

# GIS-BASED ATMOSPHERIC DISPERSION MODELLING

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## Abstract

*Atmospheric pollution due to agricultural pesticide is a major concern today, regarding both public health, sustainable agriculture and agro-systems quality monitoring. One aims to model pesticide atmospheric dispersion and to propose a useful predictive tool, using fluid mechanics equations and open-source GIS programming capabilities. This paper focuses on pesticide spray drift modelling for viticulture applications at the watershed scale. Our model tends to provide some georeferenced atmospheric transport simulation outputs at very low calculation cost using solution space reduction and reduced order modelling. This is necessary to make affordable assimilation/simulation and very helpful to quickly perform spatial based risk analysis. The coupling of fluid mechanic equations with GIS is first described, regarding spatialization of inputs/outputs and also the enhancement of the mathematical model according to GIS parameters like topography and scale variations. The GIS based predictive tool is then presented through explanations on coupling methods and technical ramblings about Quantum GIS Plugin development..*

## 1. Introduction

Let us consider environmental multi-scale phenomena presented by the atmospheric dispersion process. These are common in industrial pollutant emissions, fire smoke transport and also agricultural pesticide spray drift (see figure 1). This paper focuses on pesticide spray drift modelling over vineyards, using mathematical modelling and Geographical Information Systems (GIS). Our aim is to provide some georeferenced atmospheric transport simulation models at very low calculation cost, in order to make affordable simulations and to perform atmospheric pollution risk analysis for viticulture applications.

Atmospheric dispersion equations are based on many parameters which are strongly affected by spatial and temporal variations [1]. These variations significantly affect the spray drift's trajectory. The spatial dimension is thus essential in atmospheric dispersion modelling, but also represents the GIS paradigm [2]. GIS have so become an adequate tool to analyze and visualize spatial based environmental models [3]. The coupling of the model with such technologies is presented here, regarding both the use of DEM and the GIS role in the enhancement of the model.



Figure 1. Early morning pesticide cloud observed over vineyards at Neffiès(34)

The optimization of the mathematical model regarding the spatial dimension first appears as necessary as we wish to couple a low-complexity physical model with the landscape representation provided by GIS. This work implies to establish links between the spray drift model and GIS algorithms, by selecting the most significative geospatial parameters that can improve the calculation. Topography effects and scale variations have been naturally chosen as one needed to get an optimized height dimension, in order to implement more reality in the drift phenomenon calculation. Then, a second side of the coupling consists in integrating the model within a GIS environment in the aim to manage and automate the model inputs and to promote its outputs using cartographic rendering.

The goal of the present work is first to improve the former mathematical model regarding the long range transport calculation, and to account for non uniform topographies to get more realistic simulations. We also want to be able to locally optimize the calculation accuracy according to scales variations, by using nested numerical zoom and modifying the wind flow field construction algorithm. Thus, two main aspects are presented in this paper. The optimisation of the dispersion model according to topography and scale changes is first presented using mathematical modelling. The coupling with GIS is then detailed in a second part, regarding the model integration and the main computational tasks. Both modelling and georeferenced simulations will be illustrated through numerical examples and cartographic outputs.

## **2. Reduced Order Modeling of Atmospheric Dispersion**

### **2.1 Preliminaries**

In a previous work we have treated the problem of agricultural pesticide emission and dispersion, by coupling local (i.e. emission and near-field distribution) and global (i.e. transport over large distance) models [4], [6]. In this approach, the local model provides the inlet conditions for the levels above. The dependency between levels is a major asset to avoid the solution of partial differential equations, using model reduction. This is based on adapting search spaces for the

solution of a given model using a priori information. More precisely, a near field (to the tractor's injection device) search space is build using experimental observations. Once this local solution is known, the amount of specie leaving the atmospheric sub-layer is evaluated using analytical integration of the governing equations [5], [6]. The resulting quantity is then considered as candidate for transport over long distances. Similitude solutions are then used for mixing layers and plumes [7], and generalized in a non symmetric travel-time based metric, in the aim to account for general wind flow fields.

## 2.2 Transport and Non Symmetric Geometry

We consider the situation of a source releasing a time dependent quantity  $cinj(t)$  in the atmosphere at a given location, and aim to develop a low-complexity model to represent the dispersion of this quantity. The primary factors influencing the dispersion of a neutral plume are advection by the wind and turbulent mixing. The simplest model of this process is to assume that the plume advects downwind and spreads out in the horizontal and vertical directions. Hence, the distribution of a passive scalar  $c$ , emitted from a given point and transported by a uniform plane flow filed  $U$  along  $x$  coordinate, can be represented by:

$$c(x, y, z) = c_c(x) f(\sqrt{y^2 + z^2}, \delta(x))$$

$$\text{Where : } c_c(x) \sim \exp(-a(U)x) \quad [1]$$

$$\text{and: } f(\sqrt{y^2 + z^2}, \delta(x)) \sim \exp(-b(U, \delta(x))\sqrt{y^2 + z^2})$$

$Cc$  is the behavior along the central axis of the distribution and  $(x)$  characterizes the thickness of the distribution at a given  $x$  coordinate. An analogy exists with plane or axisymmetric mixing layers and neutral plumes where  $\delta$  is parabolic for a laminar jet and linear in turbulent cases [7].  $a(.)$  is a positive monotonic decreasing function and  $b(.,.)$  is positive, monotonic increasing in  $U$  and decreasing in  $\delta$ . In a uniform atmospheric flow field, this solution can be used for the transport of quantities over vineyards, as shown in figure 2. We would like to generalize this solution in a non-symmetric metric defined by migration times based on the flow field and hence treat the case of variable flow fields.

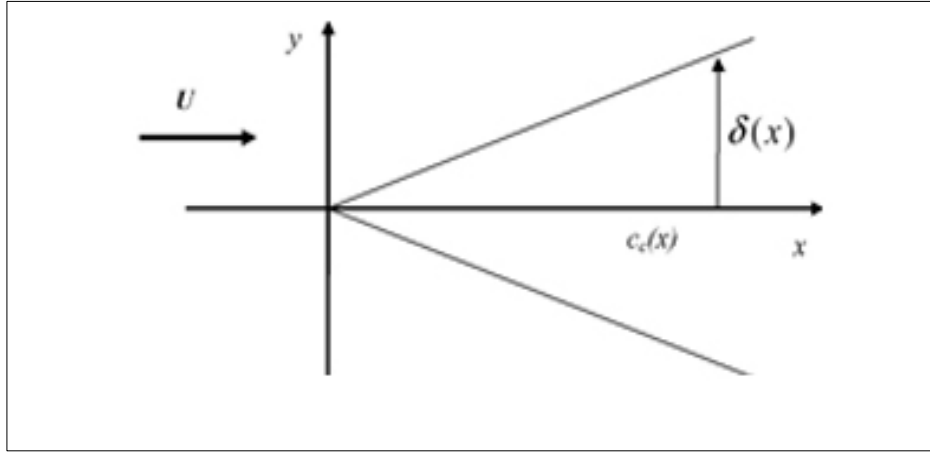


Figure 2. Plume using the Euclidean similitude

$Cc(x)$  : Concentration along the plume axis

$\delta(x)$  : Lateral distance. Thickness of the plume.

### 2.3 Non Symmetric Geometry and Migration Times

Using the Euclidean metric system, a distance function between two points A and B verifies the following relationship:

$$d(A,B)=0 \rightarrow A=B, d(A,B)=d(B,A), d(A,B) < d(A,C)+d(C,B)$$

In our case, we have chosen an original Riemannian metric M, according to which the distance between A and B is given by:

$$d_M(AB) = \int_0^1 \left( {}^t ABM(A+tAB)AB \right)^{1/2} dt \quad [2]$$

where M is positive and symmetric. If  $M=I$  with I as the identity matrix, one can recover the Euclidean geometry. The variable M allows accounting for anisotropy and non uniformity of the distance function, as shown on figure 3. Let's consider now the following distance function definition:

If A is upwind with respect to B then:

$$d(B,A) = \infty \text{ and } d(A,B) = \int_A^{B \perp} ds/u = T \quad [3]$$

T defines the migration time from A to  $B \perp$  along the characteristic passing by A. The local velocity along this characteristic is given by u, and the latter is by definition tangent to the characteristic.  $B \perp$  denotes the projection of B over this characteristic in the Euclidean metric system. We suppose that this characteristic is unique and that it avoids sources and attraction points in the flow field.

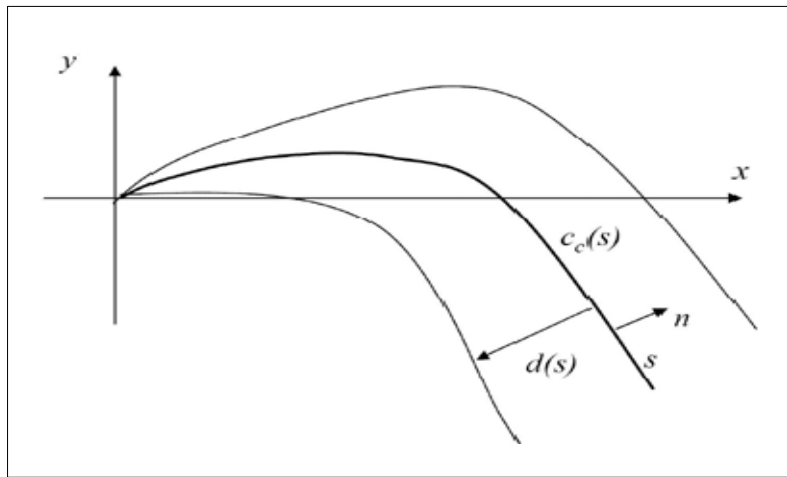


Figure 3. Plume using the the Riemannian similitude

## 2.4 Multi-Level Construction

In realistic configurations, simulation needs be carried out over several hundreds square kilometers domains. At the same time, we must be able to account for local topography variations with details provided every few meters. We saw previously that wind measurements are most of the time available on very coarse grids with only two measurements points being usually distant of several kilometers. These constraints make that it is unrealistic and inefficient to perform the whole simulation with a metric topographic accuracy. Rather we would like to account large scale variations of topography on a coarse level simulation and include gradually the details of the ground variations near the main points of interest. To perform this task, we recursively apply the modelling described above on a cascade of embedded rectangular homothetic domains, as shown on figure 4.

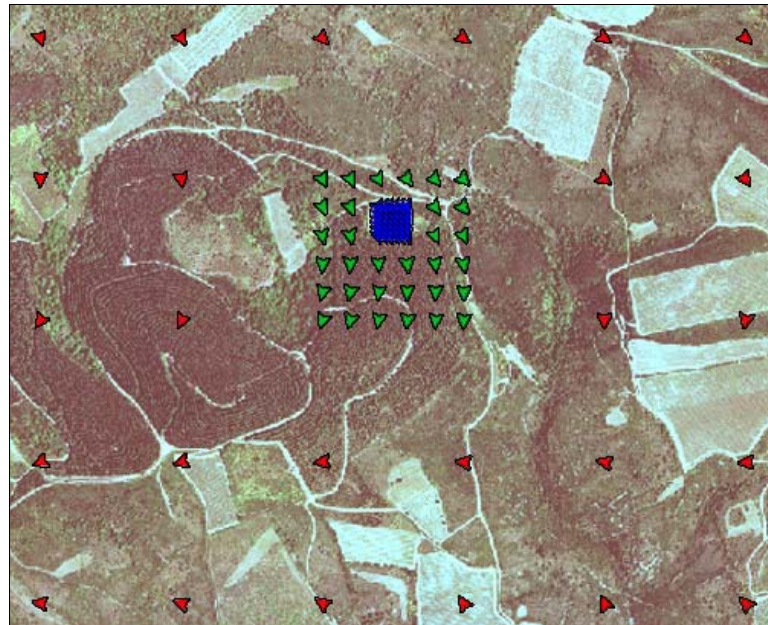


Figure 4. Three-level construction of a flow field loaded into QGIS as a vectorial layer

### **3. GIS Based Coupling**

It first be reminded that we want to couple the above physical model which involves unsteadiness and uncertainties, with GIS that are tending to provide an accurate numerical copy of the study area's surface. Thus, GIS can be used to apply the model in a richer georeferenced numerical environment. GIS capabilities regarding DEM generation and exploitation are improving the former model, as they to launch it on any local topography [8]. Furthermore, GIS permits to map directly the drift process and to get standard atmospheric concentrations at given geographical coordinates. Then it becomes rather easy to make the pesticide cloud interacts with other relevant geodata, and so to proceed to advanced risk analysis regarding for example bystanders exposure, agricultural plots or water courses contamination after treatments. Although GIS allows to gain some more precision regarding topographic impact on calculations and to georeference the model outputs, we should keep in mind that the main objective of the reduced order modeling approach is to provide mean tendencies of the spray drift with very low calculation cost, and that potential errors are duplicated into the GIS. As those limits regarding precision and application on real situation have been raised, it is now interesting to explain more precisely how the model and GIS communicate, and how we can get the best of geospatial techniques to improve the model's efficiency.

#### **3.1 Linking Spray Drift Model With GIS**

Several way to couple GIS and environmental models are known in litterature, mainly "tight" or "loose" coupling and more recently "integrating" systems [9], [10]. Each technique presents assets and limitations, and is more or less adapted depending on the complexity of the model. In our case, the loose coupling has been chosen for several reasons that have to be explained. As the latest describes an approach where interfaces are developed with minimal assumptions between the sending/receiving parties, therefore the risk that a change in one application will force a change in another application is reduced [11]. Loose coupling has also multiple assets regarding development costs, as we want to couple the model with existing GIS, and not coding a entire GIS software able to implement natively the dispersion model, as the integrated approach would suggests. As more and more GIS programs are being made available by open-source communities, we opted for Quantum GIS (QGIS) software to achieve the coupling, as it is one of the most highly capable open-source tool which offers advanced programming possibilities [12]. Indeed, QGIS has been made acessible through Python bindings, which allow a simpler programming environment for developping specific QGIS plugins that directly interact with the core source code [13]. We opted for this technical solution to propose a friendly-user atmospheric pesticide spray drift plugin. It is dedicated to agricultural atmospheric pollution prediction, and has been designed to be fast and extensible, mixing reduced-order modelling and QGIS plugin development.

#### **3.2 GIS As Input Data Provider**

The first roles of GIS deals with the automatic DEM extraction, needed by the model to compute the effects of ground variations on the windfield and so on the pesticide cloud movements. As the multi-leveled approach has been conceptualized to gain in topographic accuracy, one has to work

with several DEM resolutions and must be able to extract pixel values from any loaded DEM in the GIS. Using the Python bindings, this can simply being done with some common GDAL (Geospatial Data Abstraction Library) commands. In our case we use two successive gdal translate commands [14], as described bellow:

```
gdal_translate -ot Float32 -projwin "str(xmin) + str(ymax) + str(xmax) + str(
    ymin)+" input_dem.tif output_dem.tif
```

This first command is done to clip the loaded DEM according the user defined extent in which the calculation must be launched.

```
gdal_translate -of AAIGrid clip.tif clip.asc
```

And this one to extract the elevation value of each pixel of the extent to an ESRI grid file. The obtained grid is then converted into x,y,z triplets needed by the model as topography inputs, using the `grd2xyz` python class [15]. Theses successive commands permits to get the topographic input data for the dispersion model, overriding the user's DEM resolution and spatial projection as the Fortran program is then able to convert cartesian metric into the same values it reads in input

### 3.3 Georeferencing the Model's Topographic Input

Once those input parameters are being made available for QGIS, we must use them to provide a georeferenced environment for the model's output data. This step deals both with some basic file formats conversion, the multi-leveled equation implementation and some advanced geodata processing. The mathematical model works on a cartesian metric basis, which is not readable as is by QGIS. As we want the plugin to be able to read any resolution in any geographic projection, the spatial properties of the image DEM have to be read and understood by the model. This is done by sending the resulting file of the *gdal translate* commands to the Fortran program, which one reads the given tabular x,y,z file by accessing the standard Comma Separated Values (CSV) format. The generated DEM is then sent to Fortran using simple Fortran open, do and read commands: Each triplets (i.e each line of the former raster matrix) is then understood by Fortran and provides the elevation data on which the calculation have to be computed, for every point of the domain.

### 3.3 Introducing the Multi-Leveled Algorithm

The multi-leveled correction for ground variations let the user choose the number of levels wanted , as well as their spatial extent. This permits to define the local area where the DEM resolution must be finer in order to compute ground variations more precisely. This "micro-scale" area can be defined for example just around the considered source plot or any other area that presents particular topography or significative obstacle (like local depression, small hill or other interesting rock-formings) to the spray drift. This is done in QGIS using an adaptation of the Region Tool algorithm [16] applied in a recursive way:

```
def doneRectangle(self):
    level = self iface.getMapCanvas().setMapTool(self.saveTool)
    self.updateBounds(self.r.bb)
```

This first function permits to draw and save a rectangle on QGIS map view (map canvas) that defines the new extent.

```
def updateBounds(self,bb):  
self.xmindomain.setText(str(bb.xMin()))  
self.ymindomain.setText(str(bb.yMin()))  
self.xmaxdomain.setText(str(bb.xMax()))  
self.ymaxdomain.setText(str(bb.yMax()))  
newLevel = bb.xMin(),bb.yMin(),bb.xMax(),bb.yMax()
```

Then, the previous code allows to update the four corners of the extent and so to determine a new level for calculation. This way Region Tool can be used as many times as wanted, in order to set up the right number of levels for the calculation.

### 3.4 Cartography of Pesticide Clouds

The last step of the plugin development concerns the conversion of CSV outputs into standard GIS formats, but also the way one can enhance the cartographic rendering of the pesticide cloud. Using the QGIS API once again , we can first easily generates the model output results as ESRI shapefile (.shp) or any other OGR supported GIS vector format. This is done using the QGIS QgsVectorFileWriter class as presented bellow:

```
uri="plume.csv?delimiter=%s&xField=%s&yField=%s"%(",";"longitude","latitude")  
v=QgsVectorLayer(uri,"vectorial plume")  
QgsVectorFileWriter.writeAsShapefile(v,"vectorial-plume.shp")
```

Where plume.csv is the input CSV file that include longitude, latitude and atmospheric concentrations fields, and vectorial-plume.shp is the created point shapefile. Once this done, one can instantaneously apply some styling options to the created layer, in order to emphasize the concentrations values. This can be done using the QGIS QgsContinuousColorRenderer class, by allotting a symbol type to the geometries and a couple of minimum and maximum colors for the continuous color rendering (see figure 5).

```
r=QgsContinuousColorRenderer(v.vectorType())  
r.smin=QgsSymbol(v.vectorType(),"0","", "")  
r.smax=QgsSymbol(v.vectorType(),"1","", "")  
r.smin.setPen(QPen(Qt.green,1.0))  
r.smax.setPen(QPen(Qt.red,1.0))
```



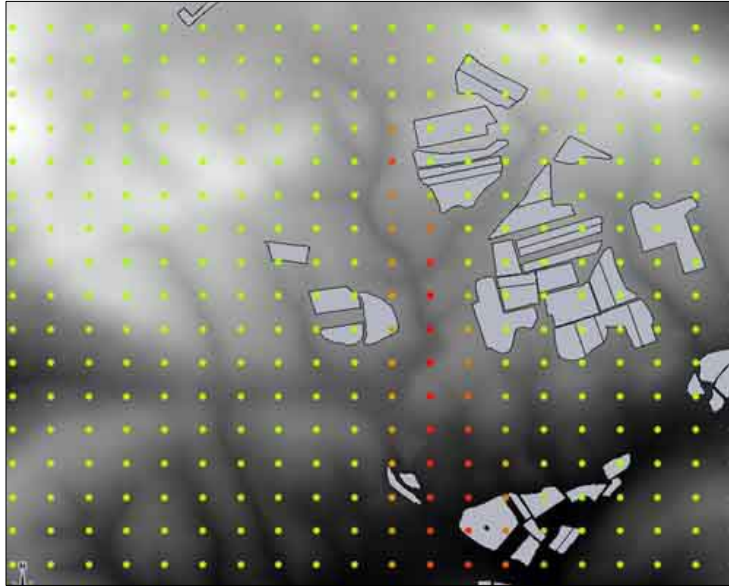


Figure 5. Vectorial pesticide cloud generated as ESRI Shapefile (.shp) with applied grated color

Another point of interest for mapping pesticide clouds is the raster generation, as the spray drift is a diffuse phenomenon and that a surfacic representation is much more readable than points in this case. The raster creation can significantly improve the cartographic message. In order to interpolate point based values, one opted for the inverse distance algorithm, assumuming that the nearer a point to be interpolated is located to a point with known value, the more similar is the value of the point to be interpolated to the known value in close distance. This can be done using the gdal grid interpolation capabilities, using the GDAL virtual format (i.e VRT driver) [14] and playing on the power and smooting values:

```
gdal_grid -a invdist:power=1.0:smoothing=50.0 -txe"+str(xmin)+str(xmax)+"-tye"
+str(ymin)+str(ymax)+" -of GTiff -ot Float64 -l driftx driftx.vrt output.tif").readlines()
```

Where -txe is the spatial extent in which to interpolate (i.e the user defined extent via the Region Tool class), -of is the desired output format and -ot the raster type. As the point-based values are interpolated over the whole domain, one has to apply a vectorial mask, in order to account only for points with values and so to kill the raster nodata. This can be done using the clipping functions of GDAL, using a *gdal -clip* command line. Finally and as for the vector outputs, one can apply coloring schemes and transparency values, using the QGIS QgsRasterLayer optionnal arguments (see figure 6), as suggested bellow:

```
r=QgsRasterLayer(fileName, baseName)
r.setDrawingStyle(QgsRasterLayer.SINGLE_BAND_PSEUDO_COLOR)
r.setColorShadingAlgorithm(QgsRasterLayer.PSEUDO_COLOR)
r.setTransparency(90)
```

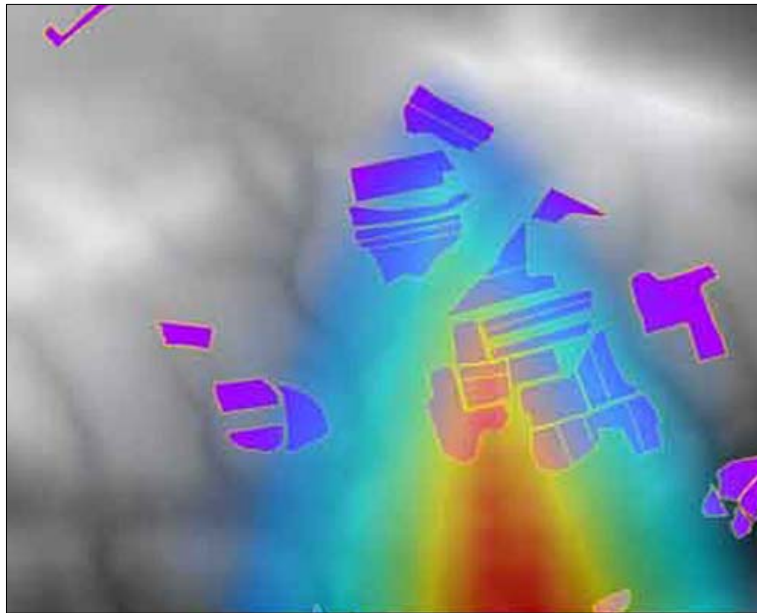


Figure 6. Interpolated and masked raster pesticide cloud with applied gratted color

#### 4. Conclusion and Perspectives

A low-complexity model for the prediction of passive scalar dispersion in atmospheric flows has been presented and coupled with open source GIS. The solution search space has been reduced using a priori physical information and a non symmetric metric based on migration times has been used to generalize injection and plume similitude solutions in the context of variable flow fields. The pesticide spray drift model has been applied on realistic topographies through coupling the inputs reading method with digital terrain models. Furthermore, the model has been integrated into a friendly-user Quantum GIS Python plugin which allows to use it on any studied area, to setup elevation and meteorological data and to visualize cartographic outputs directly into a GIS environment.

Future works will concern a more robust interaction between the model and GIS through developing an integrated dispersion Python class, as well as linking the QGIS Plugin with a “real-time” agro-meteorological PostGIS database, which one stores measurements from tractor embedded devices.

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