

Simulation of Random 3-D Trajectories of the Toxic Plume Spreading over the Terrain

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1. Introduction

An efficient software tool for purposes of simulation of random evolution of the concentration distribution of toxic admixtures originally discharged into the atmosphere is presented. The main goal of the development is its application as a pivot algorithm of the multiple recalled kernel for examination of the model error covariance structure and for Sampling-Importance-Resampling procedure for online Bayesian tracking of the plume trajectory progression. The primary quantity of interest is 3-D distribution of harmful admixtures concentration in the air on basis of which all other values in a respective release phase can be derived. In the early phase of an accident the cloud is drifting over an observed area and noxious agents (e.g. radionuclides) are depleted due to various removal mechanisms. Important indirect derived variables are for example time integral of the radioactivity concentration in ground-level of the air and radioactivity deposited on the ground. Both can be perceived as a certain projection of the primary 3-D concentration into 2-D. Any handling of 2-D output fields has unique association with 3-D trajectories inhere on background. Because of the conjugation, for example the real measurements of the activity deposited on terrain can serve as indirect observations for recursive plume tracking.

An ensemble of 3-D trajectory realizations offers good basis for uncertainty analysis (UA) and studies of sensitivity. These analyses should involve uncertainties due to stochastic character of input data, insufficient description of real physical processes by parametrization, incomplete knowledge of submodel parameters, uncertain release scenario, simplifications in computational procedure etc. Because of computational feasibility only a limited number of the most important random model parameters can be selected for parametrization of the 3-D trajectories. The rest of ones are assumed not having a random character and enter the calculations as invariants represented by their “best estimate” values. The history of each member of ensemble (called as “particle”) is always stored and can be easily and quickly reproduced when running the environmental model with corresponding recalled set of realization of random parameters and other fixed nominal inputs.

The environmental model of pollution transport is based on segmented plume-puff modification of the classical Gaussian approach which can account for hourly changes of meteorological conditions and release dynamics. Examination of uncertainty propagation through the Segmented Gaussian Plume Model (SGPM) facilitates to follow the recent trends in risk assessment methodology insisting in transition from deterministic procedures to probabilistic approach. The results mentioned in this article with a glance are related to both the probability approach of consequence assessment and generation of inputs inevitable for assimilation (prior physical knowledge included in the background fields and model error covariance structure). Real scenario of radioactivity dissemination analysed here demonstrates the complexity of the problem requiring a good degree of understanding. It covers also an introduction of necessary compromises in order to suppress excessive computational cost.

2. Outline of the environmental model SGPM of aerial transport of pollution

Various models of pollution transport in atmosphere are able to incorporate fundamental features of the problem under different approaches. It relates to dimensionality, calculation domain and grid resolution, parametrization of respective physical phenomena, initial and boundary conditions, intensive computation. Propagation of radioactive discharges in atmosphere is described by diffusion equation:

$$\frac{\partial C(\vec{r};t)}{\partial t} = -\vec{u}(\vec{r};t) \cdot \nabla C(\vec{r};t) + \nabla(K(\vec{r};t) \cdot \nabla C(\vec{r};t)) + S(\vec{r};t) - \beta \cdot C(\vec{r};t) \quad (1)$$

Here C represents 3-D distribution of specific radioactivity concentration in air [$\text{Bq}\cdot\text{m}^{-3}$]. The terms on the right side of (1) express in turns advection, turbulent diffusion (with anisotropic diffusivity coefficient K), sources of pollution S (point, linear, ...) and β designates sink (negative) terms caused by radioactive decay and removal processes of dry and wet depositions. Several approaches of solution of (1) are developed in dependency on the purpose of analysis.

Even simple, the Gaussian model is consistent with the random nature of turbulence, it is a solution of Fickian diffusion equation for constant K and wind advection velocity u , it is tuned to experimental data and offers fast basic estimation with acceptable computation effort. Proved semi-empirical formulas are available for approximation of important effects like:

- interaction of the plume with near-standing buildings,
- momentum and buoyant plume rise during release,
- power-law formula for estimation of wind speed changes with height,
- depletion of the plume activity (removal processes of dry and wet deposition, dependency on physical-chemical forms of admixtures and landuse characteristics),
- inversion meteorological situations, plume penetration of inversion, plume lofting above inversion layer,
- account for small changes in surface elevation, terrain roughness etc.

Gaussian models have long tradition of their use for dispersion predictions of continuous, buoyant air plume originating from ground-level or elevated continuous sources of pollution. Decisive criterion for its choice for our purposes is computational effectiveness which guarantees to solve the advanced data assimilation problems in real-time. Thorough control of radioactivity balance and conservation should ensure acceptable accuracy of results.

SGPM uses “source depletion” approach based on separation of the pure dispersion solution C^{disper} (the terms S and β are zeros) and “removal” component given by the plume depletion factors f_R^n, f_F^n, f_W^n due to radioactive decay (R) and dry (F) and wet (W) deposition in dependence on physical-chemical form of the nuclide n . During all elemental shifts of “Gaussian droplets” the formulation $C = C^{\text{disper}} \times f_R^n \times f_F^n \times f_W^n$ is adopted (Pecha et al. 2007).

The main objective of the modifications introduced into the SGPM model is synchronization of release dynamics with a given short-term meteorological forecast. The Czech meteorological service provides online short term meteorological forecast (point and gridded data) and real observations.

Scheme of the release dynamics have to be somewhat adopted to the hourly meteorological forecast. Real release dynamics is partitioned into equivalent number G of fictive one-hour segments of constant release source strength. Synchronization with hourly forecast of meteorological conditions is performed. Hourly segment of release is spread during the first hour as a “Gaussian droplet”. In the following hours of spreading according to available hourly meteorological forecast the droplet is treated as “prolonged puff” and its dispersion and deple-

tion during the movement is simulated numerically by large number (~ 25÷50) of elemental shifts. Each hourly segment g is consecutively modelled in its all hourly meteorological phases f ($f=1, \dots, F(g)$) and output vector s_{TOTAL} of values of interest is superposed from the particular segment-phase outputs $s^{g,f}$ as:

$$s_{TOTAL} = \sum_{g=1}^{g=G} \left\{ \sum_{f=1}^{F(g)} s^{g,f} \right\} \quad (2)$$

Transport of radioactivity is studied from the initial aerial propagation, deposition of radionuclides on the ground and spreading throughout food consumption towards human body.

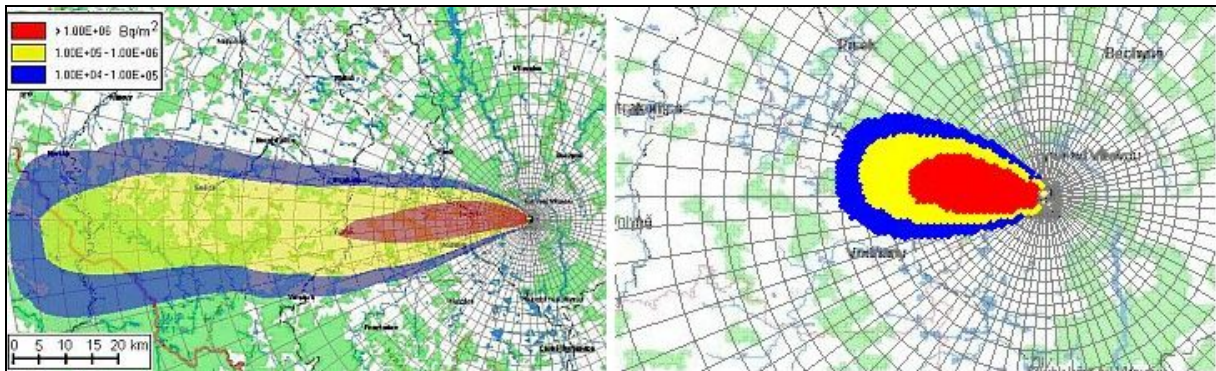


Figure 1: Deterministic model predictions (best estimate) for scenario from APENDIX. Left: total deposition of ¹³¹I after 13 hours. Right: Model prediction just 2 hours after the release start – see “best estimate” trajectory x_{Tr}^b according to Eq. (8). Legend is valid for all figures.

3. From deterministic calculations to probabilistic approach

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 parametrization, incomplete knowledge of submodel parameters, uncertain release scenario, simplifications in computational procedure etc. Simulation of uncertainties propagation through the model brings data not only for the probabilistic assessment (see next figures 2 and 3 that come out from scenario in APPENDIX), but also for another main task of analysis called assimilation of the model predictions with real measurements incoming from terrain.

Table 1: Model chain for probabilistic estimation of random quantities of interest

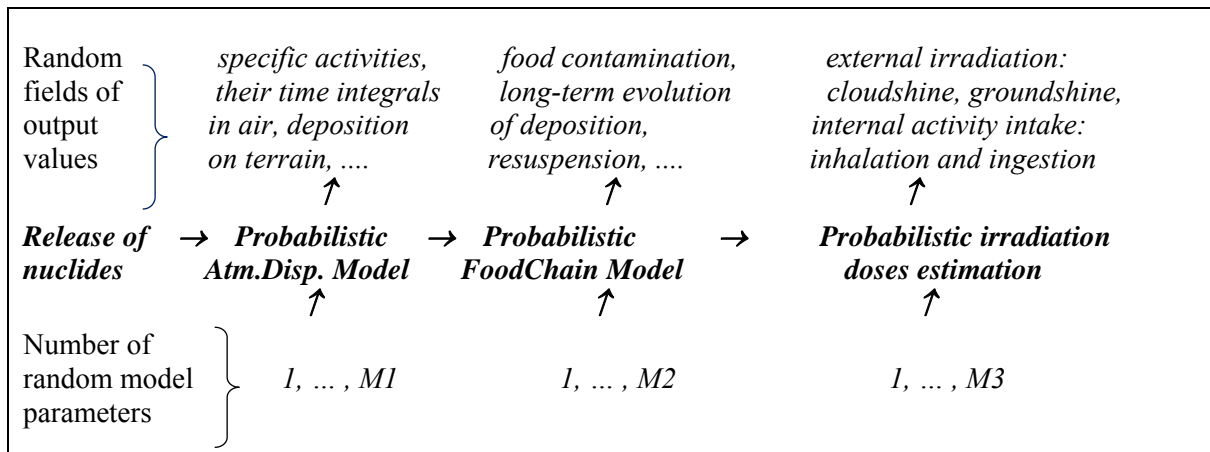


Table 2: Components of random parameter vector Θ for atmospheric dispersion module.

random parameter	unit	expressed inside code	uncertainty bounds	random parameter	unit	expressed inside code	uncertainty bounds
θ_{11} : activity release $s=1$	[Bq.h ⁻¹]	$Q = c_{11} \cdot Q^b_{11}$ Q^b_{11} in $f=1$	LU; $c_{11} \in <0.31; 3.1>$	θ_{31} : wind speed $f=1$	[m.s ⁻¹]	$V_{31} = c_{31} \times V^b_{31}$ V^b_{31} in $f=1$	U; $c_{31} \in <0.5; 3.0>$
θ_{12} : activity release $s=2$	[Bq.h ⁻¹]	$Q = c_{12} \cdot Q^b_{12}$ Q^b_{12} in $f=2$	LU; $c_{12} \in <0.31; 3.1>$	θ_{32} : wind speed $f=2$	[m.s ⁻¹]	$V_{32} = c_{32} \times V^b_{32}$ V^b_{32} in $f=2$	U; $c_{32} \in <0.5; 3.0>$
θ_{13} : ... $s=3$ θ_{1G} : ... $s=G$	[Bq.h ⁻¹]	<i>next hourly segments s of radioactivity release (if any)</i>		θ_{33} : wind speed $f=3$	[m.s ⁻¹]	$V_{33} = c_{33} \times V^b_{33}$ V^b_{33} in $f=3$	U; $c_{33} \in <0.5; 3.0>$
θ_{21} : wind direction $f=1$	[rad]	$\varphi = \varphi^b + \Delta\varphi$, $\Delta\varphi = c_{21} \times 2\pi/80$	U; $c_{21} \in <-12.0; +12>$	θ_{34} : $f=4$ θ_{3F} : $f=F$	[m.s ⁻¹]	<i>wind speed in successive meteophases f (if considered)</i>	
θ_{22} : wind direction $f=2$	[rad]	$\varphi = \varphi^b + \Delta\varphi$, $\Delta\varphi = c_{22} \times 2\pi/80$	U; $c_{22} \in <-12.0; +12>$	θ_4 : horizontal dispersion	[m]	$\sigma_y(\mathbf{r}) = c_4 \times \sigma_y(\mathbf{r})^b$	N_{trunc} ; $c_4 \in <0.89; 1.12>$
θ_{23} : wind direction $f=3$	[rad]	$\varphi = \varphi^b + \Delta\varphi$, $\Delta\varphi = c_{23} \times 2\pi/80$	U; $c_{23} \in <-12.0; +12>$	θ_5 : dry depo velocity	[m.s ⁻¹]	$vg(\mathbf{r}) = c_5 \times vg^b(\mathbf{r})$	LU; $c_5 \in <0.91; 1.10>$
θ_{24} : ... $f=4$ θ_{2F} : $f=F$	[rad]	<i>wind direction in successive meteophases f (if considered)</i>		<i>Index b stands for "best estimate" values; Distrb. type: U Uniform; LU LogUniform N_{trunc} ... Normal truncated</i>			

s – segment of radioactivity release during s^{th} hour from the release start;
 f – meteophase (hour) after the release start; V^b – wind speed at 10 m height;

4. Propagation of model parameter uncertainties

Uncertainties of model parameters Θ_i relate to imperfections of both conceptual model (algorithm limitation, simplifications during parametrization, stochastic nature of some submodel parameters, measurement errors of input data) and computational scheme (step of computation grid, averaging land-use characteristics, averaging times for dispersion parameters etc). Let $\Theta \equiv \{\Theta_1, \Theta_2, \dots, \Theta_M\}$ denotes a vector of M random model parameters Θ_m with corresponding sequence of random distributions D_1, D_2, \dots, D_M which are usually selected on the basis of commonly accepted agreement of experts (range, type of distribution, potential mutual dependencies). The value of dimension M of the parameter vector Θ is in general large, for practical reasons the further reduction of number M should be done. Computational simulation $\mathfrak{R}^{\text{SGPM}}$ based on SGPM approach enables to express random 3-D trajectory \mathbf{x}_{tr} ("particle", sometimes called also background vector) according to the parametrization:

$$\mathbf{x}_{\text{tr}} \approx \mathfrak{R}^{\text{SGPM}}(\Theta_1, \Theta_2, \dots, \Theta_M; \{\alpha_j^{\text{fixed}}\}_{j=1, \dots, J}) \quad (3)$$

α_j^{fixed} stands for invariant fixed model parameters (hereafter omitted in notations). Sampling-based method for UA consists in calculations of the k^{th} trajectory realization (for each specific sample k of the random parameter vector θ^k), repeatedly in two steps:

- 1) Generation of a particular k^{th} sample of input vector:

$$\theta^k \equiv \{\theta_1^k, \dots, \theta_m^k, \dots, \theta_M^k\} \quad (4)$$

where θ_m^k is k^{th} realisation of the m^{th} random parameter Θ_m .

- 2) Propagation of the sample k through the model, it means the calculation of the corresponding resulting k^{th} realisation of the trajectory according to:

$$\mathbf{x}_{Tr}^k = \mathfrak{R}^{SGPM}(\theta_1^k, \dots, \theta_m^k, \dots, \theta_M^k) \tag{5a}$$

or, specifically, according to the notation in Table 2:

$$\mathbf{x}_{Tr}^k = \mathfrak{R}^{SGPM}(c_{11}^k, \dots, c_{1G}^k, c_{21}^k, \dots, c_{2F}^k, c_{31}^k, \dots, c_{3F}^k, c_4^k, c_5^k) \tag{5b}$$

Adopted scheme of Monte Carlo modelling uses stratified sampling procedure LHS. Code HARP (more in (Pecha at al., 2009)) comprise interactive subsystem for generation of K LHS samples for various types of random distributions D_m of parameter vector $\Theta \equiv \{\Theta_1, \dots, \Theta_m, \dots, \Theta_M\}$. A certain technique for correlation control between components Θ_m is included. Resultant mapping of pairs of vectors is given by:

$$[\mathbf{x}_{Tr}^k ; \theta^k]_{k=1, \dots, K} \tag{6}$$

Trajectory \mathbf{x}_{Tr}^k is represented by N-dimension vector in N spatial nodes. Provided that the value of K is sufficiently high (several thousands), expression (6) offers right basis for:

- Uncertainty analysis (UA) – statistical processing of the pairs can determine extent of the uncertainty on predicted consequences and yield various statistics such sample mean and variance, percentiles of the uncertainty distribution on the quantity given, uncertainty factors, reference uncertainty coefficients etc.
- Sensitivity analysis (SA) – its strategies are applied depending on the settings (*Saltelli et al., 2001*) with further discrimination as factor screening (one-at-a-time experiments), local SA (partial derivations at a local point) and global SA (using typically sampling approach). Various techniques can be used providing different measures of sensitivity (scatterplots, regression and correlation analysis, rank transformations etc.).

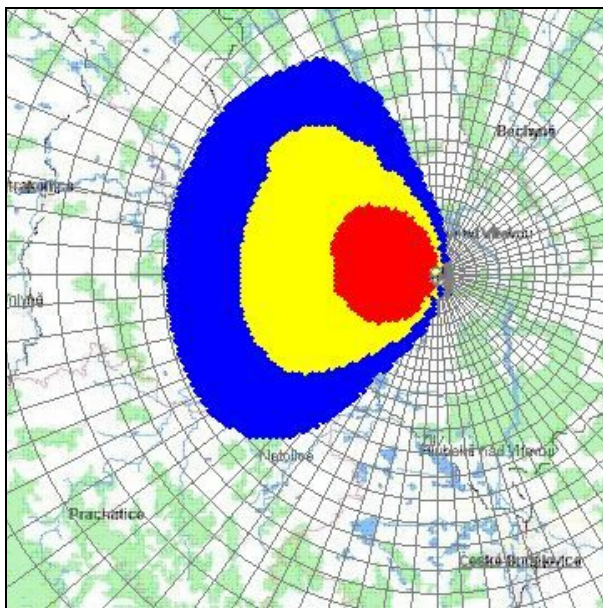


Figure 2: Sample mean from (6) (5000 samples) of random trajectories (5b) for $G=2, F=2$ (stands for just 2 hours after the release start). In contrast with deterministic Fig. 1 (right).

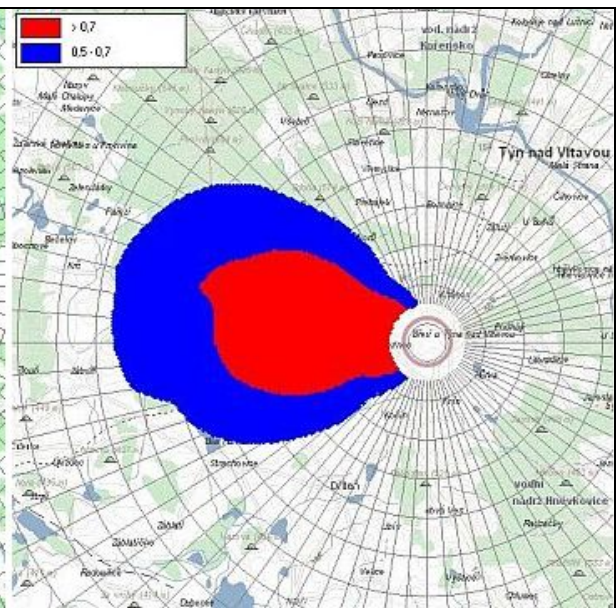


Figure 3: Illustration of probabilistic assesment based on sampling (6) from (5b), $G=2, F=2$. Isolines of probabilities of exceeding limit $1.0 \text{ E}+5 \text{ Bq.m}^{-2}$ (just 2 hours after start).

5. Particle filtering for data assimilation approach in the early stage of accident

Data assimilation represents the way from model to reality and can substantially improve the reliability of model predictions. Inevitable prerequisite for application of advanced statistical

assimilation techniques is foregoing UA which provides data for construction of covariance structure of model errors for a given release scenario.

Prospective intervention actions with purpose to avert radiation exposure of population have to be introduced with regard to the type of accidental release scenario and evolution of a failure at its all phases. Each phase is characterised by its own time scale, predominated irradiation pathways and specific countermeasures introduced for protection of persons. The DA process adapted in the later phases of accident was examined (e.g. Hofman et al., 2008, Pecha et al., 2008). Nonlinear high dimensional state-space model of early stage of an accident makes DA procedures much harder than in the later stages.

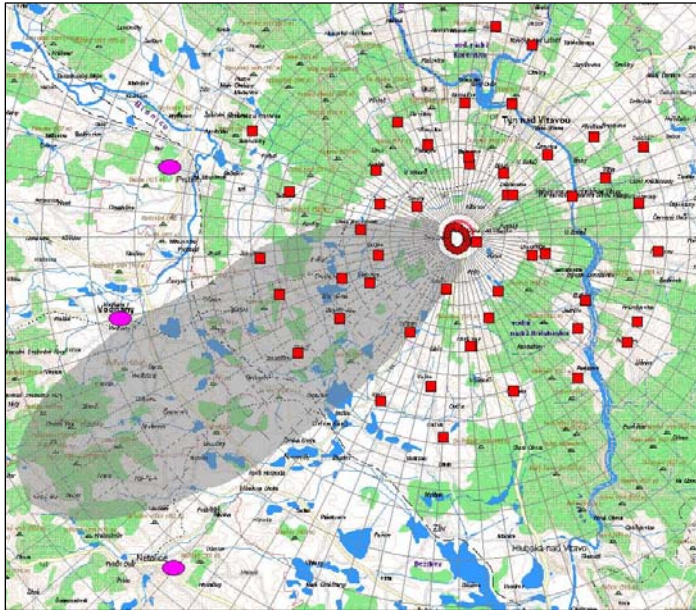


Figure 4: Part of the Early Warning Radiation Network of the Czech Republic around NPP Temelin.

- inner TDS on-fence
- outer sensors
- mobile stations

An attempt for real DA treatment requires further complementary ad hoc preconditions and developments, as follows. We shall assume conservatively a delay of two hours in recovery of radiation monitoring. The first measurements from terrain are coming just two hours after the release start. Because of a certain in-

consistency between meteorological forecast and measurements (see Table 3), the shape of the corresponding accidental trajectory close to the source should correspond more likely with observations. Without more discussion, we use this subjective assumption and generate the “artificial measurements” on basis of shadow contour in Fig. 4. It belongs to the “observation” trajectory **just 2 hours** after the release start:

$$\mathbf{x}_{Tr}^{obs} = \mathfrak{R}^{SGPM}(c_{11}^{obs}, c_{12}^{obs}, c_{21}^{obs}, c_{22}^{obs}, c_{31}^{obs}, c_{32}^{obs}, c_4^{obs}, c_5^{obs}) \quad (7)$$

The observations are simulated from the model using options $c_{11}^{obs} = c_{12}^{obs} = 0.5$; $c_{21}^{obs} = c_{22}^{obs} = 0.0$; $c_{31}^{obs} = c_{32}^{obs} = 1.0$; $c_4^{obs} = c_5^{obs} = 1.0$. Corresponding best estimate values are extracted from the Table 3 (for wind directions and speed those values in brackets). Similarly, the “best estimate” trajectory (deterministic short-term prediction) can be expressed as:

$$\mathbf{x}_{Tr}^b = \mathfrak{R}^{SGPM}(c_{11}^b, c_{12}^b, c_{21}^b, c_{22}^b, c_{31}^b, c_{32}^b, c_4^b, c_5^b) \quad (8)$$

where $c_{11}^b = c_{12}^b = 1.0$; $c_{21}^b = c_{22}^b = 0.0$; $c_{31}^b = c_{32}^b = 1.0$; $c_4^b = c_5^b = 1.0$.

The main achievement of investigations is integration of the trajectory model within the recursively repeated steps of Bayesian filtering. From all possible advanced DA techniques was chosen particle filtering (PF), which has one significant attribute convenient to our SGPM trajectory model: The ensemble of state trajectories (particles) remain unchanged during the data (observations) update step and only their weights are updated. Thus, the history of each path is not lost and the next time update is straightforward. The PF originating from the sequential Monte Carlo method is applied here for simulation of the posterior distribution of the system state. The 3-D trajectories represent the “particles” and during the resampling, those particles having small weights with regard to the measurements are eliminated.

Tracking in Bayesian concept insists in recursive evaluation of the state posterior probability density function (pdf) based on all available information. We shall mention how to launch the recursive procedure from the same beginning of the incomplete scenario described in APENDIX. The following tasks are executed:

- i) The assimilation process is initialized by determination of prior *pdf* (probability density function) $p(\mathbf{X}(t_1))$ where t_1 stands for just 2 hours after the release start. Let mention, that the sample mean in Fig. 2 and limits of exceeding in Fig. 3 can be now interpreted as expectations and other moments of the prior *pdf*.
- ii) Using measurements $\mathbf{y}(t_1)$ incoming from terrain just at t_1 , the marginal posterior density $p(\mathbf{X}(t_1) | \mathbf{y}(t_1))$ using Bayes rule and PF resampling algorithm is simulated. The expectations of the posterior distribution illustrated in Fig. 5 are evidently approaching close to the observation trajectory \mathbf{x}_{Tr}^{obs} from (7) used for simulation of artificial measurements (see also the shadow contour in Fig. 4).
- iii) Next state transition probability function $p(\mathbf{X}(t_2) | \mathbf{X}(t_1))$ describes the time update from the posterior *pdf* for t_1 forward to the next time t_2 , which means from hour 2 to hour 3 after the release start. The factors c_{23} and c_{33} are sampled, too.

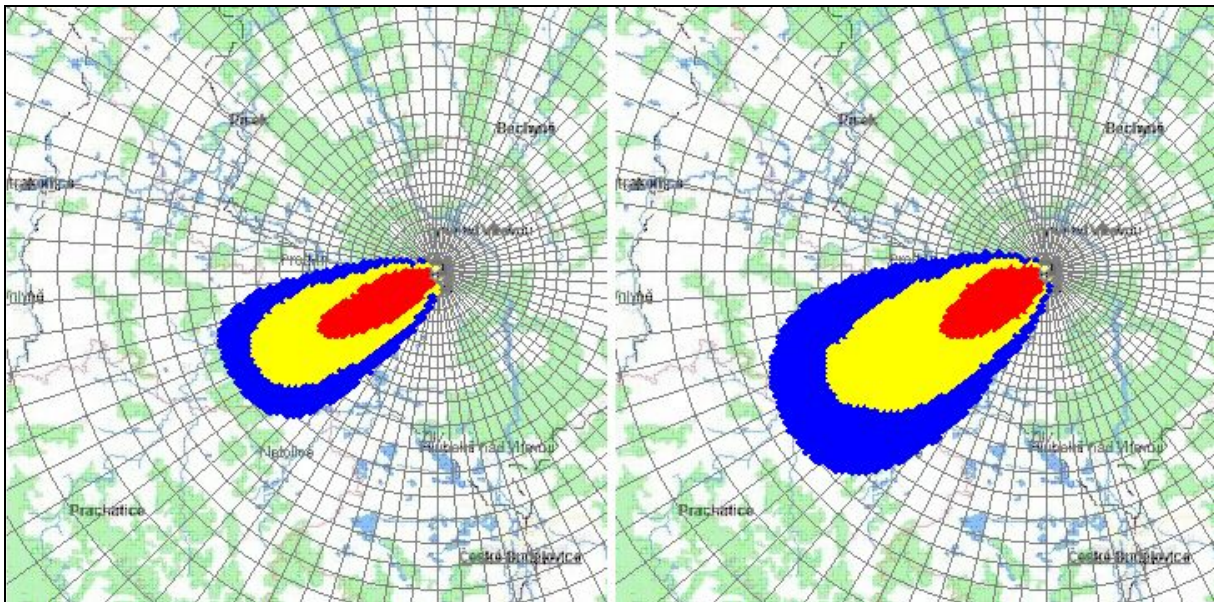


Figure 5: Expectations of posterior pdf - step ii): for small values of covariance matrix of measurements (left) and high values (less accurate measurements) – see: Pecha et al., 2009b.

Finally, after finishing step ii), the original model prediction (Fig. 2, right) is modified (Fig. 5). The step iii) of prolongation of *pdf* forward to the next time t_2 represents entry to the next time step of Bayesian recursion when posterior pdf is determined using observations incoming within the interval $\langle t_1 ; t_2 \rangle$, etc. More details are given in (Pecha et al., 2009b).

6. Persisting problems

Extensive computations have validated the presented methodology to be a proper tool for online Bayesian tracking of the toxic plume in its early phase of propagation. Ranking of the model parameters relevant for each respective step of recursion is evident from Tab. 2. Still open remain some questions on availability of online measurements. More attention should be devoted to detailed analysis of origin the model parameters that are so far predominantly related to the SGPM parametrization (see (3)). It is necessary to extract information about

SGPM algorithm imperfections itself provided that sufficiently informative measurements are available.

APPENDIX

Definition of a hypothetical accidental scenario with ambiguous characteristics

Real meteorological situation from March 31, 2009 is taken into consideration and the moment of a hypothetical accidental release is set to 10.00 UTC (see Table 3). Available real meteorological observations (in brackets) measured at the point of NPP and short term meteorological forecast are somewhat inconsistent. Following ex post analysis can give a retrospective view on the atypical actual situations (their occurrence rate is surprisingly not negligible).

Table 3: A hypothetical accidental release scenario of ¹³¹I , short-term meteorological forecast and real meteorological measurements (in brackets) for “point” of NPP Temelin (49°10'48.53"N × 14°22'30.93"E), time stamp 20090331-1000 CET.

CET hour	10.00	11.00	12.00	13.00
activity release of ¹³¹ I Bq/h	5.68 × e+14	7.92 × e+14	0	0
wind direction ^{1),2)}	95.0 (54.0)	101.0 (69.0)	84.0 (65.0)	80.0 (80.0)
wind speed ⁽¹⁾	2.0 (3.8)	2.1 (3.0)	1.9 (3.8)	2.2 (3.8)
Pasquill atm. stabil.	A	A	B	B

¹⁾ ... at 10 m heigh; ²⁾ ... blowing “from” (degrees measured clockwise from North)

ACKNOWLEDGEMENTS

This work is part of the grant project GAČR No. 102/07/1596, which is founded by Grant Agency of the Czech Republic. A lot of useful knowledge has been also acquired during RODOS customisation procedure for the Czech territory.

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