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ASSIMILATION OF GAMMA DOSE RATE AND CONCENTRATION MEASUREMENTS IN LAGRANGIAN MODEL DIPCOT

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Abstract: The variational method of data assimilation (DA) of gamma dose rate measurements in Lagrangian atmospheric dispersion model DIPCOT is presented which allows for source function correction. The method is suitable both for 'puff' mode of DIPCOT calculations and for stochastic mode, with stochastic equations of particle's movement. The DA method is validated against the field experiment on Ar-41 atmospheric dispersion.

***Key words:** inverse problems, atmospheric dispersion model, fluence rate.*

INTRODUCTION

Real-time nuclear emergency response systems (ERSs) calculate atmospheric dispersion and fallout following the accidental release of radioactivity using the atmospheric dispersion models (ADMs). In emergency phase estimated source term can differ from the true one by the factor of 10 and more (US NRC, 1990) and therefore uncertainty in source term dominates among all other sources of uncertainty. One possibility of improving source rate information is data assimilation (DA) of gamma dose measurements which are typically available around every nuclear power plant. The Kalman Filtering (KF) approaches are most widely used for that purpose. In previous works (Astrup, *et al.*, 2004, Zheng, *et al.*, 2010) the KF approach had been combined with different kinds of ADMs for source rate correction with assimilation of gamma dose measurements. Despite it's definite advantages KF approach is a computationally expensive procedure, and that circumstance becomes even more important in case of large deviations of the first guess estimation of source function from the true one. On the other hand variational approach to data assimilation which was extensively used in cases of source function correction with concentration measurements (e.g., Enting, 2002, Jeong, 2008, Bocquet, 2005) had been rarely applied for source function correction with DA of gamma dose measurements. In the present work the variational method of data assimilation is combined with Lagrangian puff model DIPCOT (Andronopoulos, *et al.*, 2009), which is used in EU nuclear ERS RODOS. The data assimilation algorithm is described. It's application to source function correction by assimilation of fluence rate measurements in field experiment on Ar-41 atmospheric dispersion in Mol, Belgium (Drews, *et al.*,2002) is presented. The comprehensive description of the method and results, presented here can be found in Tsiouri, *et al.* (2010).

DATA ASSIMILATION ALGORITHM

DIPCOT (Andronopoulos, *et al.*, 2009) is a 3D air pollution model, which simulates atmospheric dispersion estimating puff's trajectories. Puffs are transported by average wind field (puff mode) and optionally by stochastic wind field fluctuations (stochastic mode). Concentration C at an arbitrary spatial point of the 3D domain (x,y,z) at time t is calculated as sum of contributions of all puffs:

$$C(x,y,z,t)=\frac{1}{(2\pi)^{3/2}}\sum_{i=1}^{N_p}\frac{q_i\tau\cdot\gamma(t,\tau,p)\cdot\exp\left(-\lambda\left(t-(i-1)\tau\right)\right)}{\sigma_{xi}\sigma_{yi}\sigma_{zi}}\exp\left[-\frac{1}{2}\frac{(x_i-x)^2}{\sigma_{xi}^2}\right]$$
$$\exp\left[-\frac{1}{2}\frac{(y_i-y)^2}{\sigma_{yi}^2}\right]\cdot\left\{\exp\left[-\frac{1}{2}\frac{(z_i-z)^2}{\sigma_{zi}^2}\right]+\exp\left[-\frac{1}{2}\frac{(z_i+z-2z_g)^2}{\sigma_{zi}^2}\right]\right\}, \quad (1)$$

Here N_p is the total (maximum) number of puffs, (x_i,y_i,z_i) are coordinates of i-th puff, z_g is ground height above sea level, τ is time interval between releases of puffs, q_i is the release rate corresponding to the time appearance of the i-th puff, σ_{xi},σ_{zi} are the parameters characterising the spatial distribution in the puff and the function $\gamma(t,\tau,i)=\mathrm{sgn}(t-i\cdot\tau)$ eliminates the influence of non-existing puffs. The last multiplier in (1) accounts for the radioactive decay with λ being the decay constant and with time t calculated from the start of release. Total reflection of the cloud from the underlying surface is assumed in (1). Two options are available in DIPCOT for calculation of the gamma dose rate: 'infinite cloud' approximation and method of Gorshkov (1995) which transforms three-dimensional integral to one-dimensional.

Consider the problem of modelling atmospheric dispersion on time interval $(0,T)$. Assume that during that interval measurements are available from K measurement stations located in spatial points $\overline{r}^k=\left(x^k,y^k,z^k\right)^T$, $1\le k\le K$. Assume also that the source of release acts during time interval $(0,T_s)$, $T_s\le T$. Denote gamma dose rates, measured at time t by the k-th station as $d_k^o(t)$. The available measurements during interval $(0,T)$ can be used to improve the source function information thus to improve the modeling results. The adjustable parameters in the assimilation procedure compose the control vector $\bar{\psi}$ which consists of source rates corresponding to times of releases of puffs: $\bar{\psi}^T = \left(q_1,...,q_{N_p}\right) = \bar{q}^T$. The problem of data assimilation can be posed as an optimal control problem of minimizing the following objective function with respect to control vector $\bar{\psi}$ (Dhall, *et al.*, 2006):

$$J = J_1 + J_2,\ J_1 = \left(\bar{\psi} - \bar{\psi}^B\right)^T \underline{\underline{O}}^{-1} \left(\bar{\psi} - \bar{\psi}^B\right)$$
$$J_2 = \sum_{n=1}^{N_O} \sum_{k=1}^{K} \left(d_k^o\left(t_n\right) - \tilde{d}\left(\bar{r}^k\right)\right)^2 = \left(\bar{d}^o - \underline{\underline{G}}\bar{\psi}\right)^T \underline{\underline{B}}^{-1} \left(\bar{d}^o - \underline{\underline{G}}\bar{\psi}\right) \quad . \qquad (2)$$

Here $\bar{\psi}^B$ is first guess estimation of the control vector, $\underline{\underline{O}}$, $\underline{\underline{B}}$ are covariance matrices of the errors of observations and background errors respectively; vector $\bar{d}^o \in R^{N_O K}$ consists of gamma dose rates $d^o(n,k)$, measured on each subinterval Δt_n by k-th station. The elements of d^O are ordered sequentially as follows: $d_l^o = d_{(n-1)K+k}^o = d^o\left(n,k\right)$. The corresponding vector that consists of the calculated dose rates at the K stations at the N_o time intervals is denoted by $\bar{d}^M = \underline{\underline{G}}\bar{\psi}$, where matrix $\underline{\underline{G}}$ of the size $\left(N_o \cdot K \times N_p\right)$ is formally introduced relating $\bar{d}^M$ and $\bar{\psi}$. Thus the minimization of function (2) is a linear regression problem with constraint: $\bar{\psi} \geq 0$. In the present work covariance matrices are assumed to be diagonal with constant observation error σ_O^2 and background error σ_B^2. Those error parameters entering can reflect physical information concerning quality of measurements and of a priori information about background estimations of adjusted parameters. Alternatively since solution of minimization problem obviously depends on only one parameter $\sigma^{-1} = \sigma_B^2 / \sigma_O^2$ it can be tuned using different heuristics methods.

As it immediately follows from (1) concentrations at given set of points are linearly related to vector $\bar{q}$: $\bar{c} = \underline{\underline{G}}^c \bar{q}$. In case of infinite cloud approximation gamma dose rate is simply proportional to concentration in a given point, thus matrix $\underline{\underline{G}}$ can be computed simply by multiplication of the matrix $\underline{\underline{G}}^c$ on constant: $\bar{d} = \underline{\underline{G}}\bar{q} = c_{\inf} \underline{\underline{G}}^c \bar{q}$ where value of constant is easily obtained from the relationships presented in (Andronopoulos, et.al., 2010). In case of dose rate calculation method of Gorshkov (1995), computation of matrix $\underline{\underline{G}}$ is performed using more complex relation, which follows from formulas of Gorshkov (1995) and is explained in detail in Tsiouri, et.al. (2010).

The number of puffs in DIPCOT code is usually large enough. Puffs are released every 1-10 s, or so. Thus the dimension of optimization problem can become very large when data assimilation is performed in straightforward way. As it will be shown in the next section this can leed to poor performance of data assimilation. Another problem arises in case of stochastic particle mode of DIPCOT operation. In that case elements of matrix $\underline{\underline{G}}$ become random values (i.e, the same element in different runs can have different value). Up to date in case of stochastic Lagrangian ADMs variational methods had not been used, because traditional variational data assimilation approach deals with deterministic differential equations. Both the abovementioned problems can be solved with the simple 'control vector reduction' (CVR) procedure which was theoretically investigated in the context of variational data assimilation in Kovalets (2009).

Assume that during small enough interval Δt source function can be considered as constant with sufficient accuracy. In operational practice of ERSs values of $\Delta t \sim 10^3 \div 10^4 s$ are used most often. At the same time DIPCOT uses significantly smaller time step τ between appearances of neighbor particles (1-100 s) so that $\Delta t / \tau = \Pi >> 1$. Then particles could be joined in $P = N_p / \Pi$ groups with Π particles in each group being characterized by the same source function: $q_{(j-1)\Pi+1} = q_{(j-1)\Pi+2} = ... = q_{j\Pi} = \tilde{q}_j, 1 \leq j \leq P$. Here $\tilde{q}_j$ are the values characterizing source function of the $j-th$ group of particles, which form the reduced control vector: $\underline{\tilde{q}}$ of the size P.

Instead of initial problem of minimization of (2) with control vector $\bar{q}$ consisting of release rates corresponding to each puff the 'reduced' minimization problem will be solved in which the same function is minimized with respect to the reduced control vector $\underline{\tilde{q}}$. The $\underline{\underline{G}}^r$ matrix of the reduced minimization problem has size $\left(N_o K \times P\right)$. Formula for calculating the elements of the $\underline{\underline{G}}^r$ matrix from the elements of the $\underline{\underline{G}}$ matrix can be easily obtained:

$$g_{lj}^r = \sum_{m=1}^{\Pi} g_{l((j-1)\Pi+m)},\ \forall l, 1 \leq l \leq N_o K, 1 \leq j \leq P . \qquad (3)$$

Thus, when distributions of random variables g_{lp} satisfy conditions of Central Limit Theorem (Shiryaev, 1996) which are in fact quite non-restrictive and with large enough Π, sums in (3) converge to stable values. As it was discussed in (Kovalets, 2009), that circumstance allows for using of the variational data assimilation method with CVR also in case of stochastic

Lagrangian particle models. As it will be demonstrated below another important advantage of using CVR is increase in computational efficiency and accuracy because of reducing the size of the control vector by the factor of Π. The described above DA procedure had been implemented in DIPCOT code. Matrix $\underline{\underline{G}}$ is calculated during forward run mode and cost function (2) is minimized with using the IMSL ® package.

RESULTS OF CALCULATIONS

An atmospheric dispersion experiment by (Drews, *et al.*, 2002) was carried out at the BR1 research reactor in Mol, Belgium, in October 2001. In the experiment, artificial smoke was released from the 60-m reactor stack together with the routine emission of ^{41}Ar. The measurements included: a) measurements of the ^{41}Ar source term originating from the emission stack of the BR1 research reactor; b) meteorological measurements by weather mast; c) the monitoring of the gamma radiation field from the decay of ^{41}Ar. The meteorological measurements were available every 10 minutes and included wind speed measurements at heights 69 m and 78 m, wind direction at 69 m, temperatures at 48 m and 78 m.

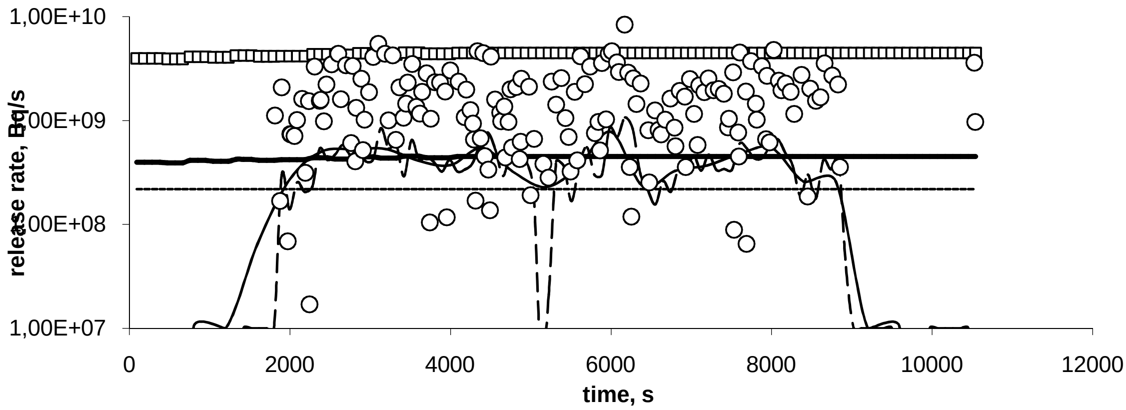

Figure 1. Source function (s.f.) estimations as result of fluence rate assimilation performed for conditions of Mol experiment , 3rd of October 2001. Method of Gorshkov (1995) had been used. Thick black line – true s.f., square symbols – first guess estimation of s.f., circles – results of DA run with P=999, dashed line – results of DA run with P=111, thin solid line – results of DA run with P=27, dotted line – results of DA run with P=1.

Table 1. Normalized mean square errors and fractional biases calculated on the basis of DTU-HPGe sensor which was not used in DA. Cases of forward run with first guess s.f., as well as cases with different values of CVR parameter (P) are presented. Zero value for 'Dose calculation method' correspond to infinite cloud approximation, alternatively method of Gorshkov (1995) had been used. Non-zero value for 'Stochastic mode' of calculations correspond to stochastic mode, while zero value correspond to puff mode of calculations.

Case	Stochastic mode of calc.	Dose calculation method	NMSE	FB
First guess	0	0	18.2	1.75
DA, P=27	0	0	0.87	-0.52
DA, P=9	0	0	1.05	-0.58
DA, P=1	0	0	0.83	-0.76
First guess	0	1	8.9	1.03
DA, P=27	0	1	0.52	-0.36
DA, P=9	0	1	0.6	-0.4
DA, P=1	0	1	0.5	-0.6
First guess	1	0	29.2	1.35
DA, P=27	1	0	12.0	-1.72
DA, P=9	1	0	8.81	-1.63
DA, P=1	1	0	5.44	-1.42
First guess	1	1	19.2	1.13
DA, P=27	1	1	6.01	-1.45
DA, P=9	1	1	4.29	-1.33
DA, P=1	1	1	1.24	-0.58

The calculations had been performed for the case of experiment on Wednesday afternoon, 3rd of October 2001. Four NAI sensors of Danish Emergency Management Agency (DK-NAI) had been used in data assimilation procedure. Data of Germanium detector of Technical University of Denmark (DTU-HPGe) had been remained for independent comparisons. Two sets of simulations had been performed – using the semi-infinite cloud approximation in calculations of the fluence rate and using the method of Gorshkov (1995). Also the calculations with both stochastic and puff mode of DIPCOT operation had been performed. The first guess source function was set by the factor of 10 greater than the true source function. The value of $\sigma = 10^{-9}$ had been used in all DA runs. Different number of groups (parameter P of CVR procedure) had been used in different runs. The total number of puffs had been set to $N_p = 999$ with time interval between puffs $\tau = 10.5\,s$ and thus the maximum value of P was 999.

Figure 1 presents examples of source function estimations as result of fluence rate assimilation. As it is seen from the figure in the case of $P = 999$ the source function is very poorly adjusted with the DA procedure. However results substantially improve with decreasing P and the adjusted source functions in those cases are much better than the first guess source function.

Table 1 present normalized mean squared errors (NMSE) and fractional bias errors (FB) calculated in first guess runs and for different DA cases on the basis of comparisons with the data of DTU-HPGe sensor. As compared to the first guess runs, DA runs in all cases significantly (by the factor of more than 10 for NMSE and by the factor of up to 3 for FB) improve the accuracy of calculations. Results of data assimilation runs with gamma dose calculation method of Gorshkov (1995) are significantly better than the results obtained with the simpler infinite cloud approximation. Results obtained in DA runs with stochastic mode of DIPCOT operation are worse than the results obtained with the puff mode. However, as it was shown by additional analysis, that fact reflects the relative merits of the turbulence parameterization, but not the drawbacks of the data assimilation method, which is equally suitable for both puff and stochastic mode of calculations. However, as follows from the results presented in Table 1 in stochastic mode the results of data assimilation runs are more sensitive to the value of control vector reduction parameter P, and generally decrease with decreasing P down to P=1. Such strong dependence on P possibly could be overcome by increasing the number of puffs in simulations.

CONCLUSIONS

The efficient algorithm is developed which allows for source function adjustment with data assimilation of gamma dose measurements in the framework of Lagrangian puff atmospheric dispersion model DIPCOT. The proposed control vector reduction allows for substantial improvement in numerical efficiency and accuracy of the data assimilation method and makes it possible to use the developed method also in the framework of stochastic Lagrangian atmospheric dispersion model. The developed method is successfully validated against the measurements in field experiment on atmospheric dispersion of Ar-41.

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