Mathematics of Air: Modelling of Pollutant Transport in the Atmosphere

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Acknowledgments

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Fraunhofer Institut Techno- und Wirtschaftsmathematik, Kaiserslautern
(Institute for Industrial Mathematics)
Teck Cominco operates one of the world’s largest integrated lead-zinc smelting operations in Trail, British Columbia, on the Columbia River.

It is a major driver of the BC economy and one of Canada’s biggest polluters (lead, arsenic, cadmium, mercury, zinc, SO₂, ...).

Annual emissions reporting is required under the National Pollutant Release Inventory [http://www.ec.gc.ca].
Historical Sidebar

- Trail was founded in 1890s as a mine supply point. A small smelter was built.
- In 1906, Cominco was formed.
- In 1941, WA state was awarded damages from Cominco for trans-border pollution – one of the most-cited international law cases.
- From 1917 to 1940, emissions of \( \text{SO}_2 \) were 100–700 T/yr. Currently down to 22 T/yr.
- Today Teck Cominco prides itself on its “clean” Trail operations.
The Problem

- Teck’s Trail operation is currently unable to directly measure Zn stack emissions in a reliable or cost-effective manner.
- Past Zn emissions reporting relied on simple “engineering estimates” of chemical processes.
- Measurements of the following particulates were made using “dustfall jars” during 2001–2002: zinc (Zn), sulphates (x-SO$_4$), strontium (Sr).
Key Questions

1. Is there a robust method that will provide *reliable* estimates of stack emission rates based on deposition measurements?

2. And what is “reliable”? ... errors of 25-50% in estimates are considered acceptable, as long as they are *overestimates*!
My Aims

To take you on a mathematical journey through . . .

- **Models:** illustrating a model of a physical phenomenon (here, model = equations).

- **Applications:** demonstrating how “classical” mathematics can be applied to a problem of direct importance to industry.

- **Generalizations:** focusing on underlying general mathematical structures.

To a mathematician, the beauty of a problem is in its **structure**!
1. Background: Atmospheric Dispersion

2. The Gaussian Plume Solution

3. Application to Trail Smelter
Atmospheric dispersion refers to transport of airborne contaminants via two processes:
1. advection by the wind, and
2. turbulent diffusion.

Reduces to solving the advection-diffusion equation

\[
\frac{\partial C}{\partial t} + \vec{u} \cdot \nabla C = \nabla \cdot (K \nabla C) + Q
\]

where
- \( C(\vec{x}, t) \) = unknown contaminant concentration \((kg/m^3)\)
- \( \vec{u}(\vec{x}, t) \) = given wind velocity \((m/s)\)
- \( K \) = turbulent eddy diffusivity \((m^2/s)\)
- \( Q(\vec{x}, t) \) = emission source term \((kg/m^3 s)\)
A variety of approaches have been used for the solving the advection-diffusion equation:

- **analytical** – Fourier series, Green’s functions, Laplace transforms, asymptotics.
- **computational** – finite difference, finite volume, spectral.

Most industry-standard software is based on Gaussian plume solutions (see “Recommended Models” at www.epa.gov).

Most previous work has focused on the **forward problem**: 

*Given a set of source emission rates, calculate deposition*

and much less on the **inverse problem**: 

*Given a set of deposition values, calculate emission rates*
Other Applications

A THEORETICAL FRAMEWORK FOR DATA ANALYSIS OF WIND DISPERSAL OF SEEDS AND POLLEN

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APPLICATION OF A GAUSSIAN PLUME MODEL OF ODOR DISPERSION TO SELECT A SITE FOR LIVESTOCK FACILITIES

Authors: Chastain, John P.; Wolak, Francis J.
Source: Proceedings of the Water Environment Federation, Odors and VOC Emissions 2000, pp. 745-758(14)
Publisher: Water Environment Federation
Ability of the Gaussian plume model to predict and describe spore dispersal over a potato crop

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Received 2 November 2000; received in revised form 24 October 2001; accepted 31 October 2001
Other Applications

- Insect infestations: locusts, mountain pine beetles.
- Radioactive particles (e.g., Fukushima reactor accident).
- Ash from volcanic eruptions.
- Dust and exhaust from automobiles.
- Contaminant transport in groundwater.
- Motion of pedestrians in crowds.
- Diffusion of languages/dialects in populations. Etc., etc…

Contaminant transport in groundwater

Mount Merapi eruption, Java (2010)
Outline

1. Background: Atmospheric Dispersion
2. The Gaussian Plume Solution
3. Application to Trail Smelter
Typical assumptions for a single, isolated stack:

- Stack is an elevated point source located at \((0, 0, H)\).
- Constant emission rate \(Q\).
- Wind velocity \(\vec{u} = (U, 0, W_{set})\) is constant with \(W_{set} \ll U\).
- Ground-level deposition is at constant speed \(W_{dep}\).
- Diffusion downwind is negligible compared to convection \((K_x = 0)\).
- Steady state – we’ll relax this later.
**Governing Equations**

**Advection-diffusion equation reduces to:**

\[
U \frac{\partial C}{\partial x} - W_{\text{set}} \frac{\partial C}{\partial z} = \frac{\partial}{\partial y} \left( K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial C}{\partial z} \right) + Q \delta(x) \delta(y) \delta(z - H)
\]

**Boundary conditions:**

\[
K_z \frac{\partial C}{\partial z} + W_{\text{set}} C = W_{\text{dep}} C \quad \text{at } z = 0 \quad \text{(deposition)}
\]

\[
C \to 0 \quad \text{as } x, y \to \pm \infty \text{ and } z \to \infty
\]
Gaussian Plume Solution

Assume no settling or deposition ($W_{set} = W_{dep} = 0$) and use Laplace transforms to obtain the Gaussian plume (GP) solution:

$$C(x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \left[ \exp\left(-\frac{(z - H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + H)^2}{2\sigma_z^2}\right) \right]$$

where $\sigma_{y,z}^2(x) = 2xK_{y,z}/U$. 
Note the peak in ground-level concentration downwind of the elevated source.
Examples: Plume Animations

Actual plume dynamics are more complex:

1. Numerical simulation of a stack plume.
2. Eyjafjallajökull volcanic eruption, Iceland.
3. Cesium-137 emissions from Chernobyl, Ukraine.

Fig. 1. Schematic of dispersion showing realizations of an instantaneous and time-averaged plume as well as the ensemble-average behavior.
Ermak’s Solution with Deposition and Settling

Ermak (1977) derived a modified GP solution with deposition and settling:

\[
C(x, y, z) = \frac{Q}{2\pi U\sigma_y\sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{W_{set}(z - H)}{2K_z} - \frac{W_{set}^2\sigma_z^2}{8K_z^2}\right) \\
\times \left[ \exp\left(-\frac{(z - H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + H)^2}{2\sigma_z^2}\right) \right] \\
- \sqrt{2\pi} \frac{W_o \sigma_z}{K_z} \exp\left(\frac{W_o(z + H)}{K_z} + \frac{W_o^2\sigma_z^2}{2K_z^2}\right) \text{erfc}\left(\frac{W_o\sigma_z}{\sqrt{2}K_z} + \frac{z + H}{\sqrt{2}\sigma_z}\right)
\]

where \( W_o = W_{dep} - \frac{1}{2} W_{set} \).

**Key:** Deposition flux is linear in \( Q \)! That is, \( W_{dep}C\mid_{z=0} = PQ \).
Outline

1. Background: Atmospheric Dispersion

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3. Application to Trail Smelter
So far, we’ve considered a single source in a constant wind.

We still need to include:

- Time-dependent wind velocity, not aligned with x-axis:
  - Shift and rotate coordinates
  - Sum over discrete time intervals to get total deposition
- Multiple sources and receptors
- Multiple contaminants (Zn, SO$_4$, Sr)
- Ultimately . . . solve the inverse problem
Multiple Sources

Four sources \((S_n)\) and nine “dustfall jars” or receptors \((R_n)\):

![Map of Trail Smelter area with marked sources and receptors](image-url)
Multiple Sources

- Sources $Q_s$ with $s = 1, 2, 3, 4$.
- Total deposition zinc $D$ from all sources is

$$D = \sum_{s=1}^{4} P_s Q_s$$

where $P_s$ depends on the location, wind, and problem parameters.
Sample Output

One month cumulative zinc deposition using actual wind data:

Contours of Zn concentration (g/m²)

Wind histogram

Due to Columbia River valley, wind is unidirectional!
Multiple Receptors

- Receptor measurements $D_r$ with $r = 1, 2, \ldots, 9$.
- Total deposition of zinc from all sources is

$$D_r = \sum_{s=1}^{4} P_{rs} Q_s$$

or in matrix-vector form

$$\vec{D} = \mathbb{P} \vec{Q}$$

where

- $\vec{D}$ is a 9-vector
- $\vec{Q}$ is a 4-vector
- $\mathbb{P}$ is a $9 \times 4$ matrix
Inverse Problem

- Equations $\vec{D} = \mathbb{P}\vec{Q}$ represent an over-determined system for the $Q$'s, consisting of 9 equations in 4 unknowns.
- We actually have three such systems for zinc, sulphate, strontium:

  
  \[
  \vec{D}^{Zn} = \mathbb{P}^{Zn}\vec{Q}^{Zn}, \quad \vec{D}^{SO_4} = \mathbb{P}^{SO_4}\vec{Q}^{SO_4}, \quad \vec{D}^{Sr} = \mathbb{P}^{Sr}\vec{Q}^{Sr}
  \]

  $\Rightarrow$ 27 equations in 12 unknowns.

- Additional linear constraints on $\vec{Q}$'s arise from chemical processes.

**Conclude:** This can be solved as a constrained linear least squares problem (Gauss again).
The ill-conditioned nature of this inverse problem is well-studied in a series of papers by Enting & Newsam (1988). When measurements are taken at very long range or at high altitudes, then ill-conditioning can be severe. 

**BUT . . .** “The relatively mild degree of ill-posedness in the [close-range] surface source deduction problem makes the numerical inversions feasible.”
Numerical Simulations

- Use Matlab’s constrained linear least squares solver `lsqlin`.
- Each run requires approx. 30 sec on a Mac laptop – fast!
- Use “engineering estimates” of zinc emissions as a guide:

\[ \vec{Q}^{Zn} \approx [35, 80, 5, 5] \text{ tons/yr} \]
Zn and SO$_4$ data are mostly consistent from month to month.

**Exception:** Zn depositions at R3.

Sr data exhibit more variation (experimental error?).
Results: Emission Rates

Measured depositions

Computed emission rates
Results: Emission Rates

Measured depositions

May 1–30, 2002

Jun 3–Jul 2, 2002

Computed emission rates

May 1–30, 2002

Jun 3–Jul 2, 2002
Conclusions (so far)

- The method seems to captures total Zn emissions well (GP approach conserves mass approximately).
- Individual Zn emission estimates still vary considerably.
- **Hypothesis:** Discrepancies in the inverse solution can be attributed to measurement errors, specifically at R3.
Results: Without R3

Emission estimates without R3 are much more consistent!
What’s the Problem with R3?

There is a debris pile containing zinc tailings adjacent to R3!
Summary

- Applied the Gaussian plume model to contaminant transport.
- Linearity in $Q$ allowed superposition of all sources.
- Emission rates can be estimated from measured deposition data using linear least squares method.
- Consistent estimates are found for total zinc emissions . . . which is all that’s required from a regulatory standpoint!
- Teck Cominco incorporated our results into their annual reporting to Environment Canada.
- These results are published in:
  
  
Summary: Mathematical Structure

- The same approach can be used for a diverse collection of phenomena involving transport of contaminants, pollen, dust, groundwater, crowds, languages, etc.
- The common thread of is the underlying mathematical structure:
  - partial differential equations (advection + diffusion)
  - over-determined linear systems
  - ill-conditioning
  - constrained optimization (least squares)
Current and Future Work

- We recommended that:
  - A full year’s wind and deposition data be collected.
  - More receptors be added.

- Teck Cominco has just completed another round of measurements (May 2010–Feb. 2011) which I am investigating right now with . . .

  **Sudeshna Ghosh**
  - PhD student
  - Internship funded jointly by MITACS and Teck Cominco

- We also plan to validate our results using direct simulations of the advection-diffusion equation (“forward problem”).
Thank-you!
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U.S. Environmental Protection Agency.