On-line estimation of dispersion model parameters using particle filter

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Introduction

After an accident in a nuclear power plant, 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 quantity *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. The concentration itself is a difficult quantity to measure, therefore the measuring devices are designed to measure the γ-dose rate. These measurements can be provided by stationary measuring sites or mobile groups.

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 [4].

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.

We have:

- Atmospheric dispersion model (ADM) C_{ADM} modeling $C(\boldsymbol{s}, t)$ in a set of grid points – vector $\boldsymbol{C}_t$
- Measurements of time integrated γ-dose rate at time t – vector $\boldsymbol{y}_t$
- ADM is a function of parameters and inputs $C_{\mathrm{ADM}} = C_{\mathrm{ADM}}(\boldsymbol{\Theta})$
- A group of most significant parameters $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ is modeled as random due to the stochastic nature of the background physics

We want to:

- On-line estimate the state $\boldsymbol{x}_t = [\boldsymbol{C}_t, \boldsymbol{\theta}_t]^T$as the cloud is passing over stationary measuring sites
- Use posterior distribution $p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t})$ to predict future evolution of the radiation situation $p(\boldsymbol{x}_{t+k}|\boldsymbol{y}_{1:t})$

Background physics

Evolution of state

We chose the Gaussian puff model (GPM) for the ADM. It is a statistical approximation of solution of the three dimensional advection-diffusion equation:

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

where $\boldsymbol{s}$ is spatial location, t is time index, Q is the total released activity in Bq, u is the wind speed, $\{\sigma_{s_i}\}|_{i=1,2,3}$ are dispersion coefficients, $f_{\mathrm{D}}(t)$ is factor of radioactive decay, dry and wet deposition. Term $R(t)$ accounts for homogenization of the vertical profile of concentration due to the reflections. Evolution of the state is given by the transition pdf:

$$\begin{aligned} p(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) &= p(\boldsymbol{C}_t, \boldsymbol{\theta}_t|\boldsymbol{C}_{t-1}, \boldsymbol{\theta}_{t-1}) \quad (2)\\ &= p(\boldsymbol{C}_t|\boldsymbol{C}_{t-1}, \boldsymbol{\theta}_t, \boldsymbol{\theta}_{t-1}) p(\boldsymbol{\theta}_t|\boldsymbol{C}_{t-1}, \boldsymbol{\theta}_{t-1}) \end{aligned}$$

Under the choice of ADM and its parameters $\boldsymbol{\theta}_t$, the evaluation of $\boldsymbol{C}_t$ is deterministic:

$$p(\boldsymbol{C}_t|\boldsymbol{C}_{t-1}, \boldsymbol{\theta}_t, \boldsymbol{\theta}_{t-1}) = \delta(\boldsymbol{C}_t - C_{\mathrm{ADM}}(\boldsymbol{\theta}_t)) \quad (3)$$

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 $p(\boldsymbol{\theta}_0)$.

Observation operator

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

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

where $\boldsymbol{D}_t$ 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

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

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 certain 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

$$\Phi(\tilde{\boldsymbol{s}}, E_\gamma) = \iiint \frac{f(E_\gamma) B(E_\gamma, \mu r) C(\boldsymbol{s})}{4\pi\, r^2}\, d\boldsymbol{s}, \quad (6)$$

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

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

where coefficients μ, a and b depend on E_γ.

Data assimilation

Bayesian approach to data assimilation is based on representing uncertainty via probability distribution. When no measurements are available the probability distribution of the considered state (the prior) is wide to cover all possible realizations of the state. Each incoming measurement is bringing information about the "true" state, reducing the original uncertainty. In effect, with increasing number of measurements, 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:

$$p(\boldsymbol{x}_t|\boldsymbol{y}_{1:t-1}) = \int p(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) p(\boldsymbol{x}_{t-1}|\boldsymbol{y}_{1:t-1}) d\boldsymbol{x}_{t-1} \quad (8)$$

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

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

Evaluation of (8) and (9) 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 [1].

Assimilation scenario

Numerical experiment is conducted as a *twin experiment*: 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.

The topology of measuring sites is similar to that of the Early Warning Network of the Czech Republic [5]. The time step of assimilation algorithm is 10 minutes and the time horizon t_{MAX}=6 (60min). Measuring devices are assumed to integrate the γ-dose in 10 minute intervals.

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 [4]. 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.

variable	parametrization
Q – released activity	$Q = \omega_t\, Q_0$
u – wind speed	$u = (1 + 0.1\,\xi_t)\, u_0 + 0.5\,\xi_t$
ϕ – wind direction	$\phi = \phi_0 + \psi_t\, (2\pi/80)$ rad
$\sigma_{s_i}|_{i=1,2}$ – dispersion	$\sigma_{s_i} = \zeta_t\, \sigma_{s_{i0}}|_{i=1,2}$

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

The comparison of initial C_{ADM} inputs with the initial setting of the twin model is in Table 2. The "real" release is smaller in magnitude, with the lower wind speed, directed by approximately 37deg anticlockwise and the puff disperses more than we apriori assumed.

variable	prior value	par. value	true value
Q	1.0E+10Bq	$\omega_t = 0.72$	7.2E+09Bq
u	3.10m/s	$\xi_t = -0.17$	2.96m/s
ϕ	310.0deg	$\psi_t = -8.3$	272.7deg
σ_{s_i}	$\sigma_{s_i} = \sigma_{s_i}(dist)$	$\zeta_t = 1.3$	$\sigma_{s_i} = 1.3\,\sigma_{s_i}$

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

Numerical experiment

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

$$TIC(\boldsymbol{s}) = \int_0^{t_{\mathrm{MAX}}} C(\boldsymbol{s}, \tau)\, d\tau. \quad (10)$$

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 choosing $\boldsymbol{\theta} = (1.0, 0.0, 0.0, 1.0,)$, 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.

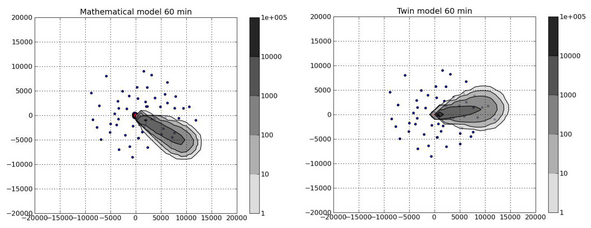

Figure 1. Predicted TIC based on initial values without the data assimilation (left) and the twin model (right).

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 converge to the twin model.

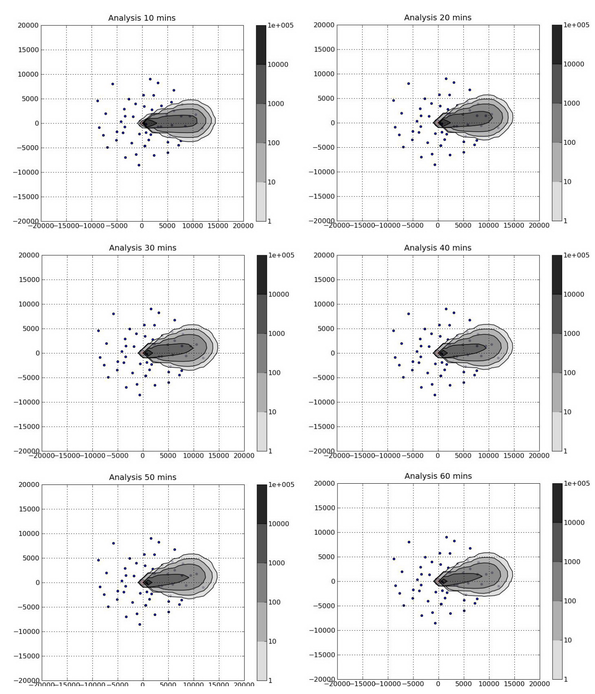

Figure 2. Predicted TIC based on assimilation at $t = 1, 2, 3, 4, 5, 6$, respectively.

Conclusion and future work

The presented scenario clearly illustrates the power of the method. Introduced Bayesian methodology has very interesting properties suitable for this scenario:

- It allows joint estimation of spatio-temporal distribution of activity and parameters of the dispersion model
- We obtain assimilated estimates of the radiation situation on the terrain
- Method provides a way how to easily extend this estimates to predictions on an arbitrary horizon

However, a lot of work is required to incorporate the method to the existing decision support systems:

- Development of more realistic models of the state evolution and the measurements
- More realistic scenarios should consider a mixture of radionuclides
- Extended set of uncertain variables should be considered

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