Data assimilation in early phase of radiation accident using particle filter

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1 Introduction

During the operation of a nuclear power plant, there is a potential for accidental release and dispersion of a nuclear material into ambient atmosphere and exposure of population to the ionizing radiation. The radiation dose received by the public as a consequence of a release comes mostly from five sources: External γ-radiation from the plume (cloud shine); external γ-radiation from radioactive material deposited on the ground, trees, buildings (ground shine); inhalation of radioactive material; external α, β and γ from radioactive material deposited on the skin and ingestion of contaminated foodstuff.

The time lapse of a nuclear release can be split into two major phases. The first phase, the early phase, covers the first few hours or days and lasts until the radioactive cloud has passed the area of interest. During this phase, the irradiation from cloud shine, ground shine, skin contamination and inhalation are most important. The second phase, the late phase, lasts until the radiation levels resumes back to levels of background. In this phase, dose from ground shine and ingestion becomes important. Negative impacts on population health are averted by the means of countermeasures introduced as soon as possible after or even before the expected release. These can be iodine prophylaxis, food bans, sheltering or evacuation.

The unavoidable condition for application of effective countermeasures is knowledge of spatial and temporal distribution of radioactive pollutants. Former accidents on nuclear facilities revealed unsatisfactory level of the decision support, both in hardware equipment (reliable communication channels, computation techniques) and also deficiencies in software decision support systems (DSS). Great attention to this topic is paid since the Chernobyl disaster. DSS is a software tool including a mathematical model for prediction of radionuclide spreading in the environment (Pecha et al. [2007]). It can embody different subsystems for evaluation of expected consequences in terms of demographic or economic statistics. Output from the system should provide to responsible authorities a rational basis for coordination of countermeasures (Rojas-Palma [2005]), (Pecha and Hofman).

Data assimilation is a way how to increase reliability of such predictions in both the early and the late phase of an accident (Smith and French [1993]). Recent development in hardware allows us to implement assimilation algorithms based on methods earlier computationally prohibited like sequential Monte Carlo methods (Hofman and Pecha [2008]). Marginalized particle filter (Schön et al. [2007]) was used here to estimate model error covariance structure in a parametrized form. Data assimilation is the optimal way how to exploit information from both the measured data and expert-selected prior knowledge to obtain reliable estimates. This paper studies exploitation of the data assimilation in the early phase of an accident when the radioactive cloud is passing over the terrain.

The outline of this paper is as follows. Problem statement is given in Section 2. Atmospheric dispersion model and methodology of calculation of cloud shine dose are described here. Section 3 briefly discusses particle filter and puts it in the scope of the Bayesian filtering. Section 4 presents a particular assimilation scenario and numerical experiment with simulated measurements. Conclusion and future work is given in Section 5.

2 Problem statement

Assume an accident in a nuclear power plant followed by aerial release of radionuclides. After the release, there is a radioactive cloud passing over the terrain. The spatio-temporal distribution of radionuclides is modeled by the means of numerical dispersion models in order to determine appropriate countermeasures. Output of such a model is a prediction of radiation situation given in terms of radiological quantities. Assume that the radiological quantity of interest is the continuous activity concentration in air $C(\boldsymbol{s},\, t)$, where $\boldsymbol{s} = (s_1,\, s_2,\, s_3)$ is a vector of spatial coordinates and $t = 1,\, \ldots,\, t_{\mathrm{MAX}}$ is the time index. Concentration of activity is important radiological quantity which can be used for calculation of some other quantities like deposition or doses from different pathways of irradiation. The concentration itself is a difficult quantity to measure, therefore the measuring devices are designed to measure the γ-dose rate. It has well developed measuring methodology. These measurements can be provided by stationary measuring sites or mobile groups (Pecha et al. [2008]).

For computational reasons, the continuous quantity $C(\boldsymbol{s},\, t)$ is evaluated only in a set of M points of a computational grid in time t. Values of $C(\boldsymbol{s}, t)$ in the grid points are aggregated in vector $\boldsymbol{C}_t$. The available measurements of time integrated γ-dose rate at time t are aggregated in vector $\boldsymbol{y}_t$. We can employ data assimilation and use the sparse measurements to improve reliability of model predictions and thus allow for introduction of effective countermeasures in the actually affected areas.

The evolution of $C(\boldsymbol{s},\, t)$ is modeled by a dispersion model which is parametrized by a set of parameters $\boldsymbol{\Theta}_t$. These parameters reflect physical processes involved in the atmospheric dispersion, atmospheric conditions and conditions of the accident in each time step t. Exact values of the parameters are uncertain due to stochastic nature of the dispersion, lack of accurate information, etc. Typically, the choice of values of these parameters is subject to an expert opinion. The subjective choice of parameter values can introduce significant errors into the predictions. To avoid this, we apply Bayesian approach and treat the parameters as random quantities. We attempt to estimate parameter distributions in consecutive time step from measurements. The number of parameters is potentially large but a restricted subset $\boldsymbol{\theta}_t \subset \boldsymbol{\Theta}_t$ of the most important parameters can be found for specific scenario (Pecha and Housa [2007]).

Since all uncertainty is modeled by probability distributions, the appropriate data assimilation methodology is the Bayesian filtering. The introduced scenario fits into the family of state-space models. Realization of the process at time t contains all the information about the past, which is necessary in order to calculate the prediction of future evolution. State vector $\boldsymbol{x}_t$ of the system comprises of the two components $\boldsymbol{x}_t = [\boldsymbol{C}_t, \boldsymbol{\theta}_t]^T$. The model of integrated γ-dose rate measurements $\boldsymbol{y}_t$ is given by the probability density function (pdf) $p(\boldsymbol{y}_t|\boldsymbol{x}_t)$.

2.1 Evolution of state

Evolution of the state is given by the transition pdf $p(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})$:

$$\begin{aligned} p(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) &= p(\boldsymbol{C}_t,\, \boldsymbol{\theta}_t|\boldsymbol{C}_{t-1},\, \boldsymbol{\theta}_{t-1}) \\ &= p(\boldsymbol{C}_t|\boldsymbol{C}_{t-1},\, \boldsymbol{\theta}_t,\, \boldsymbol{\theta}_{t-1})p(\boldsymbol{\theta}_t|\boldsymbol{C}_{t-1},\, \boldsymbol{\theta}_{t-1}) \end{aligned} \tag{1}$$

Under the choice of atmospheric dispersion model $C_{\mathrm{ADM}}(\boldsymbol{\theta}_t)$ and its parameters $\boldsymbol{\theta}_t$, the evaluation of $\boldsymbol{C}_t$ is deterministic:

$$p(\boldsymbol{C}_t|\boldsymbol{C}_{t-1},\, \boldsymbol{\theta}_t,\, \boldsymbol{\theta}_{t-1}) = \delta(\boldsymbol{C}_t - C_{\mathrm{ADM}}(\boldsymbol{\theta}_t)) \tag{2}$$

Time evolution of $\boldsymbol{\theta}_t$ is given by the pdf $p(\boldsymbol{\theta}_t|\boldsymbol{\theta}_{t-1})$. Under the choice of time invariant parameters ($\boldsymbol{\theta}_t = \boldsymbol{\theta}$), the transition pdf gets the form $p(\boldsymbol{\theta}_t|\boldsymbol{\theta}_{t-1}) = \delta(\boldsymbol{\theta}_t - \boldsymbol{\theta})$. The process is initialized with prior pdf $p(\boldsymbol{\theta}_0)$, typically covering wide range of possibilities.

We chose the Gaussian puff model (GPM) for the atmospheric dispersion model. It is based on approximative solution of the three dimensional advection-diffusion equation (Barrat [2001]):

$$C(\boldsymbol{s},\, t) = \frac{Q\, f_{\mathrm{D}}(t)\, R(t)}{(2\pi)^{\frac{3}{2}} \sigma_{s_1}\, \sigma_{s_2}\, \sigma_{s_3}} \exp\left\{ -\frac{1}{2} \left[\left(\frac{s_1\, -\, ut}{\sigma_{s_1}} \right)^2 + \left(\frac{s_2}{\sigma_{s_2}} \right)^2 + \left(\frac{s_3}{\sigma_{s_3}} \right)^2 \right] \right\}, \tag{3}$$

where t is time index, Q is the total released activity in Bq and u is the wind speed. Dispersion coefficients $\{\sigma_{s_i}\}|_{i=1,\,2,\,3}$ are functions of distance from the source. Factor $f_{\mathrm{D}}(t)$ stands for radioactive decay, dry and wet deposition. The last term $R(t)$ accounts for homogenization of the vertical profile of concentration due to the reflections from the top of mixing layer and the ground. See (Hofman et al.) for more details.

2.2 Measurement model

Measurements are assumed to be normally distributed and mutually independent given the state $\boldsymbol{x}_t$. Errors of measurements are set proportional to the their values with an offset term modeling the background radiation superposed to the actual dose measurements

$$\boldsymbol{y}_t \sim \mathcal{N}(\boldsymbol{D}_t,\, \boldsymbol{\Sigma}(\boldsymbol{D}_t)), \tag{4}$$

where $\mathcal{N}(\boldsymbol{a},\, \boldsymbol{\Sigma})$ is a multidimensional normal distribution with mean value $\boldsymbol{a}$ and a covariance matrix $\boldsymbol{\Sigma}$. $\boldsymbol{D}_t$ is a vector of measurements of time integrated absorbed γ-dose in all the measuring sites available in time t. If the released nuclide is a noble gas, there is no deposition and we don't have to assume ground shine from deposited material. In this case, the measured quantity is just the γ-dose from cloud shine. The time integral of absorbed γ-dose rate in tissue from a mixture of radionuclides emitting photons on different energy levels $E_{\gamma,j}$is

$$D_{i,t} = \int_{t-1}^{t} \sum_j \frac{K_j\, \mu_{a,j}\, E_{\gamma,j}}{\rho}\, \Phi_j(C(\boldsymbol{s}_{(i)}, \tau))\, d\tau, \tag{5}$$

where K_j, $\mu_{a,j}$ and Φ_j are conversion coefficient, absorption coefficient and effective flux of gamma rays, respectively. Subscript j stands for the fact, that the particular values depend on the energy level $E_{\gamma,j}$. Summation is over assumed energy levels and ρ is the mass density of air. Equation (5) defines the observation operator converting the concentration in $Bq\, m^{-3}$ to the time integrated γ-dose in Gy.

The general expression for Φ at a receptor located at $\tilde{\boldsymbol{s}} = (\tilde{s}_1,\, \tilde{s}_2,\, \tilde{s}_3)$ from a source of energy E_γ dispersed in air is

$$\Phi(\tilde{s}_1,\, \tilde{s}_2,\, \tilde{s}_3,\, E_\gamma) = \iiint \frac{f(E_\gamma) B(E_\gamma, \mu r) C(s_1,\, s_2,\, s_3)}{4\pi\, r^2}\, ds_1\, ds_2\, ds_3, \tag{6}$$

where $r^2 = (\tilde{s}_1 - s_1)^2 + (\tilde{s}_2 - s_2)^2 + (\tilde{s}_3 - s_3)^2$, $f(E_\gamma)$ is the branching ratio to the specific energy, μ is the attenuation coefficient of air, $B(E_\gamma, \mu r)$ is the dose build-up factor, $C(\boldsymbol{s})$ is the radionuclide concentration in $Bq\, m^{-3}$ of isotope being considered. The build-up factor can be calculated from Bergers analytical expression

$$B(E_\gamma, \mu\, r) = 1 + a\, \mu r\, \exp(b\, \mu r), \tag{7}$$

where coefficients μ, a and b depend on E_γ. Energy dependent absorption coefficient μ_a is calculated as

$$\mu_a = \mu / \left[1 + \frac{a}{(1-b)^2} \right]. \tag{8}$$

The simplicity of used Gaussian puff model (3) allows for numerical evaluation of integral (6) on a compact support where the concentration is not negligible. If the radioactive plume is large compared to the mean free path of the γ-rays, then the semi-infinite cloud approximation of effective flux can be successfully used. See (Overcamp and Fjeld [1987]) for more details.

3 Data assimilation

Bayesian approach to data assimilation is based on representing uncertainty in the state via probability distribution. When no measurements are available the probability distribution of the considered state (the prior) must be rather wide to cover all possible realizations of the state. Each incomming measurement bringins information about the 'true' state, reducing the original uncertainty. In effect, with increasing mesurements, the posterior pdf is narrowing down around the best possible estimate.

Formally, the prior distribution $p(\boldsymbol{x}_0)$ is transformed into posterior pdf $p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t})$ using measurements $\boldsymbol{y}_{1:t} = \{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_t\}$ by recursive repetition of the following steps:

$$p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t-1}) = \int p(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) p(\boldsymbol{x}_{t-1}|\boldsymbol{y}_{1:t-1}) d\boldsymbol{x}_{t-1} \tag{9}$$

$$p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t}) = \frac{p(\boldsymbol{y}_t|\boldsymbol{x}_t) p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t-1})}{\int p(\boldsymbol{y}_t|\boldsymbol{x}_t) p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t-1}) d\boldsymbol{x}_t}, \tag{10}$$

The process is initialized by prior $p(\boldsymbol{x}_0)$.

Evaluation of (9) and (10) involves integration over complex spaces and often it is computationally infeasible. Suboptimal solution can be found by the means of sequential Monte Carlo methods also known as particle filters (Doucet et al. [2001]). Particle filters numerically approximate posterior pdf $p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t})$ using a set of particles $\boldsymbol{x}_t^{(i)}$ and importance weights $w_t^{(i)}$ for $i = 1, 2, \ldots, N$:

$$p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t}) \approx \sum_{i=1}^{N} w_t^{(i)} \, \delta(\boldsymbol{x}_t - \boldsymbol{x}_t^{(i)}), \tag{11}$$

where $\delta()$ is the Dirac δ-function. The particles $\boldsymbol{x}_t^{(i)}$ are drawn from a proposal pdf $q(\boldsymbol{x}_t|\boldsymbol{y}_{1:t})$, which can be an arbitrary pdf the support of which includes the support of $p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t})$. Under this approximation, the integral equations (9)–(10) reduces to drawing new particles at each time t and simple re-evaluation of the importance weights:

$$w_t^{(i)} \propto w_{t-1}^{(i)} \frac{p(\boldsymbol{y}_t|\boldsymbol{x}_t^{(i)}) p(\boldsymbol{x}_t^{(i)}|\boldsymbol{x}_{t-1}^{(i)})}{q(\boldsymbol{x}_t^{(i)}|\boldsymbol{x}_{t-1}^{(i)}, \boldsymbol{y}_{1:t})}. \tag{12}$$

Here, $\propto$ denotes equality up to multiplicative constant. This constant can be easily computed to assure that $\sum_{i=1}^{N} w_t^{(i)} = 1$. Equation (12) can be further simplified to $w_t^{(i)} \propto w_{t-1}^{(i)} p(\boldsymbol{y}_t|\boldsymbol{x}_t^{(i)})$ by choosing $q(\boldsymbol{x}_t|\boldsymbol{y}_{1:t}) \equiv p(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})$.

The approximation is easily extendable for prediction. Predicted pdf of the state at time $t+k$ is then approximated as

$$p(\boldsymbol{x}_{t+k}|\boldsymbol{y}_{1:t}) \approx \sum_{i=1}^{N} w_t^{(i)} \, \delta(\boldsymbol{x}_{t+k} - \boldsymbol{x}_{t+k}^{(i)}), \tag{13}$$

where particles $\boldsymbol{x}_{t+k}^{(i)}$ are recursively generated from $p(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}^{(i)})$.

4 Numerical experiment

For purposes of numerical experiment was chosen assimilation scenario with an instantaneous release of ^{41}Ar. Numerical experiment is conducted as a twin experiment, where the measurements are simulated via a twin model and perturbed. Convergence of radiological quantity of interest—^{41}Ar activity concentration in air—evaluated on basis of estimated parameters to that produced by the twin model can be then assessed.

Since the argon is a noble gas, there is no deposition and consequently no ground shine. The released activity is propagated via Gaussian puff model, (3). Half life of decay of ^{41}Ar is 109.34 minutes. According to the TORI (Tables Of Radioactive Isotopes) database, there are more energy levels of γ radiation produced by isotope ^{41}Ar. We assume just the energy level $1293.57keV$ with the branching ratio 99.1%. The rest being included in the 0.9% is neglected and the summation over energy levels in (5) can be omited.

The topology of measuring sites is similar to that of the Early Warning Network of the Czech Republic (Pecha et al. [2008]). The source of simulated release is a nuclear power plant surrounded by almost fifty stationary measuring sites capable to measure time integrated γ-dose (5). Measuring sites are located more or less regularly in the area of radius 10km around the source. The time step of assimilation algorithm was set to 10 minutes and the time horizon t_{MAX}=6 (60min). Measuring devices are assumed to integrate the γ-dose in 10 minute intervals and then send measurements on-line to the quarters of crisis management. The height or release is $50m$ and the magnitude of release Q=1.0E+10Bq of ^{41}Ar. We assume no vertical velocity or any significant heat capacity of the effluent and the effective height remains $50m$ during the puff propagation. The time horizon spans up to 1 hour after the release start. It means, that we performed 6 assimilation cycles consisting of time and data update steps.

4.1 Parametrization of atmospheric dispersion model

A group of the most significant variables affecting the dispersion process (including meteorological inputs) was selected using available sensitivity and uncertainty studies performed on Gaussian dispersion models (Pecha and Housa [2007]). Variables of the dispersion model C_{ADM} treated in this numerical example as uncertain are: magnitude of release Q, horizontal dispersion coefficients $\sigma_{s_i}|_{i=1,2}$ and also two meteorological inputs: wind speed u and wind direction ϕ. Their parametrization via vector of random parameters $\boldsymbol{\theta}_t = (\omega_t, \xi_t, \psi_t, \zeta_t)$ and location parameters $(Q_0, u_0, \phi_0, \sigma_{s_{i0}}|_{i=1,2})$ is listed in Table 1. The parametrization was selected according to that in the UFOMOD code (Panitz et al. [1989]). Location parameters refer to the prior initialization of the variables. All the random parameters are treated as time constant: $\boldsymbol{\theta}_t = \boldsymbol{\theta}$, even the parameters ξ_t and ψ_t concerning uncertainty in meteorological forecast. In

variable	**physical effect**	**parametrization**
Q	magnitude of release	$Q = \omega_t\, Q_0$
u	wind speed	$u = (1 + 0.1\,\xi_t)\, u_0 + 0.5\,\xi_t$
ϕ	wind direction	$\phi = \phi_0 + \Delta\phi$, $\Delta\phi = \psi_t\,(2\pi/80)$ rad.
$\sigma_{s_i}\|_{i=1,2}$	horizontal dispersion	$\sigma_{s_i} = \zeta_t\, \sigma_{s_{i0}}\|_{i=1,2}$

Table 1: Parametrization of selected variables and inputs to the ADM.

case of time horizon of several hours, the assumption of stationarity of the meteorological condition vanishes. Parametrization of the meteorological data has to be fragmented into shorter time intervals (usually hourly intervals) where the assumption of stationarity holds.

The set of parameters $\boldsymbol{\theta}_{\mathrm{TWIN}}$ used for evaluation of the twin model simulating measurements is

$$\boldsymbol{\theta}_{\mathrm{TWIN}} = (0.72,\ -0.17,\ -8.3,\ 1.3). \tag{14}$$

The comparison of initial C_{ADM} inputs with the initial setting and the twin model is in Table 2. The real release was smaller in magnitude, with the lower wind speed, directed by approximately 37°anticlockwise and the puff dispersed more than was apriori assumed. Horizontal dispersion parameters σ_{s_1} and σ_{s_2} are functions of distance the from source. The total number of $N = 1000$ particles was initialized with random vectors $\{\boldsymbol{\theta}^{(i)},\ i = 1, \ldots, 1000\}$ with elements generated according to the pdfs in Table 3.

variable	**physical effect**	**prior val.**	**param. value**	**true value**
Q	released activity	1.0E+10Bq	0.72	7.2E+09Bq
u	wind speed	3.10m/s	-0.17	2.96m/s
ϕ	wind direction	310.0°	-8.3	272.7°
$\sigma_{s_i}\|_{i=1,2}$	horizontal disp.	$\sigma_{s_i} = \sigma_{s_i}(dist)\|_{i=1,2}$	1.3	$\sigma_{s_i} = 1.3\,\sigma_{s_i}\|_{i=1,2}$

Table 2: Values of variables of the initial model setting and the twin model.

parameter	**physical effect**	**pdf type**	**mean value**	**std. dev.**
ω_t	magnitude of release	log-normal	1.0	1.0 (3σ truncated)
ξ_t	wind speed	uniform	0.0	1.0
ψ_t	wind direction	uniform	0.0	10.0
ζ_t	horizontal dispersion	log-normal	1.0	1.0 (3σ truncated)

Table 3: Prior distributions of estimated parameters $\boldsymbol{\theta}_t = (\omega_t,\ \xi_t,\ \psi_t,\ \zeta_t)$.

4.2 Results

The results are visualized in terms of the time integral of ground level concentration of activity in air (TIC):

$$TIC(\boldsymbol{s}) = \int_{0}^{t_{\mathrm{MAX}}} C(\boldsymbol{s},\ \tau)\, d\tau. \tag{15}$$

Computational grid is a rectangular grid of dimension 41×41 grid points with the grid step $1km$. The source of pollution is placed in the center of the grid.

In Figure 1 left we can see the TIC evaluated by the atmospheric dispersion model without the data assimilation and with initial setting of variables $Q = Q_0$, $u = u_0$, $\phi = \phi_0$ and $\sigma_{s_i}|_{i=1,2} = \sigma_{s_{i0}}|_{i=1,2}$. This is done by setting $\boldsymbol{\theta} = (1.0, 0.0, 0.0, 1.0,)$, see Table 1. In Figure 1 right is the TIC evaluated by the twin model used for simulation of measurements. In Figure 2 are visualized assimilation results. Assimilation results are presented in the form of expected value of TIC with respect to the predictive densities at different time steps. Expected value of prediction of TIC displayed in Figure 2 top left are based only on the measurements $\boldsymbol{y}_1$. Even at this stage, the wind direction was correctly recognized, however other parameters, such as parametrization of Q, are still too uncertain and the prediction differs from the twin model.

With increasing time the measurements provide enough information and the expected values of TIC are converging to the twin model.

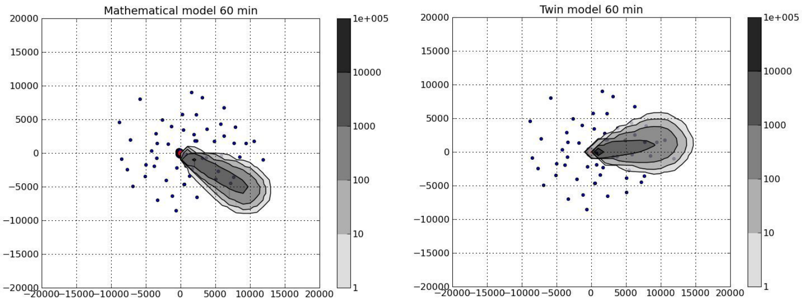

Figure 1: Predicted TIC based on initial values without the data assimilation (left) and the twin model (right).

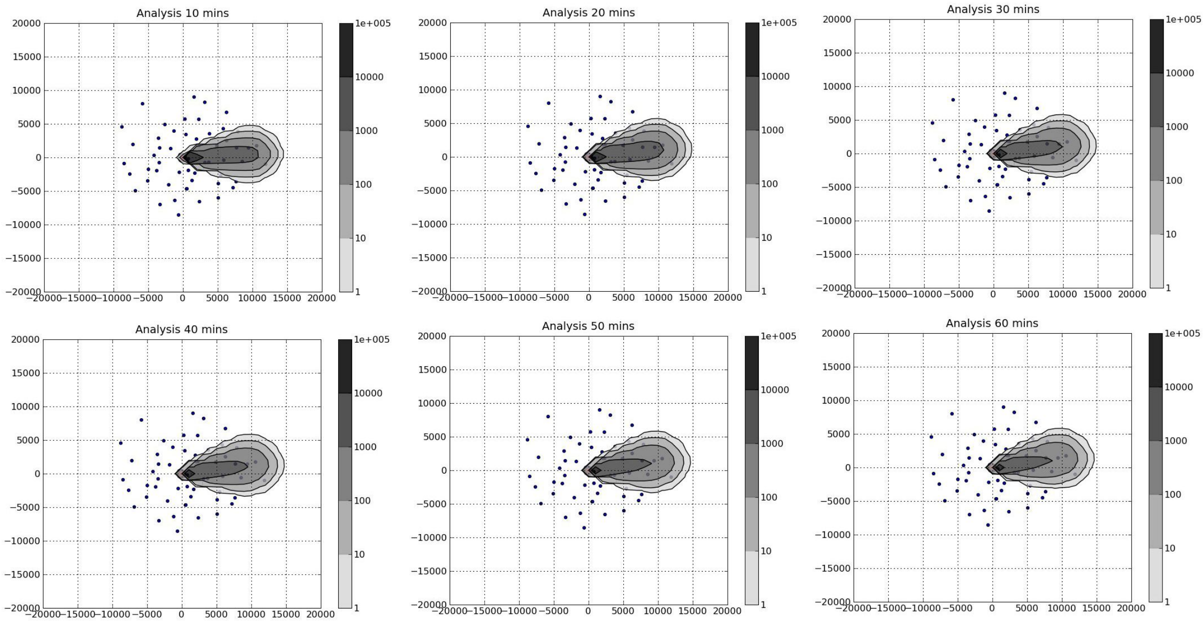

Figure 2: Predicted TIC based on assimilation at $t = 1, 2, 3, 4, 5, 6$, respectively.

5 Conclusion

Rapid assessment of the situation in case of an aerial release of radionuclides is crucial for planning of countermeasures. Introduced Bayesian methodology has very interesting properties suitable for this scenario. Specifically, it allows joint estimation of spatio-temporal distribution of activity and parameters of the dispersion model. Thus, we obtain assimilated estimate of the radiation situation on the terrain and a way how to easily extend this estimates to predictions on an arbitrary horizon. The presented scenario clearly illustrates the power of the method. However, a lot of work is required to incorporate the method to the existing decision support systems. We foresee the core of the work in development of more realistic models of the state evolution and the measurements. For example, more realistic scenarios should consider a mixture of radionuclides and extended set of uncertain variables. Such extension of the model inevitably increases complexity of the implied algorithm which may lead to computational difficulties. These may be overcome with exploitation of recent developments in the filed of sequential sampling, such as adaptive resampling or problem specific proposal densities.

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