Snapshots of modern mathematics
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Drugs, herbicides, and numerical simulation

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The Colombian government sprays coca fields with herbicides in an effort to reduce drug production. Spray drifts at the Ecuador-Colombia border became an international issue. We developed a mathematical model for the herbicide aerial spray drift, enabling simulations of the phenomenon.

1 Drugs and Herbicides

The broad-spectrum herbicide Glyphosate is used by the Colombian government to spray coca fields close to the Ecuadorian border in an effort to reduce drug production. Glyphosate was discovered in 1970 and brought to the market by the company Monsanto under the commercial name "Roundup", [10]. The patent expired in 2000. Since then, many companies have produced the herbicide and it is available in the market under several trade names, e. g. Roundup, Buccaneer, Razor Pro, etc. The Colombian sprays have taken place for a number of years and have been more frequent after 2000, when Plan Colombia started. The Plan Colombia is an initiative conceived between 1998 and 1999 by the administration of Colombian President Andrés Pastrana with the goals of ending the Colombian armed conflict and creating an anti-cocaine strategy. It was supported by US military and counter-narcotics aid. One controversial element of the anti-narcotic strategy is aerial fumigation to eradicate coca fields.

This activity has come under fire because it damages legal crops and has adverse health effects upon those exposed to the herbicides [11].

Spray drifts into Ecuadorian territory became a big issue for people living close to the border. Their negative impact on health and agriculture have been observed and confirmed by intensive studies, e. g. [1]. Hence, in 2005 Ecuador and Colombia signed an agreement to stop the sprays in a 10 km corridor along the border, see Figure 1. However, measurements on Ecuadorian territory indicated that significant amounts of Glyphosate spray had still drifted into Ecuador. The sprays stopped in 2007 and a trial at the International Court of Justice started.

In September 2013 the case was settled with an agreement that "sets out operational parameters for Colombia's spraying programme, records the agreement of the two governments to ongoing exchanges of information in that regard, and establishes a dispute settlement mechanism" [7]. In the settlement, Colombia also agreed to pay 15 million US dollars to Ecuador [5].

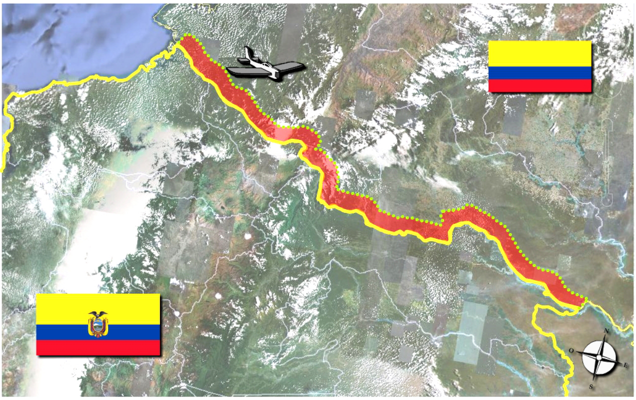

Figure 1: Illustration of the 10 km corridor along the Ecuador-Colombia border. (Airplane not to scale.)

2 Sprays at Ecuador-Colombia border

Spray application procedures and general guidelines have been proposed in the context of agriculture in order to maximize the effectiveness of plant protection products and minimize risks to public health and the environment. For the sprays at the Ecuador-Colombia border, some of these guidelines either cannot be followed, e. g., the maximum aircraft spray height due to the topography of the zone, or they were not followed, e. g., the droplet size, see [1] and references therein. These issues result in demands for a new mathematical model (see section 3) that considers the particular spray procedures at the border and deals with technical difficulties such as the size of the spray zones and the accuracy required. Most of the earlier models like the AgDrift [9] require at least input data representing:

a) aircraft flight conditions,
b) the nozzles,
c) the droplet size distribution,
d) the spray material properties, and
e) the meteorology conditions.

For the sprays at the Ecuador-Colombia border: a), b) and c) are not known. Moreover, d) and e) are difficult to estimate due to the facts that the exact composition of the herbicide is not known and that there are no weather stations near the zones of interest, i.e., the areas where the sprays took place. These regions were chosen in cooperation with an interdisciplinary team of biologists, engineers, and geophysicists investigating the effects on human beings, animals and the grounds. In Figure 2, these zones as well as the direction of the average wind are visualized. Table 1 contains the location of the zones.

Place	Area (km^2)	Longitude	Latitude	Wind (km/h)
El Conejo	8.8 x 10	0.23	-76.90	7
San Marcelino	12.9 x 10	0.24	-76.76	6
Chanangue	16.0 x 10	0.23	-76.60	5

Table 1: Area, location and average wind for the zones of interest

The following are some international guidelines for aerial sprays [6]: verify the direction of the wind, no application within 46 m of an unprotected person, use largest droplet size (the minimum recommended size is 500 μm), spray when wind speeds are between 4.7 and 16.2 km/h, avoid spraying in low humidity and high temperature conditions, do not spray during temperature inversions, maximum spray height of the aircraft is 25 m. In the particular case of the sprays at the Ecuador-Colombia border, the average droplet size was 150 μm, the spray height of the aircrafts was up to 80 m [1], in some zones there are low humidity and high temperature conditions.

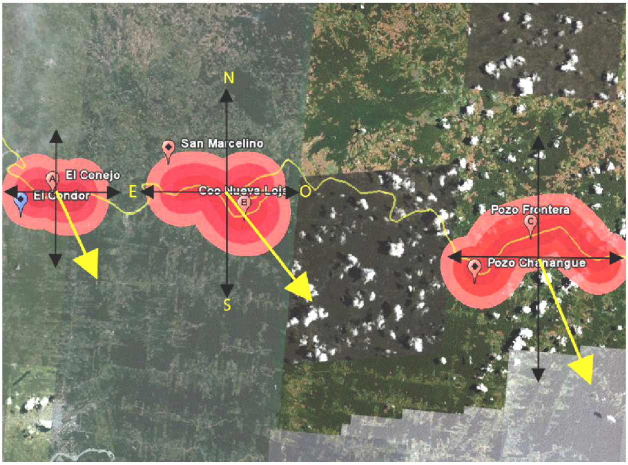

Figure 2: Illustration of the sensitive zones at Ecuador-Colombia border and direction of average wind

3 Mathematical model

Our aim is to link the data we obtained from observations in the real world to our mechanistic understanding of how spray drift happens. This is where a mathematical model comes into play. It allows us to encode our observed data into mathematical language and interpret the output with the help of statistics and partial differential equations. We aim to find patterns in the observed data and extrapolate new knowledge about the underlying processes. Of course, the accuracy of such a mathematical model depends on the quality of the used data as well as on the focus we laid during in the model, i. e., which ingredients we consider central in the process.

Most studies of spray drift so far have focused on the extent of near-field drift under varying meteorological conditions and application methods. Taking into account into our mathematical model the particular procedure of the sprays close to the Ecuador-Colombia border, we conclude that a model for the Glyphosate aerial spray drift has to fit the following criteria: small droplet size, diffusion and transport are the dominant phenomena, simulation domains are considerably large compared to the size of the droplet sources, sprays take place at a height higher than the recommended maximum (25 m) which implies more evaporation and more drift, many input parameters are unknown.

If we tried to take the full physical dynamics of the spray into account, we would have to solve the so-called Navier-Stokes equations, a very complicated system of partial differential equations. This, however, is not feasible with current computational resources. Instead, we propose a simplified model to characterize the spray drift both qualitatively and quantitatively. We assume that the spray plume released by the aircraft is composed of a range of droplet sizes whose distribution is dependent on actual operation conditions, e. g., break-up of droplets due to turbulence.

The larger droplets will fall down within a relatively short distance of the release point, and thus are not relevant to the presumed phenomenon of significant amounts of herbicide drifting 10 km or more.

Very small droplets, however, have a very low mass in relation to their surface area. Thus, they do not just fall down, but behave more like mist droplets, suspended in the surrounding air. Their movement is primarily dictated by the motion of the air they are suspended in. These droplets can travel long distances, transported by the wind.

As we are not primarily interested in the paths of individual droplets, we move on to averaged concentrations of droplets in the air, and even further, to concentration of the herbicide in the air. The dynamics of the concentration over long timescales are mainly described by two effects:

1. transport (convection) due to the mean flow field velocity of the surrounding air and the (very slow) fall of the small droplets, and
2. diffusion, i.e. local smoothing of concentration contrasts due to small scale random particle motion and turbulence of the surrounding air (short length and timescale velocity fluctuations).

This leads to the following *convection-diffusion equation*,

$$f = \frac{\partial}{\partial t}c - k_x \frac{\partial^2}{\partial x^2}c - k_y \frac{\partial^2}{\partial y^2}c - k_z \frac{\partial^2}{\partial z^2}c + b_x \frac{\partial}{\partial x}c + b_y \frac{\partial}{\partial y}c + b_z \frac{\partial}{\partial z}c \qquad (1)$$

in $\Omega \times (0, T)$, where

- $f = f(x, y, z, t)$ is the concentration release rate of the airplane,
- $c = c(x, y, z, t)$ is the (unknown) concentration as function of spatial location (x, y, z) and time t[1],
- $k_x, k_y, k_z > 0$ are the diffusion coefficients,
- b_x, b_y, b_z are the components of the wind speed vector,
- Ω is the spatial area under consideration for spray drift, and
- T is the time horizon.

A full description of the equation can be found in [4, 3].

[1] Since c is a function of several variables, it can be partially differentiated with respect to x, y, z, and t. We denote the derivatives with $\frac{\partial}{\partial x}c$, $\frac{\partial}{\partial y}c$, $\frac{\partial}{\partial z}c$, and $\frac{\partial}{\partial t}c$, respectively.

Our model (1) is a partial differential equation (PDE, i. e., an equation relating the partial derivatives of a function to the function itself)[2]. While mathematics provides fairly simple tools to show that this equation has a unique solution c, it is in general not so simple at all to compute this solution. However, there are known numerical methods allowing sufficiently accurate approximation of the solution. The application of these methods leads to a **numerical simulation** of the phenomena, for which we present some results in the following section.

While our model (1) as a PDE is of the same kind as a full-physics model (multi-phase Navier-Stokes equations), it is a far simpler variant of a PDE. The numerical approximation of the solution of the simplified model (1) is far less demanding in computer cycles and memory than for the full-physics model. This makes our model (1) tractable (albeit still challenging) while the full-physics approach is outside of reach and will remain so for the foreseeable future.

4 Numerical simulations

As an illustration we present the simulation using use the finite element[3] software package `FEINS` [8] on a two dimensional domain. For a detailed discussion see [4, 3]. We consider the zone of Chanangue, see Table 1, a square domain of size 16 km $\times$ 10 km with wind 5 km/h. In Figure 3, the spray drift simulation at different times is plotted. Early in the simulation, high concentrations can be observed where the airplane releases the herbicide. With time progressing, the herbicide is spread to a wider area at a lower concentration (dispersion and diffusion), while being transported due to the wind (convection). [4]

5 Conclusions

The main inputs of our mathematical model have to be estimated, e. g., the meteorology conditions are only available as averaged values at nearby locations due to the geographical location. The resulting lack of reliable information and the simplifications constrain the accuracy of the results of the model. Nevertheless, the model allows to study the influence of some parameters such

[2] An example for an easier mathematical model using ordinary differential equations (ODEs) instead of PDEs can be found in the snapshot 10/2013: "The mystery of sleeping sickness – why does it keep waking up" by Funk.

[3] More information about the finite element method can be found for example under http://en.wikipedia.org/wiki/Finite_element_method.

[4] A three dimensional simulation with realistic parameters is currently under way in [2].

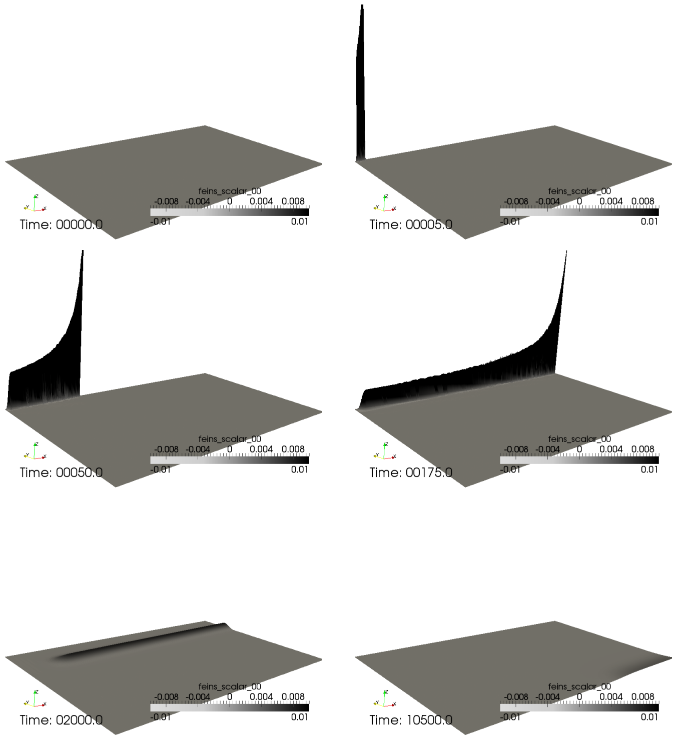

Figure 3: Spray drift simulation on 16 km × 10 km domain, herbicide concentration c in the domain at different times

as the release position on the spray drift. Overall this project shows that applied and numerical mathematics may be used to tackle questions with significant societal impact, and may even help to settle political quarrels on international levels. The project also had the important side effect of advancing the status of Applied Mathematics research in Ecuador, a country where mathematics did not have an overwhelming reputation so far.

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