An Inversion Algorithm for Multiple-Source Dispersion and Deposition of Particulate Matter

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ABSTRACT

Our project investigates the dispersion and deposition of pollutant particles under the influence of diffusion, advection by the wind and gravitational settling effects. The primary aim is to aid Teck Cominco Ltd. in obtaining better estimates of yearly releases into the atmosphere of certain pollutants in the smelting area of Trail, B.C.

This Inverse problem is often referred to as "inverse source modeling and computation". We explain a new approach for estimating the emitted quantity of particulate matter for each chemical, from each stack. Our model incorporates an exact solution to an idealized steady-state of the 3-D advection-diffusion equation, into an optimization solver to find the emission rates from the amount of monthly deposited matter in the receivers. The model allows input site-specific constraints derived from the chemical processes, which help decrease the error in the solution.

1 BACKGROUND AND MOTIVATION

The problem description:

- 4 stacks emitting Zn, Pb, etc., at an unknown, constant rate.
- very expensive to measure release rates directly.
- difficult to estimate due to the complicated processes.
- pollutant particles are dispersed into the area under the influence of diffusion, advection by the wind and settling effects.
- local wind profile is known through measured data.
- known monthly pollutant accumulation in 10 receptors/ 'dustfall jars'.
- information from the processes give some constraints
- need to estimate the emission rates given these data and constraints.

Targets of this project are:

- Modelling the dispersion and deposition of the pollutant particles.
- Research mathematical methods to solve the problem.
- Build an optimization code that approximates the release rates.
- Develop a method to be used in similar problems.

The 4 Source (S) and 10 Receiver (R) locations in the map:

2 MATHEMATICAL MODEL

The advection-diffusion equation for the concentration C of one pollutant from one source:

$$C(x,y,z,t)_t + \nabla \cdot (U(x,y,z,t) - W)C(x,y,z,t) = \nabla \cdot (K(x,y,z)\nabla C(x,y,z,t)) \quad (1)$$

where U is the wind velocity, W the (vertical) constant settling velocity and K_i the difussion coefficients.

For a steady-state solution, we use the following assumptions:

- U is constant and in the x-direction.
- diffusion coefficient $K(x,y,z) = K(x)$.
- W, the settling velocity, is approximated by Stokes' Drag Formula for spherical objects.
- Since the advection due to the wind is much larger than diffusion in the x-direction, we can safely neglect the later.
- Boundary Conditions: $C \to 0$ as $|x| \to \infty$, $|y| \to \infty$ or $z \to \infty$
- continuous point source with constant strength/rate Q at $(0,0,h)$: $C(0,y,z) = Q\delta(y)\delta(z-h)/U$.
- Deposition on the ground boundary condition: $[K\frac{\partial C}{\partial z} + WC]_{z=0} = VC|_{z=0}$, where V is a deposition velocity.

An exact formula for the steady-state solution of the concentration:

$$C(x,y,z) = \frac{Q}{2\pi U\sigma_y\sigma_z}\exp\left(\frac{-y^2}{2\sigma_y^2}\right)\exp\left(\frac{-W(z-h)}{2K} - \frac{W^2\sigma_z^2}{8K^2}\right)\left[\exp\left(\frac{-(z-h)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z+h)^2}{2\sigma_z^2}\right) - \sqrt{2\pi}\frac{V_1\sigma_z}{K}\exp\left(\frac{V_1(z+h)^2}{K} + \frac{V_1^2\sigma_z^2}{2K^2}\right)\operatorname{erfc}\left(\frac{V_1\sigma_z}{\sqrt{2}K} + \frac{z+h}{\sqrt{2}\sigma_z}\right)\right] \quad (2)$$

where $V_1 = V - \frac{1}{2}W$ and $\sigma_y^2 = \sigma_z^2 = \frac{2}{U}\int_0^x K dx'$.

The deposition flux on the ground is $-J_z(x,y,z=0)$ where:

$$J_z(x,y,z) = -K_z\frac{\partial C}{\partial z} - WC. \quad (3)$$

The deposition per unit time in a receptor located at position (r_i) having a cross-sectional area A (assumed very small) is approximated by:

$$D_A = \int_A -J_z(x',y',z')\mathbf{dx'} \approx -AJ_z(r_i).$$

3 KEY IDEAS

- The source strength Q is a linear constant factor in the solution for the concentration C and the ground deposition flux $-J_z(z=0)$.
- To use these solutions, we need the steady-state assumptions to hold.
- The assumptions hold for small enough Δt time units , e.g. $5-10$ mins when changes in the wind velocity are negligible.
- We use component of the velocity in the source-receptor direction.,
- Hence, $J_z(x,y,z,U) = QF(x,y,z,U)$, where F is some function derived from equation **2** and **3**.

Based on this 1-source, 1-particulate solution information, we can:

- sum up a sequence of depositions at a receptor with area A, over a number N of discrete time steps

  $$D_A = -A\Delta t Q\sum_{k=1}^{N} F(x,y,z,U_k)$$

  where U_k are wind components at time step k
- the source strength Q still appears linearly in the deposition.
- can directly determine the source strength Q if we know D_A.

4 HANDLING MULTIPLE SOURCES

- We have: ten receptors located r_i, $i = 1,\ldots,10$ and four sources with strength Q_j located at s_j, $j = 1,\ldots,4$.
- We subdivide the total time interval of interest into N equal time intervals Δt, in each of which the wind velocity U_k, $k = 1,\ldots,N$ is known.
- All the receptors are the same, with cross-sectional area A.

The deposited material D_i into receptor at r_i over the total time interval is:

$$D_i = -A\Delta t\sum_{j=1}^{4}\sum_{k=1}^{N} J_z(r_i,s_j,U_k) = -A\Delta t\sum_{j=1}^{4} Q_j\sum_{k=1}^{N} F(r_i,s_j,U_k) = A\Delta t\sum_{j=1}^{4} Q_jG_{ij} \quad (4)$$

where F and G are explicit known expressions from the explicit concentration solution 2. They are still linear in the Q_j, and easily computable.

This information can be written in terms of a matrix-vector system:

$$\begin{pmatrix} G_{1,1} & G_{1,2} & G_{1,3} & G_{1,4} \\ G_{2,1} & . & . & . \\ . & . & . & . \\ G_{11,1} & . & . & G_{11,4} \end{pmatrix}\begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{pmatrix} = \frac{1}{A\Delta t}\begin{pmatrix} D_1 \\ D_2 \\ \ldots \\ D_{11} \end{pmatrix}$$

where G is an 10×4 computable matrix, Q is an unknown 4×1 vector, and D is an 10×1 vector known from measured data.

The underdetermined system above can be solved for Q_j using a linear least squares method.

5 MULTIPLE PARTICULATE SPECIES

The sources in our problem emit a number of different particulates:

- Source 1 emits Zn^{2+}, SO_4^{2-}
- Source 2 emits Zn^{2+}, SO_4^{2-}, Ca^{2+}
- Source 3 and 4 emit Zn^{2+}, SO_4^{2-}, Sr^{2+}

which represent a total of 11 discrete source rates to be determined.

Using the model above for one chemical species, we construct a large matrix-vector system for all 11 emission rates at each source and their net deposition over a one-month period at each receptor:

$$\begin{pmatrix} G_{Zn^{2+}} & 0 & 0 & 0 \\ 0 & G_{SO_4^{2-}} & 0 & 0 \\ 0 & 0 & G_{Sr^{2+}} & 0 \\ 0 & 0 & 0 & G_{Ca^{2+}} \end{pmatrix}\begin{pmatrix} Q_{Zn^{2+}} \\ Q_{SO_4^{2-}} \\ Q_{Sr^{2+}} \\ Q_{Ca^{2+}} \end{pmatrix} = \frac{1}{A\Delta t}\begin{pmatrix} D_{Zn^{2+}} \\ D_{SO_4^{2-}} \\ D_{Sr^{2+}} \\ D_{Ca^{2+}} \end{pmatrix}$$

The G, Q and D terms represent the matrices and vectors defined previously for each of the individual chemicals.

We can solve the resulting sparse system for the emission rates from each source using a linear least squares solver.

6 SITE-SPECIFIC CONSTRAINTS

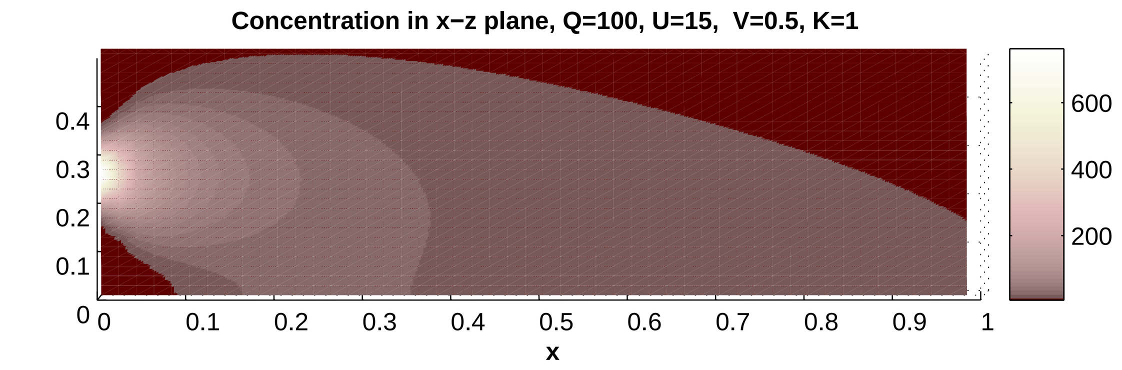
We have identified some site-specific constraints coming from the chemical and industrial processes that can be inputted into the solver:

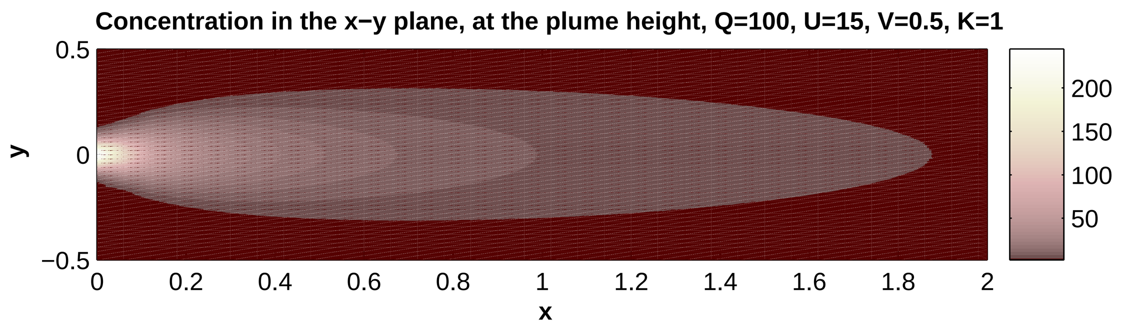
- At Source 1, Zn^{2+} is emitted at the same rate as SO_4^{2-}.
- At Source 2, SO_4^{2-} comes from both $ZnSO_4$ and $CaSO_4$. So we expect $Q_{Zn^{2+}} + Q_{Ca^{2+}} = Q_{SO_4^{2-}}$.
- At Sources 3 and 4, we expect $Q_{Zn^{2+}} \leq Q_{SO_4^{2-}}$.
- At Sources 3 and 4, Sr is emitted at the same rate.

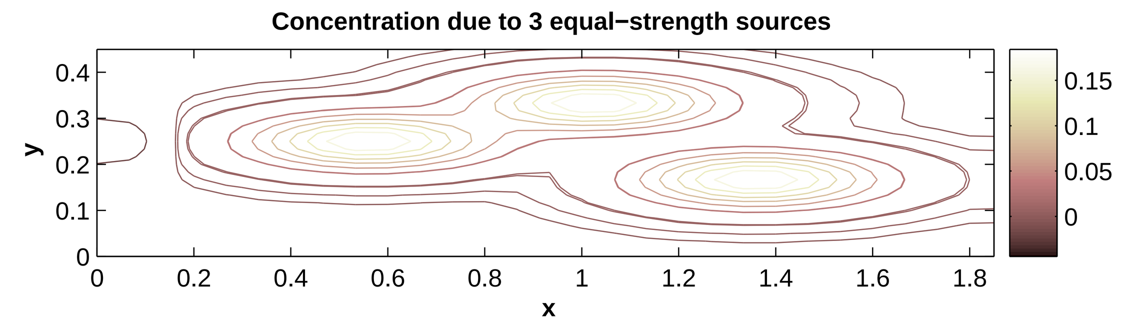
The equality constraints can reduce the number of unknowns from eleven to seven, and there exist minimization methods flexible enough to handle the remaining inequality constraints.

7 SOME FIGURES

Plots of concentration C, due to one or more sources:







8 CONCLUSIONS AND FUTURE WORK

- Modelled correctly the physics of dispersion and deposition.
- Included an exact steady-state solution idea into a linear solver.
- Can accommodate the effects of rain, insolation, ground diversity .
- Versatile to suit other similar problems, with many sources, receptors, particulates.
- Can include constraints depending on the problem.

Work in progress or for the near future:

- Run the algorithm with the real data and analyze results.
- Investigate the numerical stability of the algorithm (inverse problems are ill-posed) and suitably determine the optimization methods to use.
- Perform tests to determine the efficiency and accuracy of the algorithm.

References

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CREDITS

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