# Real time solution of forward and inverse air pollution problems with a numerical dispersion model based on short-term weather forecasts

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## Introduction

One of demanding applications of the short-term weather forecast is a real-time emergency modelling of nuclear and chemical hazardous events. Current paper presents an operational system developed in FMI in co-operation with other institutes and authorities aimed at short-term forecast of the potential areas of risk in case of accidents at the nuclear power plants.

In addition to the operational emergency forecasts, the developed framework has shown capability to address various inverse problems appearing when the actual source of the observed pollution episode is unknown.

## Forward and inverse problems of atmospheric dispersion

Classical atmospheric dispersion problem is based on certain information about an emission source and an emitted substance. Minimum source description includes its location and time variation of the emission rate. In some cases extra details like a source height, fractionation and temperature of the exhaust fumes can be also provided. Information about the emitted species includes their chemical and physical properties, phase state (gas, aerosol), etc.

Using the above information and meteorological data from an NWP model it is possible to solve the atmospheric transport and transformation equation and obtain the time- and space-resolved distribution of the pollutants.

Such problem can be classified as a forward one. In general case the transport equation can be written in a form of advection-diffusion equation with additions reflecting chemical and physical transformations, removal of species by deposition, and their emission from the source:

**( 1)**

$$L\varphi \equiv \frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x_i}(u_i \varphi) - \frac{\partial}{\partial x_i} \mu_{ii} \frac{\partial \varphi}{\partial x_i} + \sigma \varphi = f$$

Here $\varphi$ is unknown distribution function (usually, concentration), $u_i$ is a wind component in *i-th* direction, $i=1,2,3$; $\mu_{ii}$ is a semi-empirical turbulent diffusion coefficient in *i-th* direction; $\sigma$ represents all sorts of sink mechanisms for particular species – deposition, chemical transformations, sorption/desorption, radioactive decay, etc. Finally, $f$ is the emission intensity. Denoting this differential functional as $L$ one can write the equation in a short form:

**( 2)**

$$L\varphi = f$$

Boundary conditions for the emergency modeling problem are usually set to zero:

**( 3)**

$$\varphi(t=0) = 0; \;\; \varphi(\partial D) = 0$$

where ∂D is a boundary of the calculation domain D. In more general case these conditions can be set to some non-zero functions.

It is worth mentioning that the functional $L$ in ( 1) - ( 2) is linear, which does not always correspond to reality. However, below we shall explicitly use the linearity feature, so it has to be assumed at the very beginning. The non-linear dependencies, if any, can be linearised at every point of the phase space with further application of the below formalism. For the forward problem this step is not necessary because the equation ( 1) can be solved numerically in a straightforward way also in the non-linear case.

The solution of the transport equation ( 1) – the function $\varphi$ - is often inconvenient for the risk assessments. Usually, a more convenient parameter is a load, which can be computed from $\varphi$ with some weight (or sensitivity) function $p$. Physically it means that pollution mass in air is less important than e.g. actually consumed amount of species. Another example is deposition, which can be more important than atmospheric concentrations.

Assuming linear dependence of the load $M$ on $\varphi$ (also not strictly true but acceptable in many practical applications) it can be written as a functional:

**( 4)**
$$M = \int_0^{\infty} \int_D \varphi(t,\vec{x})\, p(t,\vec{x})\, d\vec{x}\ dt$$

Equation ( 4) together with ( 1), ( 2) conclude the forward problem formulations for the unknown load $M$.

Inverse problem of the atmospheric pollution appears when some measurements show presence of contaminants, which origin is unknown or uncertain. The task of determining the responsible emission source then forms the essence of the inverse problem.

In the above terms it means that some part of the load $M$ is measured and it is necessary to find the unknown emission function $f$. Such formulation is evidently not constructive and can not be approached in a straightforward way. In order to derive more convenient set of equations let's generalize the functional ( 4) by putting $p \equiv 0$ outside the domain $D$ and for negative time $t$. Then the integrals can be taken over the whole 4-D space and the functional becomes just an inner product of functions $\varphi$ and $p$ both belonging to some Hilbert space $H$, where the inner product is defined as the following:

**( 5)**
$$(\eta,\psi) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty}\int\int \eta(\vec{x},t)\,\psi(\vec{x},t)\, d\vec{x}\ dt$$

Using the features of the inner product we can write:

**( 6)**
$$M = (p,\varphi) = (L^*\varphi^*,\varphi) = (\varphi^*, L\varphi) = (\varphi^*, f)$$

Here $\varphi^*$ is a new variable formally satisfying the equation

**( 7)**
$$L^*\varphi^* = p$$

and $L^*$ is an adjoint to the differential operator $L$.

It is straightforward to show that the adjoint equation has the following form:

(8) $$L^*\varphi^* = -\frac{\partial \varphi^*}{\partial t} - \frac{\partial}{\partial x_i}(u_i\varphi^*) - \frac{\partial}{\partial x_i}\mu_{ii}\frac{\partial \varphi^*}{\partial x_i} + \sigma\varphi^* = p$$

With zero conditions for $\varphi^*$ at infinity and $t=0$.

Comparing the forward and adjoint equations one can notice that they differ only by signs of time and wind velocity, which enables to use the same model for computation of both problems if sufficient internal flexibility of the program is maintained.

The sensitivity function $p$ should be set to zero everywhere but the points where the observations show the presence of the pollutant. The solution of corresponding adjoint equation provides the sensitivity distribution function $\varphi^*$ outlining the area and time period where the responsible source can be located. The next steps mainly depend on the obtained $\varphi^*$ and a-priory information about possible source locations. If this information is sufficient – the source can be localized and its time-dependent emission is determined.

Some additional tuning can be obtained by solving another adjoint problem with the sensitivity function corresponding to the stations where the pollutant was NOT found. Evidently, the obtained sensitivity distribution outlines the regions and time periods where the source can NOT be located.

Below example presents the first results of the test application of the above theory. Both forward and inverse simulations were performed with the Finnish emergency model SILAM, which outline opens the next section.

## Overview of SILAM dispersion model

SILAM is a Finnish Operational Emergency Modelling Framework consisting of the following main parts:

- Lagrangian particle dispersion model with the Monte-Carlo random walk diffusion representation
- Meteorological data pre-processor
- Separate radio-active dose assessment module

The model handles two types of the sources: point source (e.g. leakage from the store, stack emission or other types of ground-based or elevated emission from a small area) and nuclear bomb explosion source (the mushroom cloud is computed from the yield of the bomb).

The model can provide the results in 5 different formats:

- GrADS plain binary suitable for treatment with Grid Analysis And Display Software (GrADS);
- GRIB universal binary;
- Vis5d coded binary (obsolete) for treatment with Vis5d visualization software (no longer supported by the developers);
- Trajectory text file containing an arbitrarily selected set of random-walk trajectories from the main cloud;
- Ready-made maps drawn by GrADS and stored in Acrobat pdf file.

The model is comparably quick – 48-hours forecast for one point source emitting a passive tracer takes about 5 minutes of Intel Pentium IV 1.4 GHz. The model is programmed as a single-processor application and can be run under both UNIX and Windows NT.

Physical size of the program code is ~2.4 MB located in 83 FORTRAN-90 modules (totally about 30,000 operators).

## Operational solution of the forward problem

Above described SILAM model is used at Finnish Meteorological Institute as an operational tool for real-time solution of the forward dispersion problems. It is linked to the HIRLAM runs and starts immediately when the new forecast is ready.

Automatic runs cover 5 closest nuclear power plants and provide 48-hours forecasts of potential areas of risk in case of some accident on any of those plants. Model also supports manual runs with flexible setup and user-defined source characteristics.

The results of the simulations are automatically uploaded to the Finnish Nuclear safety authority.

## A case study with combined forward and inverse modelling

The SILAM model is programmed in a flexible way allowing straightforward solution of both forward and adjoint equations ( 1) and ( 8). The case study presented in this section consisted of the test problem with "known solution" constructed in the following way.

Forward calculations show that hypothetical 1-hour release of passive tracer from the nuclear power plant Sosnoviy Bor started at 6:00 30.10.2001 would result in a short-time peak of concentrations near Helsinki harbor at 24-th hour since the release – around 6:00 31.10.2001, which is below called as a "reference time" $\tau_R$ (see Figure 1).

It was assumed that some measurement device has registered this peak with somewhat disturbed shape – non-zero concentrations were reported only for 1-hour period ending at the reference time.

Additional a-priory information includes exact knowledge about the nuclear power plant locations and assumption that there are no other sources of the observed concentrations. Second, it was assumed that inside Finland there exists a reliable information about the plant conditions, so the local installations were excluded from the consideration.

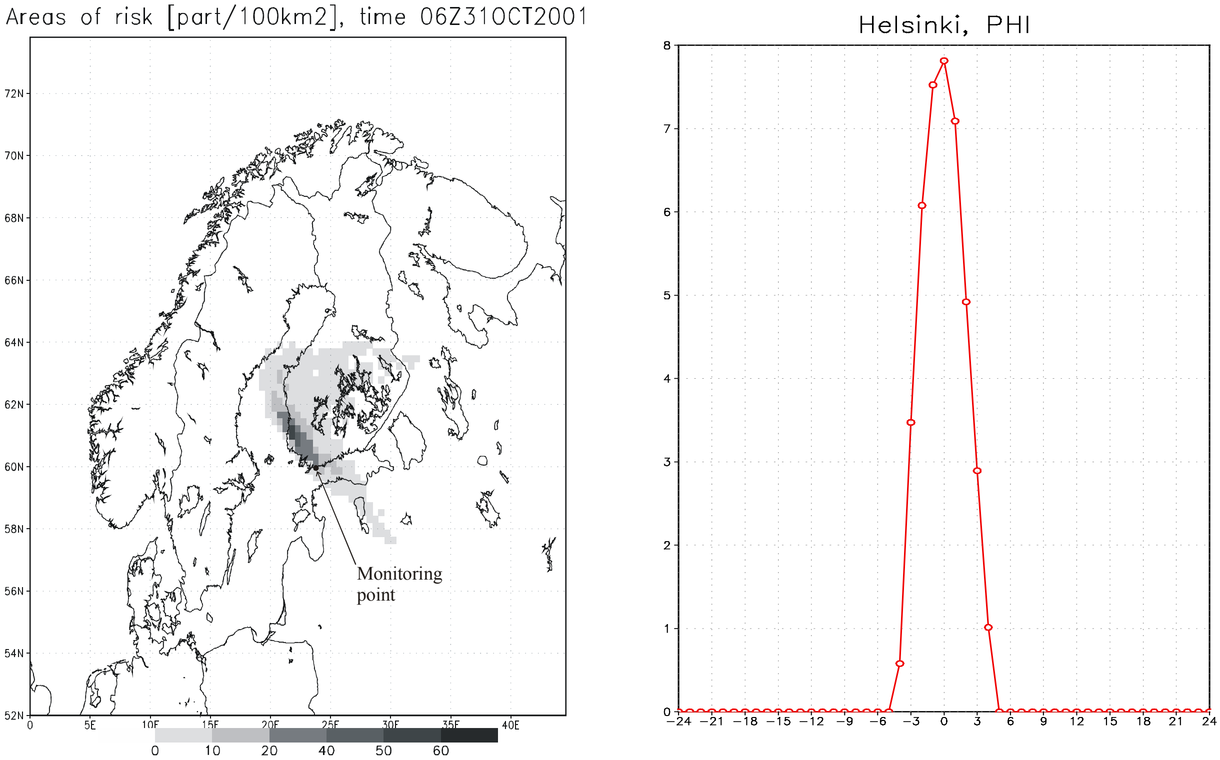
The inverse problem was approached in two steps.

First, the adjoint equation was solved for 48 hours period, thus covering the range [$\tau_R$–48 h; $\tau_R$]. In order to be consistent with the forward model run, the same single 48-hours long forecasting set of the meteodata was taken – in below figures referred as a "single-analysis" data set. Analysis time of the data set was equal to the moment of emission: $\tau_R$ -24 h.

Second, the sensitivity distribution function $\varphi^*$ was compared with the locations of the installations, which provided a suspected time periods for each plant. The results are aggregated in Figure 2, where the sensitivity distribution is computed for the above-stated 1 hour concentration peak during the period [$\tau_R$ -1h; $\tau_R$].

As shown in Figure 2, the inverse problem solution appeared to be almost exact. The sensitivity function highlights the 1-hour period of the release as the only period when the source at Sosnoviy Bor affects the reception point at the reference time. The other potential sources (nuclear power plants) were not covered by $\varphi^*$, which means that they could not create the observed concentration peak.

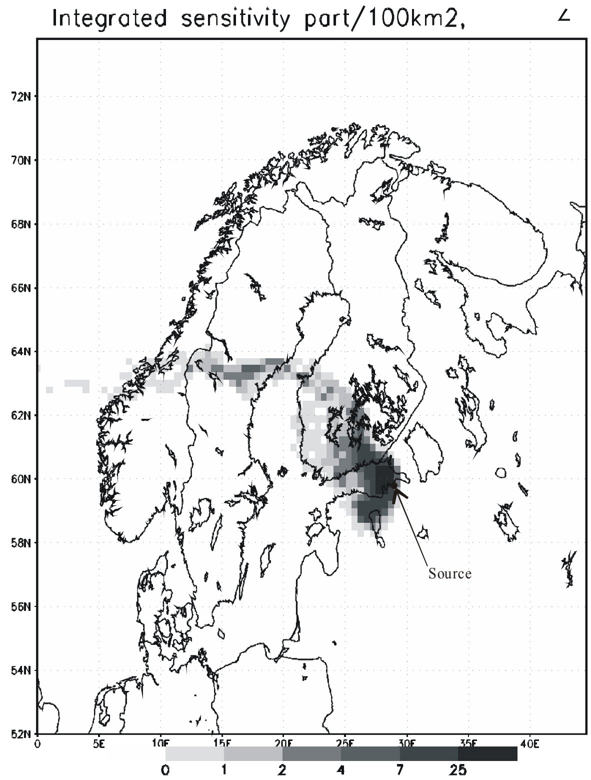
This time chart does not, however, contain information whether the emission itself was limited by that 1-hour period, it is just stated that the sensitivity to that emission is zero outside this time. For more detailed conclusions about the time variation of the emission rate the provided information is not sufficient. To get a complete picture it is necessary to involve measurements before and after the observed peak and/or use information from the other monitoring sites. Corresponding extensions are expected in the next studies.



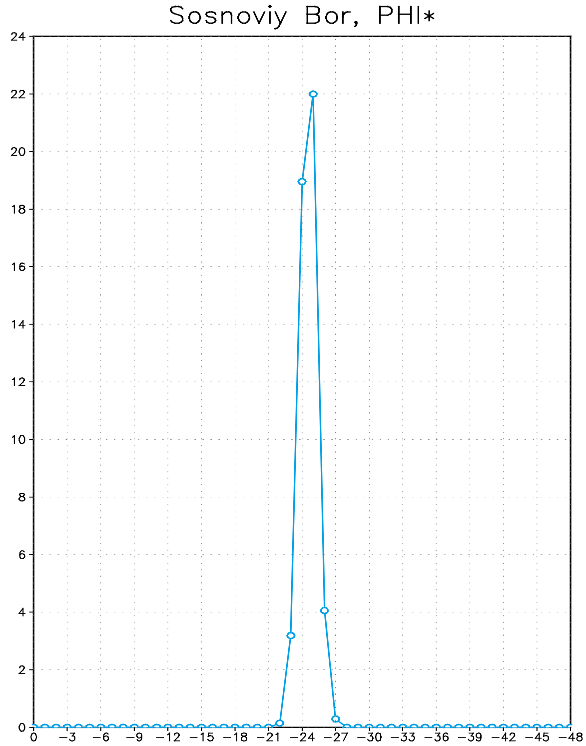

Concentration map 6:00 31.10.2001 (reference time)

Concentration time chart at Helsinki harbour

**Figure 1.** Forward dispersion of the passive tracer – concentrations at 7:00 30.10.2001 and 6:00 31.10.2001(the reference time). Single-analysis meteodata, 1-hour time step. Relative units




Sensitivity distribution at 6:00 30.11.2001 ($\tau_R$ – 24 h)

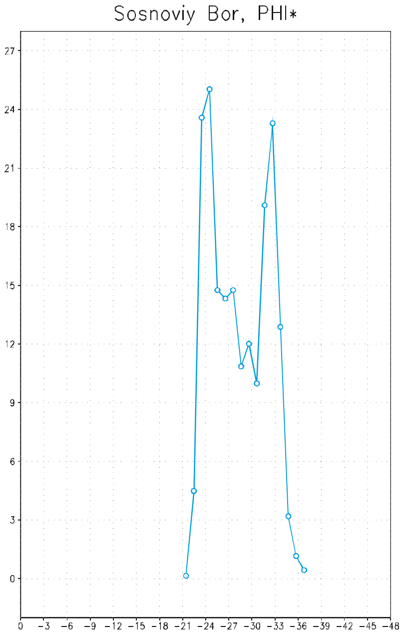



Sensitivity time chart for Sosnoviy Bor

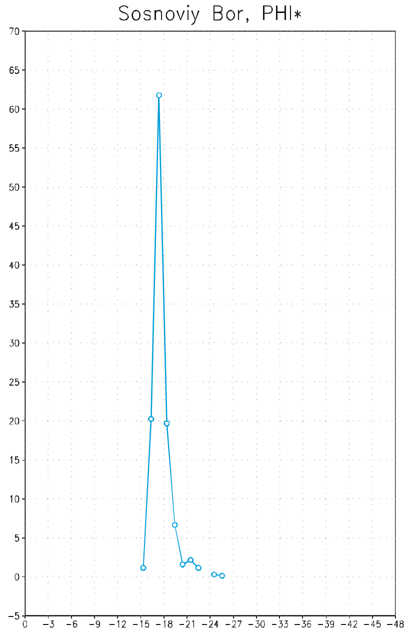
**Figure 2.** Inverse problem solution – the sensitivity distribution function for $\tau_R$ -1h and $\tau_R$ -24 h. Single-analysis meteodata, 1-hour time step. Relative units

The second important specific of the time charts in Figure 1 and Figure 2 is that both of them are obtained from the same model using the same input meteorological data. This makes them consistent with each other but does not reflect the reality where the forward and inverse "tools" are essentially different – forward dispersion is driven by actual atmospheric processes, while the inverse run is performed by the model sourced by the numerical forecast data or meteorological observations.

In order to get a qualitative impression about the sensitivity of the current case to the variations of the meteorological information, two more inverse runs have been made. First, the same meteodata set was squeezed to 6-hour time step with linear interpolation in-between. This reflected some poor data set with low time resolution. Second, the multi-analysis data set was taken with analysis update every 6 hours and the time step between the fields of 1 hour. The last data set reflects high time resolution and best-possible fit to synoptic measurements. The results of the simulations are shown in Figure 3.




Sensitivity time chart for Sosnoviy Bor with 6-hour step of the single-analysis meteodata




Sensitivity time chart for Sosnoviy Bor with 1-hour step of the multi-analysis meteodata (analysis update every 6 hours)

**Figure 3.** Time charts for the sensitivity distribution for different meteorological input fields. Relative units.

As expected, the sensitivity of the time charts to the input data variations is high – in both cases the response is significantly different from that shown in Figure 2. The reason for this is quite evident as well – it is well seen that the observation point happens to be at the edge of the pollution cloud. Consequently, the source point is at the edge of the sensitivity distribution. As a result, small variations in the wind pattern may severely affect the concentrations / sensitivity at these points. This qualitative consideration highlights the necessity to build a comprehensive statistical inversion solution, which would not only determine the source but also provide some estimates of the confidence of this solution. However, the statistical approach would require an appropriate input data – for example, ensemble forecasts.

# Summary

• The forward dispersion problem can be covered with numerical model driven by short-term forecast meteofields in a straightforward way

• An inverse dispersion problem may be covered by adjoint model if

- The forward differential operator is linear
- There exists a convenient linear load functional
- Sufficient quality of input meteorological fields is provided

• There is a strong implication that deterministic approach may be not accurate enough demonstrating high sensitivity to (small) variations of the input information. In this case statistical inversion model has to be built using, e.g. ensemble of the meteorological input data or other ways for creation a set of stochastically perturbed inverse problems.

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