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Separation problem of industrial particles emissions using a stationary scattering model

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Abstract

This paper deals with some methods used to separate and to evaluate emission of dust particles coming from various industrial origins. Locations of all sources are supposed to be known by their 3D-Cartesian coordinates and steady-state dispersion is assumed to be reached. Our main contribution is to combine a particular stationary dispersion model with some efficient separation methods. The estimation of particles flow for the case of point sources over flat terrain is first addressed and then it is extended to line or area sources. Anyway, the approach is divided into two specific steps: the stationary model presentation and the separation techniques applied to the previous model. Finally, simulation results show the performances of the different methods in case of point. It turns out that small variations on the wind angle lead to large errors on flows estimate. Robust techniques with respect to model uncertainties appear to be of prime interest.

Keywords: Particles flow estimation; Inverse problem; Regularization; Particles transport model; Estimated errors

1. Introduction

Pollutant, particles may be emitted by a great number of industrial plants. The particles plume is moving in the air but dry deposition regularly affects the particles' plume displacement. This deposition is caused by gravitational settling or ground absorption by the soil. Measuring this deposition at particular locations may be of prime importance to evaluate the impact on the local ecosystem. In addition, these measures are useful to estimate pollutant flow source. This paper addresses the problem of estimating pollutant flow source by combining a dry deposition model and some inverse techniques.

In this study, the amount of particles depositions are provided by specialized sensors located at ground level. In addition, the mineral nature of a class of particles, their size and their weight are known. The deposition rate is associated with the previous quantities. All these data are collected into an analytical dry deposition model.

Some deposition models may be used to compute a source flow estimate for a specific class of particles. In the absence of any removal mechanisms, the Gaussian plume dispersion model is the classical model used to investigate air pollution concentrations from a point source in steady state conditions (Pasquill, 1976). Turner (1994) modifies Pasquill–Gifford's model to involve the use of appropriate atmospheric stability class. This Gaussian plume has been widely used because of its simplicity and a good fitting to practical measurements.

The problem of atmospheric transport when gravitational settling cannot be neglected has been studied primarily by Calder (1961). It is assumed that both the gravitational settling flow and the ground deposition flow are proportional to the local air concentration. Gravitational settling velocity and deposition velocity are these proportionality factors.

Usually, they are different from each other. Unfortunately, the complexity of the solutions has limited their use.

Subsequently, two types of models have received great interest. The source depletion approach considers the ground deposition as a disturbance to the Gaussian plume dispersion (Pasquill, 1976). The constant source

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strength is replaced by a virtual source of decreasing strength.

The second (Ermak, 1977) is a more physically realistic solution and yet remains as simple as the Gaussian plume. Analytical solutions for pollutant air concentrations and ground deposition flow are developed in Ermak (1977). This model has been chosen to solve our estimation problem for the sake of simplicity.

For line and area sources, the Caline3 model (California DTI, 1979) is derived from the previous model.

Anyway, the sources–receptors link is described by linear matrix relations whose coefficients can be computed under known conditions.

Using data measurements and the previous model, it is possible to compute flow sources: many inverse techniques exist and the choice of which one depends on the nature of application. However, we focus here on a few techniques: a least square method and a regularized least square method. Data measurements are usually corrupted with noise so that regularization techniques appear to be necessary.

Moreover, atmospheric conditions and particles attributes are roughly estimated so that matrix components are mixed with errors. The effect of imprecise conditions on the source flow has to be quantified.

Errors on source location, wind velocity, wind angle may be investigated. According to these accuracies, it is possible to provide an upper bound for the relative error.

The purpose of this work is to develop a technique able to compute coach source flow. First, the sensor principle is presented and source assumptions are then developed. Under these specific assumptions, the dry deposition model proposed by Ermak will be discussed. This enables to tackle inverse techniques where the use of regularization appears to be necessary. However, the accuracy of the estimation needs to be evoked. Finally, simulation results illustrate the previous remarks.

2. Sensor principle

The aim of this section is not to study the measurement principle but to understand what important information is delivered by the sensor. So, we only describe the functionality proposed by the used sensors.

The sensor collects a set of particles, all of them are classified according to their chemical nature, their size class, and a sphericity factor by color analysis and pattern recognition techniques. For the particles belonging to the previous class, the sensor computes a deposition rate averaged on one or three hours depending on the particles concentration. Such a sensor has been developed by Aloa Technologies[1] and is currently tested by a public pollution surveillance network (Opal' air) in sub-town industrial Dunkerque (France). More generally, some sensors are located at various places of the monitored domain, all of them provide synchronously a deposition rate (in mg/m^2 h) for a specific class of particles. The numerical information delivered is used to explain the origin of the pollution.

3. Basic sources assumptions

In most cases, we consider the size of the source as a point comparatively to the size of the monitored area. It is the case of a chemical or metallurgical chimney which throws out a major type of particles in significant quantities varying from 10 to 200 kg/h. However, as regards material roughly thrown on the floor by mechanical shovel or conveyor belt alongside a quay embankment, and being lifted by the wind, it then makes up a source considered as line or area and emitting particles in kg/(m/h) or kg/(m^2/h). The geometrical characteristics (length, width, location) are also well known. Each source flow is supposed to be slowly varying and steady state dispersion is reached in less time than the sample one. This assumption enables to consider a stationary dispersion model.

Usually, the number of sources is smaller than the receptors. This enables to compute a best solution according to a specific criterion. Sometimes the number of sources may be greater than the receptors. Then the separation algorithm needs a priori extra information, such as the upper bound of each source flow, to deliver a plausible solution.

4. Stationary dispersion model

4.1. Point source case

Measurement method (average deposition on a time period) and length of the sample time (1 or 3 h) lead to consider a stationary dispersion model. Pollutant transport is assumed to be ruled by the atmospheric advection diffusion differential equation:

$$\frac{\partial C}{\partial t}=-U_x\cdot\frac{\partial C}{\partial x}+\frac{\partial C}{\partial x}\left(K_x\cdot\frac{\partial C}{\partial x}\right)+\frac{\partial C}{\partial y}\left(K_y\cdot\frac{\partial C}{\partial y}\right) \tag{1}$$
$$+\frac{\partial C}{\partial z}\left(K_z\cdot\frac{\partial C}{\partial z}\right)+V_{\mathrm{g}}\cdot\frac{\partial C}{\partial z}+Q(x,y,z,t)$$

where C denotes the pollutant, concentration at any location (x,y,z) and time t. Q stands for a source flow

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located at (x,y,z), and time t. (K_x,K_y,K_z) are the eddy diffusivity coefficients (m^2/s), V_g the particle gravitational settling velocity (m/s) and U_x, is the constant average wind speed (in x direction) and simply noted U in the following text. When the last value is sufficiently large, Ermak (1977) assumes that diffusive transport is negligible in wind direction with respect to advection. Moreover, the coefficients K_y, and K_z, only depend on the downwind distance x and are therefore independent of the crosswind distance y and height z. This leads to a simplification of the expression of diffusive terms. In addition, when the source strength is constant with time, a steady state solution can be used resulting in a simplified equation as follows:

$$U\cdot\frac{\partial C}{\partial x}=K_y\cdot\frac{\partial C^2}{\partial y^2}+K_z\cdot\frac{\partial C^2}{\partial z^2}+V_g\cdot\frac{\partial C}{\partial z}+Q(x,y,z,t) \quad (2)$$

Some boundary conditions must be joined to the previous equation. They are:

(i) a continuous point source at (0, 0, h) of constant strength Q: $C(0,y,z)=\frac{Q}{U}\delta(y)\delta(z-h)$, where h is the source height,
(ii) the pollutant concentration approaches zero far from the source in y and z direction : $C(x,\pm\infty,z)=0$; $C(x,y,\infty)=0$
(iii) on the ground, the pollutant deposition is supposed to be proportional to the local air concentration. The proportionality factor is called the deposition velocity U_d. It is defined by the following relation:

$$\left[K_z\cdot\frac{\partial C}{\partial z}\right]_{z=0}=[U_d\cdot C]_{z=0}. \quad (3)$$

The deposition velocity U_d is a function of the particles nature, their size, the nature of the ground and the atmospheric stability. Sehmel and Hodgson (1978) propose an expression of U_d as a function of the gravitational settling velocity V_g, the inverse Monin–Obukhov distance, the surface friction velocity, the effective particle diameter, the sensor height and temperature. The algorithm which computes U_d has been implemented in the soft FDM developed by TRC (1990).

At large downwind distance (typically a distance source–receptor greater than one kilometer), the gravitational settling velocity V_g can be computed using Stokes law (Green and Lane, 1964):

$$V_g=\frac{\rho g d^2}{18\eta\psi} \quad (4)$$

where ρ is the particle density, g is the gravitational acceleration, d is the disk diameter with the same area as the projected particle, ψ is the sphericity factor (ψ=2 for sand particle, ψ=2.25 for coal and (coke particle, ...) and η is the atmospheric viscosity.

According to the following assumptions, the classical formulation of Gaussian plume (Pasquill, 1976) is adapted to integrate the transfer gradient deposition algorithm of Ermak (1977). Finally, the concentration is

$$C(x,y,z,U)=\frac{Q}{2\pi\sigma_y\sigma_z U}\cdot e^{-\frac{y^2}{2\sigma_y^2}}\cdot \mathrm{disp}(U_d,V_g,\sigma_z,z) \quad (5)$$

where

$$\mathrm{disp}(U_d,V_g,\sigma_z,z)=e^{\left[\frac{-V_g(z-h)}{2k}-\frac{V_g^2\sigma_z^2}{8k^2}\right]}\left\{e^{-\frac{(z-h)^2}{2\sigma_z^2}}+e^{-\frac{(z+h)^2}{2\sigma_z^2}} - \sqrt{2\pi}\frac{V_1\sigma_z}{K}e^{\left[\frac{V_1(z+h)}{K}+\frac{V_1^2\sigma_z^2}{2K^2}\right]}\mathrm{erfc}\left(\frac{V_1\sigma_z}{\sqrt{2}K}+\frac{z+h}{\sqrt{2}\sigma_z}\right)\right\} \quad (6)$$

$C(.)$ denotes concentration (g/m^3). Q is emission rate (g/s), U wind speed in x direction (m/s). σ_y, σ_z are empirical standard deviations in respectively y and z direction obtained by Turner formulae for a variety of atmospheric stabilities (i.e.: A, AB, B ,... DE, E) as a function of meteorological and terrain conditions and are dependent of the source–receptor distance x in wind direction (Turner, 1994). V_g is the gravitational settling velocity (m/s) and h the plume centerline height (m). $K=\frac{\sigma_z^2 U}{2x}$ is the eddy diffusivity (m^2/s) assumed to be constant, $V_1=U_d-V_g/2$. The sensor coordinates (x,y,z) are given in the local orthogonal basis where O_x is parallel to wind direction, and origin O is attached to the source.

Finally, a deposition flow ($g/m^2/s$) can be obtained using the deposition velocity:

$$d(x,y,z,U)=U_d\cdot C(x,y,z,U). \quad (7)$$

4.2. Linear and rectangular source case

Sometimes, a point source is not representative of a real source. To overcome this disadvantage, we extend the formulation to line sources. Let us assume that the source segment is orthogonal to wind direction. A line source may be divided into m point sources, each of them emitting a source flow equal to $Q_j=\lambda_j\cdot\Delta_y$ at the central location y_j, where Δ_y is the segment width associated with the point source and λ_j (g/m/s) stands for the segment source j uniform strength. It can then easily be stated that the concentration obeys the following relation:

$$C(x,y,z,U)=\frac{1}{2\pi\sigma_y\sigma_z U}\sum_{j=1}^{m}\lambda_j e^{-\frac{(y-y_j)^2}{2\sigma_y^2}}\Delta_y\cdot \mathrm{disp}(U_d,V_g,\sigma_z,z) \quad (8)$$

This model requires the line sources to be orthogonal to the wind. The California Department of Transportation Institute proposes an extension which takes into account a rectangle divided into n source segments oriented with an angle ψ with respect to the wind (see Fig. 1). However, it only applies to gas transportation. The extension to particles transport can be carried out without difficulty. Each part of the rectangular source may be replaced by a finite equivalent line source as defined previously in Fig. 1. The whole concentration may be deduced by applying Eq. (8) to each finite equivalent line source:

$$C(x,y,z,U)= \frac{1}{\sqrt{2\pi}U}\cdot\sum_{i=1}^{n}\frac{1}{\sigma_{yi}\sigma_{zi}}\cdot\sum_{j=1}^{m}\lambda_j e^{-\frac{(y-y_j)^2}{2\sigma_{y_i}^2}}\Delta y\sum_{k=-cnt}^{cnt}\mathrm{disp2}(h,L,k,\sigma_z,z) \tag{9}$$

the function disp2(.) can be written as:

$$\mathrm{disp2}(h, L, k, \sigma_{zi}, Z)=e^{\left[\frac{-V_g(z-h)}{2k}-\frac{V_g^2\sigma_z^2}{8k^2}\right]}\left\{e^{\frac{-(z-h+2kL)^2}{2\sigma z^2}}+e^{\frac{-(z+h+2kL)^2}{2\sigma z^2}}-\sqrt{2\pi}\frac{V_1\sigma_z}{K}e^{\left[\frac{V_1(z+h)}{k}+\frac{V_1^2\sigma_z^2}{2k^2}\right]}erfc\left(\frac{V_1\sigma_z}{\sqrt{2}K}+\frac{z+h}{\sqrt{2}\sigma_z}\right)\right\} \tag{10}$$

where h is plume centerline height, L is mixing height, k index of reflection term, σ_{yi} and σ_{zi} are standard deviations computed for each distance x_i between sensor and source element, i. For details, the reader is invited to refer to Benson (1979), the technical report (California DTI, 1979) or the Ph.D. thesis of Bennouna (1988). Anyway, the important idea is that an area source can be replaced by a set of point sources judiciously chosen.

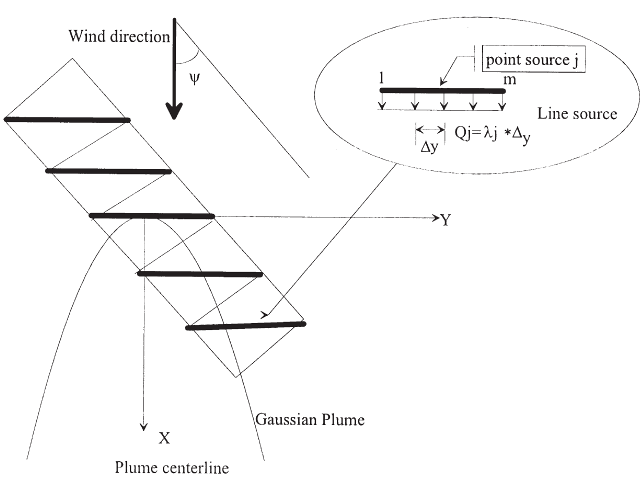

Fig. 1. Rectangular source represented by a serie of finite segment sources.

All these relations Eqs. (7)–(9) are linear forms with respect to source strength, the only change is the increase of the sources number. Also, it is possible to compute the emission flow for each line source. The following thought process is exactly similar. Subsequently, we focus only on the case of point sources.

These models enable to compute the sources–receptors transfer matrix which becomes the kernel of the inverse separation problem, which method is described in the next section. Once sources are identified, the iso-concentration curves are computed with the direct model Eq. (7) on the monitored domain.

5. Sources separation problem

The main algorithm consists in computing the emission flow of each source with knowledge of the perceptual system measurements.

The point source–sensor analytic model can be written in the same form as Eq. (11). In fact, the theoretical deposition $D(r)$ at sensor r (from 1 to R), is a sum of elementary depositions issued from each source among P sources:

$$D(r)=\sum_{p=1\ldots p}U_d(r)\cdot C(p,x_r,y_r,z_r,U) \tag{11}$$

Sources and sensors are located on a global basis but each analytic expression is calculated on a local basis where sources are at origin and x direction is spanned by wind direction. On the other hand, $U_d(r)$ depends on sensor height r, particle diameter and Monin–Obukhov distance.

As Eq. (11) is linear with respect to emission flows, the deposition rate at sensor r can be explicated by linear combination of sources strength as Eq. (12):

$$D(r)=\sum_{p=1\ldots P}Q_p\cdot unit-dep(r,p) \tag{12}$$

where

$$\mathrm{unit-dep}(r,p)=U_d(r)\cdot\frac{1}{2\pi\sigma_y\sigma_zU}\cdot e^{-\frac{y^2}{2\sigma_y^2}}\cdot\mathrm{disp}(U_d,V_g,\sigma_z,z) \tag{13}$$

unit-dep($\cdot$) represents a proportionality factor depending on the source strength Q_p, and operating on the sensor r. The vectorial solution of P sources emission flow minimizing the quadratic criterion J_1 is obtain in solving a least squares inverse problem Eq. (14):

$$Min_QJ_1(Q)=Min_Qe^Te=Min_Q(M-G\cdot Q)^T(M-G\cdot Q) \tag{14}$$

where $Q=[q_1,q_2,\ldots,q_p]^T$ is the vector of p sources strength, $M=[m_1,m_2,\ldots,m_r]^T$ is the measurements vector issued from R sensors, and $G=\begin{bmatrix} g_{I1} & \cdot & \cdot & g_{IP} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ g_{R1} & \cdot & \cdot & g_{RP} \end{bmatrix}$ the kernel matrix (or mixing matrix) whose elements g_{rp} are given by the function unit_dep(·) defined in Eq. (13).

Assuming that $[G^TG]^{-1}$ exists, we have the following solution:

$$Q_{\text{est}}=[G^TG]^{-1}G^TM \quad (15)$$

However, data m_r issued from the receptor r are noised due to measure imprecisions. Model parameters imprecisions (i.e. wind angle and velocity, sources locations, $U_{\text{d}}(r)$, V_{g}) involve some errors on matrix G elements. Consequently, the solution of Eq. (14) is unstable with respect to measures and parameters due to ill-conditioning of G.

Assuming $M=M_{th}+\Delta m$ where $M_{th}=G\cdot Q$ is the measure vector without noise, a small measure variation $\|\Delta m\|$ involves an error $\|\Delta Q\|$ on the solution Q_{th} as:

$$Q_{\text{est}}=Q_{th}+\Delta Q=[G^TG]^{-1}G^T[M_{th}+\Delta_m] \quad (16)$$

$$=\sum \mu_i^{-1}(w_i|M_{th})v_i+\mu_i^{-1}(w_i|\Delta_m)v_i \quad (17)$$

where $\{\mu_i{:}i=1\ldots g\}$ are singular values of G assuming to be ordered in increasing sense, w_i, eigenvector of GG^T and v_i eigenvector of G^TG. $\|\cdot\|$ is vectorial norm and $(\cdot|\cdot)$ is dot product.

Since G is ill-conditioned, some singular values of μ_i are very small. Consequently, μ_i^{-1} are high enough to amplify the measured noise $\|\Delta m\|$. Sensibility of least squares solution can be analysed with respect to measure uncertainties by:

$$\frac{\|\Delta Q\|}{\|Q_{th}\|}=K(G)\frac{\|\Delta m\|}{\|M_{th}\|} \quad (18)$$

$K(G)$ is a conditioning number defined by:

$$K(G)=\|G\|_2\|G^{-1}\|_2=\frac{\mu\text{max}}{\mu\text{min}} \quad (19)$$

$\|\cdot\|$ stands for the ℓ_2 matrix norm.

Instability problem can be damped using regularization techniques as it is proposed in Groetsch (1993), Tarantola (1987) and Theodor and Lascaux (1993). This method contributes to achieving an acceptable solution with respect to the inverse problem. This solution consists in combining data and a priori information. The new solution is the argument minimum of the criterion:

$$J(Q,\alpha)=J_1(Q)+\alpha\cdot J_2(Q) \quad (20)$$

$J_1(Q)$ used in previous development Eq. (14), estimates the relative fidelity to the measures. Criterion J_2 yields a distance between solution and a priori information. α is a non-negative regularization factor determining the relative importance of each part of the criterion (J_1, J_2). If α is set to zero, the prediction error will be minimized, but, no a priori information will be provided to single out the undetermined part of the solution. Miller (1970) suggests using the following criterion:

$$J(Q,\alpha)=(M-GQ)^T(M-GQ)+\alpha\cdot\|CQ\|^2 \quad (21)$$

where C is a linear operator characterizing a type of a priori information. This term invokes to reach a minimal filter norm solution. In this procedure, minimizing $J(Q,\alpha)$ with respect to flow Q leads to the solution:

$$Q^{\text{est}}=(G^TG+\alpha\cdot C^TC)^{-1}G^TM \quad (22)$$

The matrix I increases the smallest singular value of $G^TG'=G^TG+\alpha\cdot C^T\cdot C$. The singular value decomposition of Eq. (22) leads to the expression:

$$Q_{th}+\Delta Q=\sum_{i=1}^{r}\frac{\mu_i}{\mu_i^2+\alpha\cdot\eta_i^2}(w_i|M_{th})v_i \quad (23)$$

$$+\frac{\mu_i}{\mu_i^2+\alpha\cdot\eta_i^2}(w_i|\Delta m)v_i$$

η_1 is the singular value of C^tC ($\eta_i=1$ if $C=I$). If μ_i is low (because G is ill-conditioning) then $\frac{\mu_i}{\mu_i^2+\alpha\cdot\eta_i^2}$ leads to zero and the error term $(w_i/\Delta m)$ stays at low value for any Δm. Then the solution is stable.

On the other hand, a question about α can be asked. Which value to choose for α to have a good trade off between low prediction error and flatness of the solution? There is no simple method of determining what this compromise should be. Nevertheless, the following conditions have to be checked:

$$\|CQ^{est}\|=\|Q^{\text{est}}\|\leq E \quad (24)$$

and

$$\text{e}^T\text{e}\leq\epsilon^2, \quad (25)$$

then it would be judicious to choose $\alpha=\left(\frac{\epsilon}{E}\right)^2$ where ϵ is the prediction error upper bound, and E the maximum norm solution. E and ϵ have to be chosen so that Eqs. (24) and (25) are fulfilled. Obtaining a relative prediction error no more than 5% of measures norm ($\epsilon=0.05\cdot\|M\|$) is considered as a good estimation. In addition, knowing the *a priori* maximum flow $Q_p^{\max}$ of each source, the estimate vector norm $|Q^{\text{est}}|^2$ is less than $\sum_{p=1\ldots p}(Q_p^{\max})^2$. For the implemented algorithm in the software, typical value of Q is then:

$$\alpha=\frac{(0.05\cdot\|M\|)^2}{\sum_{p=1\ldots p}(Q_p^{\max})^2} \quad (26)$$

Moreover, when the number of sources is greater than the sensors, the under-determined system Eq. (14) can be informed by a priori considerations average about sources (Menke, 1984). Note that this relationship Eq. (26) is empirical and approximate to obtain a result close to the prediction error specifications (ϵ^2 and E), but it does not give the certainty to have the best source flow estimate of each one. It is, then, important to provide some error information on the estimates.

6. Errors

Flows estimate determination cannot be proposed without an associated errors valuation. These errors may be brought by either measurement, imprecisions provided by particles deposition rate sensors or transport model parameters uncertainties. Wind velocity and direction, stability class, particles plume height, particle diameter or sphericity factor, point sources location may be cited as sensible model parameters which cause significant variations on estimates.

6.1. Measurement errors

As shown in expression Eq. (18), a relative error $\frac{\|\Delta Q^{measurement}\|}{\|Q^{\mathrm{est}}\|}$ on flows estimate Q^{est} may be calculated by the knowledge of relative measurement error $\frac{\|\Delta m\|}{\|M_{th}\|}$. In a regularized case, conditioning number $K(G')$ of the equivalent regularized matrix G' is:

$$K(G')=\frac{\mu'_{\mathrm{max}}}{\mu'_{\mathrm{min}}} \quad (27)$$

where the greatest and smallest values are

$$\mu'_{\mathrm{max}}=\max_{\mu_i}\frac{\mu_i^2+\alpha\cdot\eta_i^2}{\mu_i} \text{ and } \mu'_{\mathrm{min}}=\min_{\mu_i}\frac{\mu_i^2+\alpha\cdot\eta_i^2}{\mu_i} \quad (28)$$

Let us note that $\eta_i^2=1$ if identity matrix stands for the matrix C.

Then applying the expression Eq. (18) to G' gives an estimated flows relative error (assuming ΔQ and Δm are low enough):

$$\frac{\|\Delta Q^{\mathrm{measurement}}\|}{\|Q^{\mathrm{est}}\|}=K(G')\frac{\|\Delta m\|}{\|M\|} \quad (29)$$

6.2. Model errors

When the model of a kernel matrix is disturbed (i.e model matrix G is affected by ΔG deviations), inverse problem gives biased flows estimate Q^{est}. For a least squares inverse problem, solution variation norm $\|\Delta Q^{\mathrm{mod}}\|$ and residue ($M-GQ^{\mathrm{est}}$) of the measurement are presented in Theodor and Lascaux (1993).

Let Q^{est} be the solution of Eq. (14).

Let residu$=M-GQ^{\mathrm{est}}$ be the measurement residue and let:

$$\sin\theta=\frac{\|\mathrm{residu}\|}{\|M\|} \quad (30)$$

Let $Q_{\mathrm{est}}=Q_{th}+\Delta Q^{\mathrm{mod}}$ be the solution of:

$$Min_Q J_1(Q)=Min_Q \mathrm{e}^T\mathrm{e}=Min_Q[M-(G+\Delta G)\cdot Q]^T[M-(G+\Delta G)\cdot Q] \quad (31)$$

where ΔG is the kernel matrix deviation brought by parameters uncertainties. Assuming $\varepsilon=\frac{\|\Delta G\|}{\|G\|}$ is small, then the relative error norm is upper bounded as following:

$$\frac{\|\Delta Q^{\mathrm{mod}}\|}{\|Q\|}\leq\varepsilon\cdot[\tan(\theta)\cdot[K(G)]^2+K(G)]+O(\varepsilon^2) \quad (32)$$

Let us note that, $K(G')$ can replace $K(G)$ if the mean square solution is obtained by a regularized method.

Global model uncertainty $\|\Delta G\|^2$ which is numerically computed, can be estimated by a quadratic sum of each variational term issued from sensible parameters:

$$\begin{aligned}\|\Delta G\|^2\leq&\|\Delta G(\delta\theta)\|^2+\|\Delta G(\delta U)\|^2\\&+\|\Delta G(\delta \text{ stability factor})\|^2+\|\Delta G(\delta d)\|^2\\&+\|\Delta G(\delta \text{ source location})\|^2\end{aligned} \quad (33)$$

where $\delta\theta$, δU, δ(stability class), δd, δ(source location) stand respectively for error in wind direction, wind velocity, atmospheric stability factor chosen, particle diameter and 3D-source coordinates.

7. Software description

The current version of the software, named '*Particle Flow Identification*', is organized into six available functionalities from the main menu. The first one concerns *file*: transfer of pictures, context, definitions (source and sensor characteristics), print, …. The atmospheric conditions (stability class, temperature, wind angle and velocity) are entered in *Atmospheric data* field. Particles sub-menu specifies parameters about, their size, density and sphericity factor concerning the observed particle. In addition, default computed values of V_{g} and U_{d}, are adjustable if they do not correspond to the reality. Deposition measurements at sensors are entered in *Inverse*

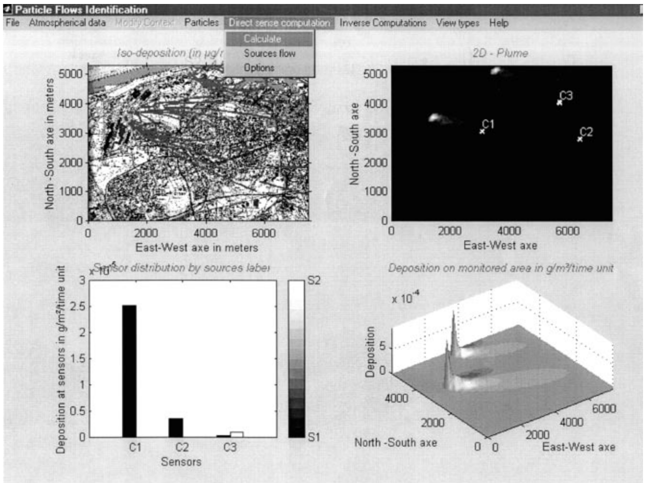

Fig. 2. Software view after a direct session.

computation field. One of the three inverse methods (*least square*, *regularized least squares*, and *constraint least squares*) must be chosen; in *option*, the default regularization parameter value is displayed and is also adjustable. Computation results are displayed by four graphic windows (see Figs. 2 and 3) giving information on iso-deposition plot (see Fig. 4), flow estimates, sensor measurements and sensor observations as a function of sources label. Direct *sense computation* can be applied to simulate some experiences with the knowledge of real source flows provided by flux measurement at sources (ex: thrown out of chimney) see Fig. 2.

8. Simulation results on particles flow identification

The previous models and some inverse techniques have been implemented. It is assumed that the soil is flat, so that the dry deposition model is reasonably suited

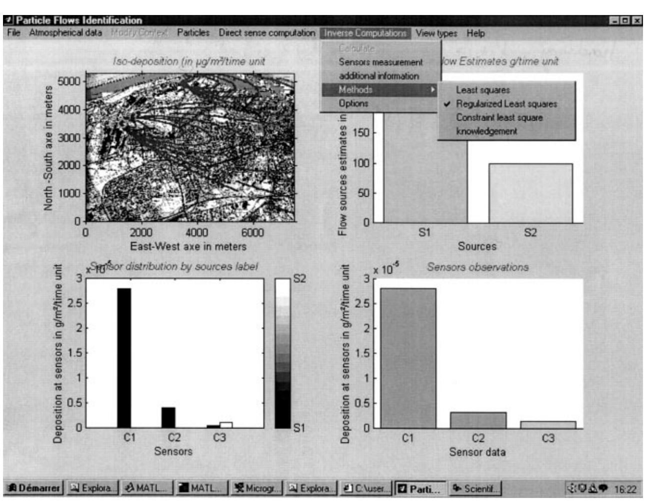

Fig. 3. Software view after an inverse session.

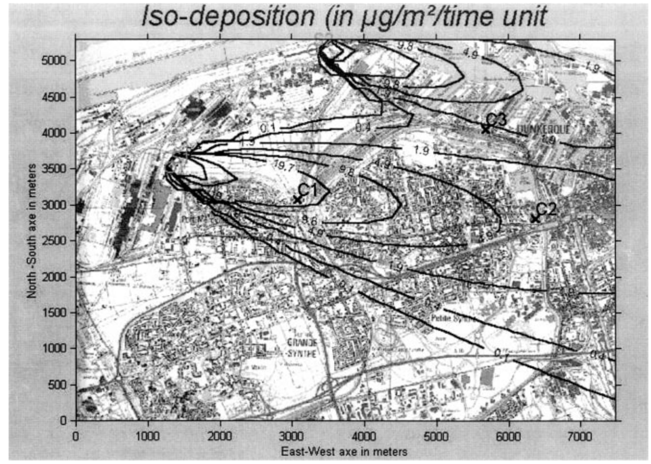

Fig. 4. Geographical sensors location and iso-deposition plot.

to a practical situation. Depositions have been computed at the receptor location by using the Ermak point source model. Operating conditions are listed below. They gather wind intensity and angle, atmospheric stability class, temperature, sources location and sensors location, particle characteristics:

- Atmospheric conditions : U=40±10 km/h, θ=280°±10, stability class 'B', Temperature: 20°C
- Sources data Table 1
- Sensor data Table 2
- Particles characteristics: particle diameter d=100 μm, sphericity factor $\psi\simeq 1$, volume density ρ=2.5 g/m^3

  For accurate positions, the reader is invited to look at the Fig. 4. Let us notice that, the wind definition corresponds to a north-west coming wind (meteorological definition). Other conditions are classical atmospheric data. We can easily notice that sensors are 1 km or greater from the industrial point source.

Ideally, when all these data are accurate (simulated data), the inverse technique provides an estimation of the source flow. With a least squares technique, estimation flux is roughly equal to theoretical source flow.

With the noised measurements of the previously described experiment, the return result of the estimated flows is given in Table 3.

As previous considerations indicated, the greatest estimates error are decreased from 21.6 to 7% due to reg-

Table 1
Sources data

Sources	Location (x,y,z) in m	Theoretical average flow in g/s
Q1	(1317; 3514; 20)	200
Q2	(3296; 5144; 3)	100

Table 2
Sensor data

Sensor	Location (x,y,z) in m	Simulated data (μg/m²/s)	Measures (μg/m².s)	Relative error $\frac{\Delta m}{M_{th}}$ (%)
C1	(3082, 3065, 1)	25.1	27	8
C2	(6377, 2806, 1)	3.57	3.2	10.2
C3	(5692, 4046, 1)	1.27	1.5	18

Table 3
Return result of estimated flows

Sources	Theoretical flow (g/s)	Estimates by LS	$\frac{\|\Delta Q\|}{\|Q^{est}\|}$ %(LS)	Estimates by RLS	$\frac{\|\Delta Q\|}{\|Q^{est}\|}$ % (RLS)
Q1	200	214	7%	214	7%
Q2	100	121.6	21.6%	101	1%

Table 4
The following variations are obtained with around average wind conditions (280°; 40 km/h)

Wind variations	Kernel variation ε	A priori $\frac{\|\Delta Q^{mod}\|}{\|Q\|}$	A posteriori $\frac{\|\Delta Q\|}{\|Q\|}$	Q^1_{est} ; Q^2_{est} in g/s
+10 km/h	2%	35%	9.3%	218 ; 90
-10 km/h	0.5%	8.4%	7.7%	212 ; 88
+5°	14%	159%	20%	190 ; 57
−5°	38%	212%	92%	120 ; 35
+10 km/h, −5°	74	328%	220%	65 ; 85

ularized least squares (RLS) with α=1.7×10^{-7}. The corresponding relative prediction error is 7.3%, lightly up to the 5% minimum weighted in Eq. (26).

Concerning modelling errors, simulation shows the estimates' large sensibility with respect to the relative variation ε% of the kernel matrix G. Some results are gathered in Table 4 in which we observe the maximum relative estimate error $\frac{\|\Delta Q^{mod}\|}{\|Q\|}$ computed a priori by Eq. (32) and the relative real error $\frac{\|\Delta Q\|}{\|Q\|}=(Q^{est}-Q)/Q$ calculated a posteriori. We have to etablish that wind angle is more sensible on kernel matrix G than wind speed, inducing large variations and inacurrate source flow estimates.

Let us note that, with average effect of the norm, *a posteriori* error is smaller than the *a prior error* which is however a good prediction of the maximum error encountered on the worst estimate.

9. Conclusion

This paper has created an opportunity to bring to the fore the regularized least squares method in the flow estimation of particles emission. Initially, a particles transport model adapted for our problem was presented. Then, the least squares method is repeated in its regularized derivation. Error considerations have been considered to show how to associate an imprecisions evaluation with estimated flows. Finally, some simulation results are presented to evoke the robustness problem with respect to wind direction and speed.

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[2] Matlab, is registered trademark of the Mathworks, Inc

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