dangerous endpoints are modified by measurements in such a way, that resulting respond surface is fitting towards measurements through the iterative adjustment of a certain set of model input parameters. Thus, in all iterations the physical knowledge expressed by model algorithm is preserved. The method provides reasonable results for smaller set of aforementioned selected input "manipulation" parameters provided that the measurements are well positioned and sufficiently dense. In spite of this limitation this approach is assumed to be applicable for the first preprocessing of model predictions and available measurement providing for example better initial conditions for application of further advanced statistical techniques. At the same time it can support robustness of decision making and can contribute to early detection of possible fatal decision maker errors due to misinterpretation of input parameters for an accidental release scenario.

Keywords: Pollution spreading; Gaussian plume; Simplex minimisation; Data assimilation.

1 ASSESSMENT OF ACCIDENT CONSEQUENCES

Potential failures occurred in man-made processes can lead to dangerous phenomena resulted in accidental releases of harmful substances into the living environment. Hazard evaluation and decision-making focused on early warning and protection of population is in charge of emergency management teams. Reliable and up to date information represents basic inevitable conditions for effective management of intervention operations targeted on consequence mitigation during such emergency situations. This appeared to be a basic lesson for further progress of emergency preparedness procedures, which has arisen from Chernobyl accident where lack of reliable information has shown to be the main reason of poor effectiveness of countermeasures. Decision making has to be supported by proper user-friendly software tool complied with advanced theoretical methodology with access to all necessary relevant latest data. Crisis management should come out from reliable picture of space and time of accident evolution, which should take into account all available information including physical knowledge of problem, expert judgement of input data, online measurements from terrain and others. The subject of investigation concerns evaluation of consequences of radioactivity propagation after an accidental release from nuclear facility. Nevertheless, the presented approach can be adopted to general problems of harmful substances dissemination. Transport of activity is studied from initial atmospheric propagation, deposition of radionuclides on the ground and spreading through food chains towards human body. Corresponding model of atmospheric dispersion and advection is based on segmented Gaussian plume model (SGPM) approach that can account approximately for dynamics of released discharges and short-term forecast of hourly changes of meteorological conditions. Implemented numerical difference scheme enables to approximate simulations of important parent-daughter pair formation. Subsequent deposition processes of admixtures and food chain activity transport are modelled. Hazard estimation based on radiation doses resulting from external irradiation and internal activity intake is integrated into the software system HARP (more detailed description was published on 6th EUROSIM Congress by Pecha et al. [2007a]).

2 FROM DETERMINISTIC CALCULATIONS TO PROBABILISTIC APPROACH AND DATA ASSIMILATON

Recent trends in risk assessment methodology insist in transition from deterministic procedures to probabilistic approach which enables generate more informative probabilistic answers on assessment questions. Corresponding analysis should involve uncertainties due to stochastic character of input data, insufficient description of real physical processes by parametrisation, incomplete knowledge of submodel parameters, uncertain release scenario, simplifications in computational procedure etc. Simulation of uncertainty propagation through the model brings data not only for the probabilistic assessment mentioned above but also for another main task of analysis called assimilation of model predictions with real measurements incoming from terrain. Data assimilation represents the way from model to reality and can substantially improve the reliability of model predictions. As advanced statistical assimilation techniques are capable account for model and measurement errors, inevitable prerequisite for their application is probabilistic modelling which provides data for construction of covariance structure of model errors for a given release scenario. The main problem such analysis inheres in necessary compromise between computer code speed and attained precision of the results.

There are several important sources of information that can enter the assimilation procedures. Basic physical knowledge is included in prior fields (resulted vectors) predicted by the model. Assumptions related to the random characteristics of model inputs can be supported by some kind of expert judgements. Substantial benefit can result from accessibility of data incoming from terrain. Merging of all these contending resources is a principle of assimilation and had shown to be very promising in many branches of contemporary Earth sciences. Each such resource can be known on a certain degree of details (e.g. dense or rare measurements in space and time, complete or only partial knowledge of model error covariance structure, cases with indirect observations). Thus, available information determines the option of suitable assimilation technique. At a present time we are constructing user-friendly assimilation subsystem, which is incorporated within the HARP system. For a certain accidental scenario the user can select from a palette of particular assimilation techniques starting from simple interpolation (no model prediction, dense and precise observed data) up to advanced statistical methods (full description of resources including the error structure have to be available). Principles of integration of assimilation subsystem were published on conference HARMO11 by Pecha at al. [2007b].

3 DATA ASSIMILATION USING MINIMISATION TECHNIQUE

This article deals with one particular method based on nonlinear optimisation technique. The objective multi-dimensional function F of N variables (subjected to bounds) is minimised starting at initial estimate. Simple Nelder-Mead direct search or Powell minimisation methods based on the concept of a simplex, that are tested here for elementary scenarios of accidental pollution releases, gave satisfactory results at acceptable time of computation.

3.1 Principles of application within atmospheric dispersion and deposition modelling.

Even for the simplest formulation of atmospheric dispersion and deposition in terms of Gaussian straight-line admixtures propagation the model $\boldsymbol{M}$ is nonlinear. In the following paragraphs we shall concentrate on accidental radioactivity release into atmosphere and its further deposition on terrain. Approximation in terms of source depletion scheme accounts for removal mechanisms of admixtures from the plume due to radioactive decay and dry and wet deposition on terrain. Let us proceed directly to the examination of the resulting fields of radioactivity deposition of a certain nuclide on terrain. The output is assumed to be represented by vector $\mathbf{Z}$ having dimension equal to the number N of total calculating points in the polar grid (in our case N= 2800, what means 80 radial sections and 35 concentric radial zones up to 100 km from the source of pollution). General expression for dependency of $\mathbf{Z}$ on model input parameters θ_1 , θ_2 , …. , θ_K can be formally written as

$$\mathbf{Z} = \boldsymbol{M}(\theta_1 ,\ \theta_2 ,\ \ldots ,\theta_K) \tag{1}$$

Let there are R receptor points on terrain where the respective values are measured. Generally, the number of receptors is much lower then N and we meet the problem with rare measurements expressed by observation vector $\mathbf{Y} \equiv (y_1,\ y_2,\ \ldots,\ y_R)$. Positions of sensors generally differ from the points of calculation grid. We shall use terminology from data assimilation for introduction of observation operator $\boldsymbol{H}$, specially for its linear observation matrix H. Construction of observation operator is done according to Kalnay [2003]. H is R × N matrix and transforms vectors $\mathbf{Z}$ from model space (having length N) into corresponding vector $\dot{\mathbf{Z}}$ in observation space (having length R) according to matrix notation $\dot{\mathbf{Z}} = H \cdot \mathbf{Z}$. Components $\dot{z}_r$ of vector $\dot{\mathbf{Z}}$ represent model predictions interpolated at the positions of observations r =1, … , R. We shall define innovation vector $\mathbf{D}$ that describes observation increase according to $\mathbf{D} = \mathbf{Y} - H \cdot \mathbf{Z}$.

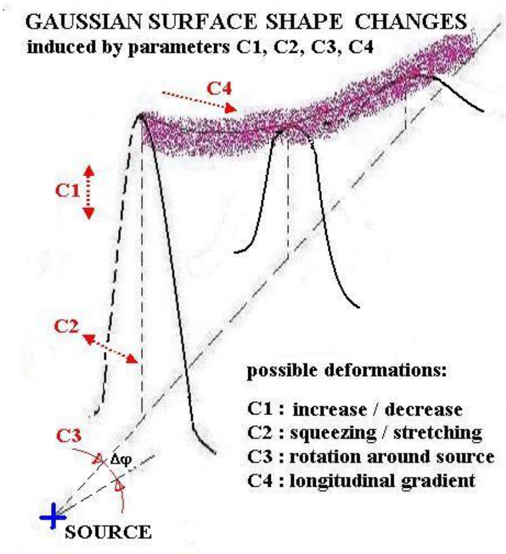

Figure 1. Gaussian surface shape fitting

surface modifications

Number K of input parameters is rather high (several tenth) and then for practical purposes only S of them are treated as random. Let rest of them are assumed to be less important from viewpoint of uncertainty propagation through the model and we assign them their best estimate values. Equation (1) is then simplified to the form $\mathbf{Z} = \boldsymbol{M}(\theta_1 ,\ \theta_2 ,\ \ldots ,\theta_S, \theta^b_{S+1}, \ldots , \theta^b_K)$. In other words a certain number S of selected problem-dependent optimisation parameters $\theta_1, \theta_2, , \ldots, \theta_S$ are considered to be uncertain and subjected to fluctuations within some range. The function F is constructed as a sum of squares in the measurement point positions between values of model predictions and values observed in terrain expressed as:

$$F(\theta_1,\ldots,\theta_S) \quad = \quad \sum_{r=1}^{r=R}\left(y_r - \dot{z}_r(\theta_1,\ldots,\theta_S)\right)^2 \tag{2}$$

Minimisation algorithm finds a minimum of scalar function F on S parameters starting at an initial "best estimate". In brief glance, the test points $[\theta_1 ,\ \theta_2 ,\ \ldots ,\theta_S]$ of the objective function F are arranged as a S-dimensional simplex and the algorithm tries to replace iteratively individual points with aim to shrink the simplex towards the best points. Further specific analysis concerns the resulting spatial fields of radioactivity deposition of a certain nuclide on the terrain. Model predictions of the deposition are done with the assistance of Gaussian solution and then the resulting deposition fields can be interpreted as Gaussian surface (or mixture of partial Gaussian extents) over the terrain. Our objective is to take into account both model predictions and available measurements incoming from the terrain and to improve spatial description of deposited radioactivity. We can imagine the iterative process of minimisation of function F such consecutive adjustment of the resulting respond surface, always according to the new evaluation of the parameters [θ_1 , θ_2 , …. , θ_S]. Thus, the predicted respond surface of results is gradually "deformed by permissible manipulations" directly driven by changes of problem-dependent optimisation parameters θ_s as long as the best fit of modified surface with observation values is reached. Important feature of the method consists in preservation of physical knowledge, because the new set of parameters [θ_1 , θ_2 , …. , θ_S] evaluated by minimisation algorithm always enters the entire nonlinear environmental model ***M*** according to equation (1).

3.2 Practical implementation and results

Investigation of applicability of minimisation assimilation technique was tested on "twin experiment", when lack of real observations is substituted by simulation of measurements artificially. Moreover, if for this purposes we use the same environmental model (e.g. for a fix one set of parameters) we can examine the problem convergence issues. In application part of the paper the results of two simulation experiments TWIN1 and TWIN2 are illustrated. TWIN1 relates to release of nuclide ^{131}I and its further straight-line propagation and deposition on terrain is described according to simple straight-line Gaussian plume model scheme. TWIN2 experiment deals with the problem of long-term evolution of ^{137}Cs deposition on terrain. Direct search complex algorithm represented by subroutine BCPOL was taken from IMSL Math/Library, Vol. 1. At the same time the procedure *fminsearch* from Optimization Toolbox of MATLAB was tested with similar results.

3.2.1 TWIN 1 experiment for simple release scenario described by Gaussian straight-line propagation

Accidental one-hour release of radionuclide ^{131}I with total radioactivity 1.28 E+11 Bq discharged into atmosphere from nuclear facility is analysed. Release height is 100 m, propagation continues under constant meteorological conditions (straight-line propagation in direction North-East, mean plume velocity 1.6 $m.s^{-1}$, Pasquill category D of atmospheric stability, no rain). Atmospheric dispersion coefficients are calculated according to KFK-Jülich semi-empirical formulas.

In the first step all input parameters are assumed to be represented by their best estimate values denoted by θ_i^b and then the corresponding output vector $\mathbf{Z^b}$ presents deterministic solution of deposited activity of selected nuclide on terrain. At the same time $\mathbf{Z^b}$ represents initial estimate for starting of minimization iterative search (input array GUESS(1:N) of subroutine BCPOL). In the second step we shall further reduce the number of parameters S from equation (2) to four parameters. Corresponding four uncertainties c_1, c_2, c_3, c_4 are introduced into the model according to scheme $\theta_i = c_i \cdot \theta_i^b$ or $\theta_i = \theta_i^b + c_i \cdot f(\theta_i^b)$. Specifically, their meaning and real choice is done according to the Table 1.

Table 1. Introduction of uncertainties for four important input model parameters

parameter	unit	expression	uncertainty bounds	influence on shape
θ_1: Source release rate	[$Bq.s^{-1}$]	$Q = c_1 \cdot Q^b$	$c1 \in$ <0.1;2.9>	increase / decrease
θ_2 : Horizontal dispersion	[m]	$\sigma_y (x) = c_2 * \sigma_y (x)^b$	$c2 \in$ <0.1;3.1>	squeezing/ stretching
θ_3 : Wind direction	[rad]	$\varphi=\varphi^b + \Delta\varphi$, $\Delta\varphi=c_3*2\pi/80$	$c3 \in$ <-5.0; +5.0>	rotation
θ_4 : Dry deposition velocity	[$m.s^{-1}$]	$vg = c_4 * vg^b$	$c_4 \in$ <0.1;4.0>	longitudinal gradient

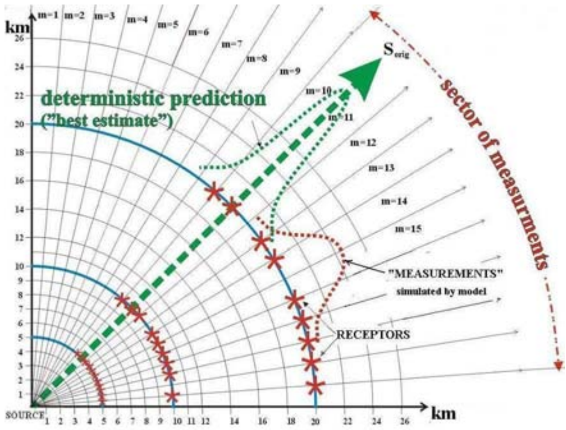

Figure 2. Artificial simulation of observations

The function $F(\theta_1, \theta_2, \ldots, \theta_S)$ from (2) now has form $F(c_1, c_2, c_3, c_4)$ and minimisation algorithm handles with 4-dimensional simplex. For purposes of construction of function F we have used slight modification of probabilistic version of existing environmental model HARP where original random inputs c_1, c_2, c_3, c_4 now play more general role of uncertainties characterized only by their range of possible fluctuations (see column 4 in Table 1). Procedure BCPOL uses this constraints such lower and upper bounds for permissible manipulations with values of variables c_1, c_2, c_3, c_4 (see arrows in Figure 1). During TWIN experiments the observation vector $\mathbf{Y} \equiv (y_1, y_2, \ldots, y_R)$ is simulated artificially, the simplest way is utilization of the same environmental model $\boldsymbol{M}$. For TWIN 1 experiment we follow scheme on Figure 2. Deterministic best estimate distribution $\mathbf{Z}^{\mathbf{b}}$ generated on the polar calculation grid in original wind direction S_{orig} (North-East) is drawn in green. At the same time it corresponds to the best estimate values $\{c_1, c_2, c_3, c_4\}_{best} \equiv \{1.0, 1.0, 0.0, 1.0\}$. Selected positions of observations are labelled by red asterisks. We select properly (for illustration purposes) one fixed quartet of $\{c_1, c_2, c_3, c_4\}^{obs} \equiv \{1.73, 1.51, +4.00, 1.98\}$ and generate vector $\mathbf{Z}^{\mathbf{obs}} = \boldsymbol{M}(\{c_1, c_2, c_3, c_4\}^{obs})$ - see dotted red curve on Figure 2. Then the values are transformed into observation positions according to $\dot{\mathbf{Z}}^{\mathbf{obs}} = H \cdot \mathbf{Z}^{\mathbf{obs}}$. Final simulated observation vector is obtained by assignment $\mathbf{Y} \equiv \dot{\mathbf{Z}}^{\mathbf{obs}}$.

Minimisation algorithm in successive iterations j brings newly generated quartets $\{c_1, c_2, c_3, c_4\}^j$ closer and closer to the $\{c_1, c_2, c_3, c_4\}^{obs}$. Fast convergence of assimilated model predictions towards simulated observations has been found. 220 iterations are calculated during about 6 minutes and the following values has been found: $\{c_1, c_2, c_3, c_4\}^{j=220} = \{1.731, 1.514, +4.003, 1.982\}$. It demonstrates very good consent with "simulated" observations generated by $\{c_1, c_2, c_3, c_4\}^{obs}$. The results are illustrated in Figure 3.

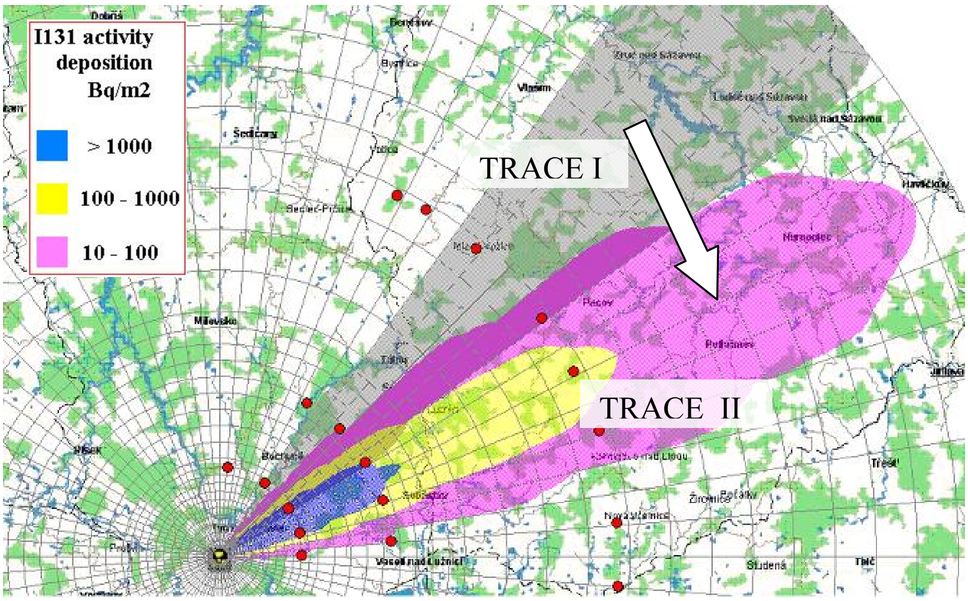

Figure 3. TWIN I experiment using Gaussian straight-line model. TRACE I and TRACE II are initial best estimate and resulting assimilation with simulated measurements (at red circles). Picture of ^{131}I deposition levels [$Bq.m^{-2}$] related to the end of plume progression.

Original best estimate deposition on terrain (and at the same time initial guess entering BCPOL) is labelled as TRACE I. Deposition after 220 iterations is calculated as $\mathbf{Z}^{j=220} = \boldsymbol{M}$ $(\{ c_1, c_2, c_3, c_4\}^{j=220})$ and its isoplets illustrates TRACE II. The assimilated respond surface TRACE II is at the same time practically identical with $\mathbf{Z}^{\mathbf{obs}}$ generated according to $\boldsymbol{M}$ $(\{ c_1, c_2, c_3, c_4\}^{obs})$ originally used for artificial simulations of measurements. The shapes of TRACE I and TRACE II reflect imposed changes in values of c_1^{best} to c_1^{obs} (higher nuclide discharge), c_2^{best} to c_2^{obs}(higher peripheral dispersion), c_3^{best} to c_3^{obs}(twist by 18°), c_4^{best} to c_4^{obs}(more intensive dry deposition causing steeper longitudinal gradient).

Conclusion I: Direct search algorithm connected with Gaussian straight-line propagation model has proved fast convergence provided that the measurements are well positioned. Its applicability depends on validity of model itself. Basic uncertainty propagation in plume dispersion models is discussed in Hanna et al.[1982]. Profound treatment and some results of expert studies we have found e.g. in Goossens at al. [2001] or Irwing and Hanna [2004], where limitations of the models are declared. However, the TWIN 1 results could be useful for preliminary fleeting estimation in near distances or during constant meteorological conditions.

3.2.2 TWIN 2 experiment accounting for short-term meteorological forecast

TWIN2 scenario complies with hourly changes of short-term weather forecast and uses segmented Gaussian plume scheme (model SGPM marked as $\boldsymbol{M}^{SGPM}$), which is much more complicated then straight-line spreading (more detailed on our approach of SGPM is in Pecha [2007a]). The first two consecutive release segments of ^{137}Cs discharge (each with 1 hour duration) with released amount 2.0 E+17 Bq and 1.0 E+17 Bq has dangerous power close to severe LOCA accident with partial fuel cladding rupture and fuel melting. Short-term meteorological forecast for the next 48 hours is provided by the Czech meteorological service. Then, for each hour since the release initiation there is prediction of wind direction and speed, category of atmospheric stability according to Pasquill classification and rain precipitation. Omitting other details, we are declaring for TWIN II the following plan:

1. Number of uncertainties is increased from four to five as c_1, c_2, c_3, c_4, c_5. c_5 stands for fluctuation of mean wind velocity. If we suppose wind direction and velocity fluctuations to be independent between hourly phases, then c_3 and c_5 split to 6 independent uncertainties c_{31}, c_{32}, c_{33} (for wind direction predicted for hour 1, 2 ,3) and c_{51}, c_{52}, c_{53} (for wind velocity predicted for hour 1, 2 ,3).
2. Each of the two hourly segments is modelled up to third hour after the release start taking into account short-term hourly meteorological forecast. The situation just after 3 hours is given by superposition of both segments in their successive meteorological hourly phases. Resulting best estimate fields are calculated in analogy with equation (1) according to scheme $\mathbf{Z}^{\mathbf{b}}_{\mathbf{3hour}} = \boldsymbol{M}^{SGPM}$ $(\{ c_1, c_2, c_{31}, c_{32}, c_{33}, c_4, c_{51}, c_{52}, c_{53} \}_{best})$ and is illustrated in Figure 4a.
3. Let simulate artificially fictive "observation surface" according to $\mathbf{Z}^{\mathbf{obs}}_{\mathbf{3hour}} = \boldsymbol{M}^{SGPM}$ $(\{ c_1, c_2, c_{31}, c_{32}, c_{33}, c_4, c_{51}, c_{52}, c_{53}\}^{obs})$. Vector of simulated measurements at observation positions (see black filled squares in Figure 4b) are calculated by help of linear observation operator as $\mathbf{Y}_{\mathbf{3hour}} \equiv H\, \mathbf{Z}^{\mathbf{obs}}_{\mathbf{3hour}}$. Let us suppose their incoming in one stroke just at hour 3 after the accident start. The "observation surface" nearly corresponds with TRACE II formation in Figure 4c.
4. Accomplish assimilation of the model predictions $\mathbf{Z}^{\mathbf{b}}_{\mathbf{3hour}}$ in compliance with measurements $\mathbf{Y}_{\mathbf{3hour}}$ in analogy with equation (2) using BCPOL procedure of minimisation.

Deposition of ^{137}Cs on terrain after 728 iterations is calculated as $\mathbf{Z}^{\mathbf{j=728}}_{\mathbf{3hour}} = \boldsymbol{M}^{SGPM}$ $(\{ c_1, c_2, c_{31}, c_{32}, c_{33}, c_4, c_{51}, c_{52}, c_{53}\}_{j=728})$ and its isolines illustrates in Figure 4c a trail on terrain marked as TRACE II. The results represent a new prediction just at third hour after release start, which is corrected by observations. Minimisation algorithm is initiated by the best estimate solution (TRACE I) and gradually approaches to the simulated observations. In short numerical summary, TWIN2 experiment required to prepare in advance sets of parameters { c_1 ,c_2 , c_{31}, c_{32}, c_{33} ,c_4, c_{51}, c_{52}, c_{53}} for:

best estimate: $\{ \ldots \}^b$ = 1.0, 1.0, 0.0, 0.0, 0.0, 1.0, 0.0, 0.0, 0.0 $^{(*)}$
"measurements": $\{ \ldots \}^{obs}$ = 7.0, 2.0, -4.0, -5.0, -6.0, 2.55, -0.5, -0.6, -0.7 $^{(**)}$

Here are examples of results achieved during iteration process for a particular iteration j :

$\{ \ldots \}^{j=728}$ = 7.18, 2.49, -3.94, -5,80, -6.34, 2.49, 0.21, -0.28, -0.59 (***)
$\{ \ldots \}^{j=1201}$ = 7.25, 2.03, -4.14, -5,80, -6.39, 2.59, 0.27, -0.36, -0.58

$^{(*)}$ TRACE I in Figure 4a, $^{(**)}$ close to TRACE II in Figure 4c, $^{(***)}$ TRACE II in Figure 4c

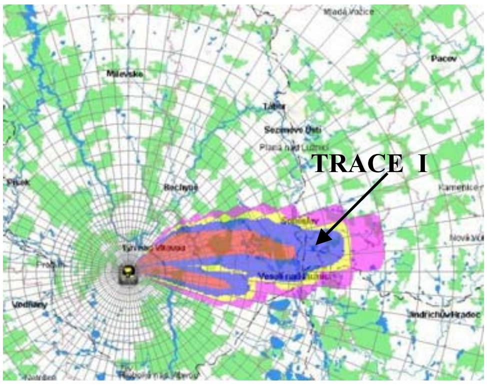

Figure 4a. Nominal deposition of ^{137}Cs (just 3 hours after release start)

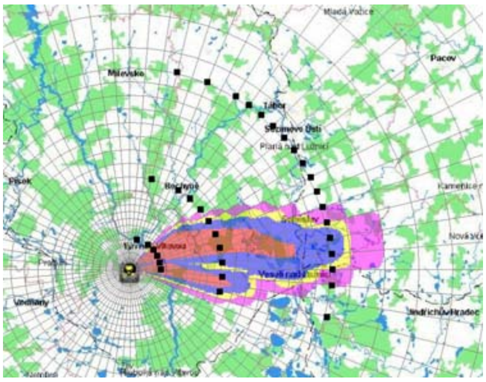

Figure 4b. Positions of artificially simulated measurements (black squares)

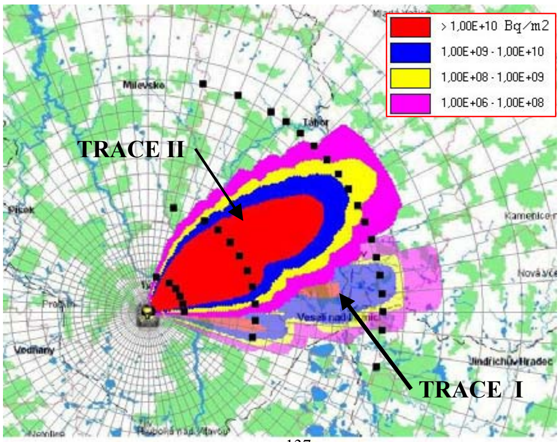

Figure 4c. Assimilation of ^{137}Cs model prediction and simulated measurements just after 3 hours

Meaning of the parameters c_1 to c_4 is the same as described in Table 1. c_5 stands for uncertainty of the mean velocity of the plume. Further spliting to c_{5i}, i=1,2,3 holds true for independent fluctuations of the mean velocity $\bar{u}_i$ forecasted for hours *i*. Uncertain $\bar{u}_i$ is then expressed according to $\bar{u}_i = \bar{u}_i^{best}$ (1+0.35* c_{5i}). c_{5i} bounds are <-1; +1>. More detailed recommendations for uncertainty bounds arising from expert judgement were found for example in Goossens at al. [2001].

<u>*Conclusion II*</u>: TWIN II experiment took into consideration 9 optimisation parameters with constructive idea to discriminate according to their global or local effect (introduced into the wind vector). System HARP is connected to the ORACLE server for online access to meteorological forecast, but for scenario TWIN II was used a certain historical meteorological forecast sequence. Satisfactory convergence is illustrated, but more detailed analysis related to the criterion of match between model and measurements (e.g. Eleveld [2004]) is so far pending.

4 FINAL REMARKS

Our latest tests have included also local effect of atmospheric precipitation and have confirmed its decisive role on character of picture of deposition on terrain. Our experience related to applicability of minimisation techniques indicates that number of selected optimisation parameters c_i should not be too high in order to avoid the poor convergence or even further algorithm "wander" (more sophisticated algorithms have to be searched). At this stage we recommend to consider five optimisation parameters included in the TWIN II experiment (where wind velocity vector is global, it means no further splitting of c3 to further c3i and c5 to c5i) and link the 6th parameter c6 representing uncertainty in precipitation intensity with local effect.

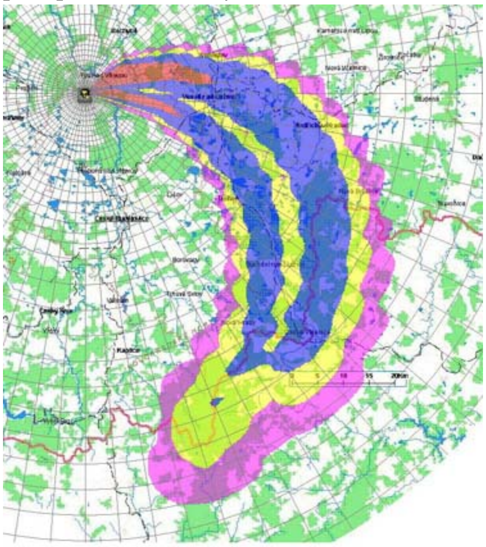

Figure 5. Nominal deposition of ^{137}Cs on terrain (just 9 hours after release start)

Presented minimisation technique fits results on a certain specific situation described by incoming observations, whereas in this process always preserve physical knowledge. But in no case it cannot be confused with parameter calibration. Real signification of our effort insists in achieving a reasonable capability to improve model predictions on basis of assimilation with observed values. Realistic prediction of evolution of radiation situation during emergency gives decision makers necessary time on judgement and introduction of efficient countermeasures on population protection. In Figure 5 is model prediction according to $\mathbf{Z}^{\mathbf{b}}_{\mathbf{9hour}}=\boldsymbol{M}^{SGPM}(\{\ldots, c_i, \ldots\}_{best})$. It represents a simple extension of $\mathbf{Z}^{\mathbf{b}}_{\mathbf{3hour}} = \boldsymbol{M}^{SGPM}(\{\ldots, c_i, \ldots\}_{best})$ illustrated in Figure 4a or 4b as TRACE I from hour 3 to hour9 after the release start. But we can easily anticipate, that if we extend propagation from assimilated TRACE II staying for hour 3 to hour 9 after release, we shall meet different but more reliable picture. Interventions introduced on the basis of earlier description according to Figure 5 could lead to fatal consequences on population health.

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