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MODELLING AND NUMERICAL SIMULATION OF THE ATMOSPHERIC DISPERSION OF POLLUTANTS FROM AN INTEGRATED IRON AND STEEL COMPLEX - PART I

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ABSTRACT

The Iron and Steel Complex processes handle, store and undertake important amounts of raw materials (iron ores, coals, etc.) energy, fuels, waste waters, slags and other different types of wastes. These activities have an important environmental impact; therefore significant amounts of pollutants (gases, waste waters and wastes) are resulted.

In case of accidents involving emission of pollutants in the atmosphere, health authorities and local administrations often need to know what areas could be affected by dangerously high pollutant concentrations. The goal of the paper is to evaluate a ready-to-use and modelling system, including meteorological parameters and a dispersion model using FLUENT® 6.3, a flexible software and reliable to be used for such real-time evaluations, especially for trans-border regions.

KEYWORDS: pollutants dispersion, numerical modelling, chemical substances, air, water, soil

1. Introduction

The mathematical and numerical modelling of the pollutants dispersion in the terrestrial atmosphere has known along the time a continuous evolution. From the simplest mathematical models at the beginning of the 20th century (the Gaussian model, 1936), it reached over today the use of extremely complex models such as CFD type ("Computational Fluid Dynamics").

2. State of the art in air quality modelling

As described above, the aim of this work was to develop a model that has certain quality characteristics. This means that there currently exists no available method that suits this demand. In the following state of the art analysis, available methods are checked with regard to the required criteria.

2.1. Dispersion modelling

With dispersion models the dispersion of pollutants starting from one or more emission sources that might be point, line or area sources is calculated. Depending on the requirements, dispersion models are able to consider the topography, the development, the velocity-, turbulence- and temperature-field, chemical and physical alterations and other parameters [1].

There are different possibilities to classify dispersion models:

- Mathematical and physical models [2]
- Mesoscale or microscale models [3]
- Models with a diagnostic or prognostic flow field pre-processor
- Simple models with homogenous terrain, models that consider the relief and land usage, models that consider the development [1]

Today's models are usually combined with a pre-processor, which calculates the flow field – the end result depends strongly on the beforehand-calculated flow field. For local scale considerations, CFD (computational fluid dynamics) models are first choice today [4, 5].

Generally it should be emphasized that the requirements for the input data are very high [6].

Their preparation and acquirement very usually is time consuming, as well as the final calculation run on the computer, which may take several days depending on the model and the regarded problem.

Table 1 gives a summary of the currently available dispersion models. The classification here follows the mathematical principle of the method.

2.2. Interpolation methods

In many countries, simple interpolation algorithms are officially applied, e.g. Kriging, Inverse Distance Weighting, Modified Shepard’s Method and Radial Basis Function [7].

Input parameters are the geographical coordinates and the pollutant concentration values. The calculated concentrations at a certain site are a function of the distance to the measurement points [1]. According to the implemented approach, the number, direction and distance to the real concentration values can be considered.

With Kriging, it is moreover possible to include the spatial variation of the measured concentrations by using variograms [8].

One can differentiate between statistical and non-statistical approaches or “exact” (the input value is preserved in the output) and “inexact” methods. Single cases are normally not considered, the adjusted interpolation parameters are valid for all cases. Therefore, the result depends strongly on the geographical location of the measurement sites that should not be influenced by local emission sources [3].

Table 1. *Classification and assessment of dispersion models*

Model Type	Theoretical background	Advantages	Disadvantages
The Box model	The pollutants distribution is homogeneous, calculating thus the medium concentration of every pollutant in any point of the studied air volume.	It is used for a range of wind directions and speeds and a range of mixing heights.	- extremely limited; - the pollutant is uniformly distributed in the box across the area.
Gaussian models	- Gaussian plume model: analytical solution of the steady-state advection - diffusion equation [13]; - Gaussian puff model: analytical solution of the time varying advection diffusion - equation [14].	- short computing time; - easy to handle; - input data requirements are low.	- theoretical simplifications (homogeneous velocity and turbulence field); - not suitable for hourly values; - mainly suitable for homogeneous terrain.
Eulerian grid models (k-models)	- numerical solution of the advection diffusion using a finite difference technique.	- flexibility to process flow and turbulence inhomogeneities over time and space; - higher-order chemical transformation considered; - variable time scale.	- problems treating the advection (numerical diffusion, mass deficits, negative mass densities); - long computing time; - input data requirements are high.
Particle models (Lagrange)	- the model tracks point-like particles representing a trace species on their path; - the vector of the turbulent velocity is varied for each particle at each time step using a Markov process [2].	- natural phenomena involved in turbulent diffusion are largely reflected; - no numerical diffusion; - mass conserving; - delivers non-negative mass densities - consideration of complex geometry; - consideration of large areas; - physical and chemical alterations considered; - variable time scale.	- sampling error associated with the particle count; - long computing time; - input data requirements are high.

The utilization of these mathematical models in pollutants dispersion simulation especially in the urban areas became a real necessity, the number of this kind of studies growing from a year to another. Although the necessary hardware resources for high scale simulation exceeds for the moment the possibilities of common user, this kind of simulations were and still are realized in research centres that own high capacity computers.

3. The geometric modelling of the studied geographic region

3.1. The virtual topographic description of the Galaţi – Cahul trans-border region

Every numeric simulation requires first the realization of a virtual, convenient mathematical description of the physical space in which are realized the fluid flow and pollutants dispersion phenomenon. Because the dispersion process is a three dimensional one and for a correct reproduction of the altitude variation effects between different geographical areas analyzed, the virtual space in which the simulation is made has to be 3D-like.

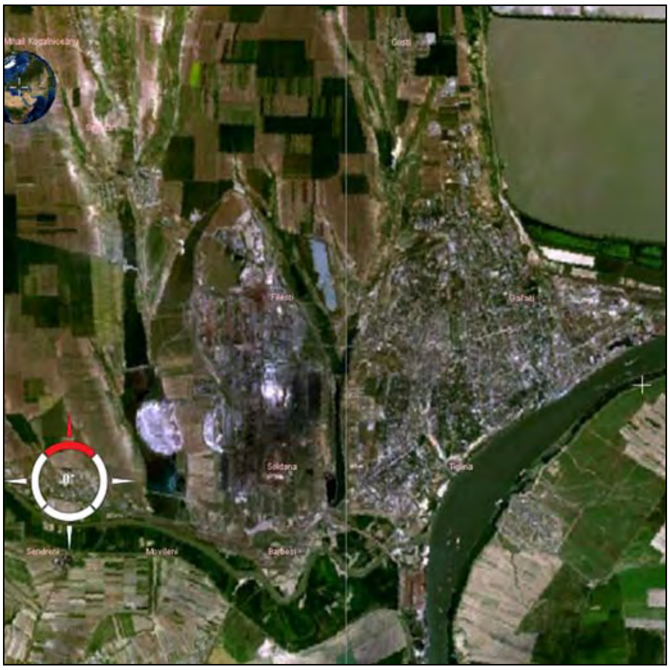

Fig. 1. *Satellite view of geographic sector included in the numeric simulation.*

For the area around Galaţi it was took into consideration an almost rectangular area with a side of 13 km. This area includes also the whole sector corresponding to the Arcelor Mittal iron and steel complex. Fig. 1 presents the geographic aria taken into consideration (approximately), seen from above. The geographic coordinates of the area are detailed in Tab. 2.

Tab. 2. *Geographic coordinates of the analyzed sector*

	Upper – left corner	**Down – right corner**
Lat.	45° 30′ N	45° 22′ N
Long.	27° 55′ E	28° 05′ E

The sector geometry, the basis of calculation domain, was taken from the NASA SRTM-90 database with specialized programs (with a precision of 3 seconds arch ≈ 90 m) obtained by cartography with radar technology.

The SRTM models representation precision is remarkable considering the scale from which the data were taken (approximately 80% from the solid surface of Earth is covered), the average marking error for the Romania territory being approximately 5 m.

3.2. The import, the rectifying and export of geometry using TGRID® 5.0 numerical processing program

The FLUENT® package pre-processing programs can not directly process the data contained in the SRTM models.

The information transfer must be realized in a compatible format, converting the original data in the STL format being the chosen modality. To avoid the subsequent errors, the local elevation information export resolution was imposed to be identical with the final numerical grid resolution.

Fig. 2 contains a graphic representation of the STL geometry imported in the TGRID®5.0 processing program.

It is seen that, in reality, the STL format is a geometry discrete, triangulated representation. It is obvious the fact that the representation precision is proportional with the clearly separation resolution.

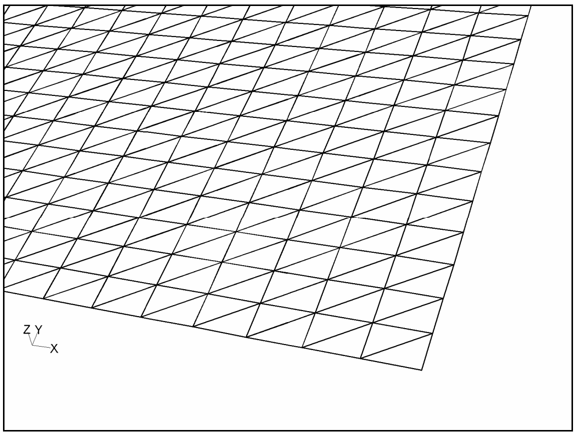

Fig. 2. *The STL format geometry imported in TGRID®*

For the scale in which the numerical simulations were made, it was considered sufficient a resolution of 50 m in the ground surface plane.

The resulting geometry from the direct data import in V TGRID® can not be used in the initial format, being necessary some rectifying operations:

a) „the welding" of triangles nodes situated in the same geographic place, with a specified tolerance (in STL geometrical format, the triangles are considered free, not connected to the neighbours);

b) the displacement of entire surface with a corner in the coordinates system origin (to minimize the rounding errors generated by the numbers of representation limits in the electronic calculus systems);

c) the scaling of surface dimensions from the geographic coordinate system used to protect the SRTM model to SI of units (arch degree → meters).

All these operations are very quickly realized with help from specific functions offered by the TGRID® program.

Finally, the rectified geometry is exported in a format that is compatible with GAMBIT® processing program (.msh), to be further processed.

4. Geometrical modelling and clear separation of the analyzes sector using GAMBIT®2.4 processing program

4.1. The modelling of control volume geometry (the calculus domain)

As mentioned earlier, a series of three-dimensional flow effects prevents the correct modelling of the dispersion phenomena in a limited 2D space in the sector near the ground.

Even if some types of presented mathematical models allow this kind of approximations, they are acceptable only if the dispersion is simulated over smooth geographic sectors, or if IT is previously known, precisely, the wind speeds distribution (the simulation being reduced to a simple equation solving that is modelling the dispersion).

Considering the following:

- there is a substantial inequality between absolute elevations of different analyzed surface points, which conduct to uneven distribution of wind speed and of atmospheric turbulence; this also determines an uneven dispersion of pollutants (the turbulent dispersion is faster then the molecular one);
- due to the ground surface interaction, in the lower atmospheric layers is formed a "limit layer" (boundary-layer flow), within which the wind speed varies very fast in height, according to an approximately logarithmic law;
- the height to which ground level interactions influence is felt (the thickness of boundary-layer flow) is about 500 – 700 m in the geographic areas as the analyzed ones,
- there was constructed a rectangular control volume, having as basis the analyzed surface and the absolute maximum height of approximately 1000 m (see Fig. 3).

4.2. Clear separation of the calculus domain and the numerical grid export

The control volume clear separation operation was realized using specific functions of GAMBIT® processing program.

This operation consists in distribution of the initial volume, of certain shapes, in smaller elementary cells. The final purpose is to obtain a three-dimensional network, used to make the mathematic model equation of the clear separation.

Due to the offered advantages:

- minimum number of cells for a given resolution;
- minimum deformation of the web for rectangular shaped domains cases;
- maximum precision for an imposed resolution (the numeric schemes are better adapted to structured networks);

it was chosen for realization of a structured type of clear separation network.

The detailed network parameters are given in Tab. 3.

Tab. 3. *Clear separation network parameters*

Network's resolution	X	261 nods ($\Delta x = 50$ m)
	Y	261 nods ($\Delta y = 50$ m)
	Z	51 nods (variable)
The distribution of nods	X	Homogeneous
	Y	Homogeneous
	Z	geometric, growth rate = 1.1
First cell layer height	$Z_0 = 0.6$ m	
Total number of cells	260 x 260 x 50 = 3,380,000	

In Fig. 3 is presented, as can be seen from the program's graphic interface, the clear separation grill of ground surface and that of calculus domain lateral borders. The following can be seen:

- the ground surface geometry was clearly separated again with quadrilateral elements (these has as a matter of fact the same resolution as the STL type initial clear separation);

- the grid nods are distributed on height according to a geometric law, being more frequent in the ground vicinity (the height of the first cells layer is 0.6 m), for two reasons:

- speeds distribution and turbulence parameters (turbulent kinetic energy, especially) in the atmospheric limit layer are strongly dependent on altitude, the gradients being maximum on the ground vicinity;

- the part with the most interest of the pollutants dispersion process is produced in the immediate vicinity of the ground.

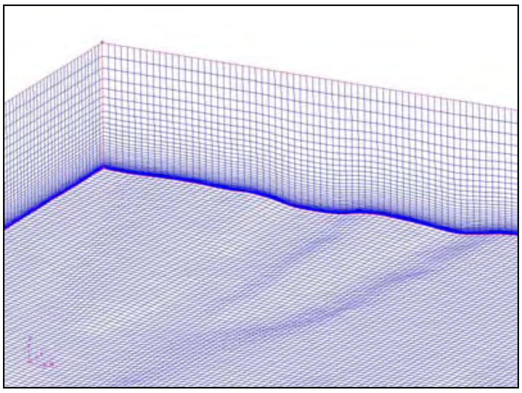

Fig. 3. *Clear separation of ground surface and the lateral borders of the calculus domain.*

To the calculus domain borders (exterior surfaces) were arrogated limit conditions specific to the FLUENT® program. These are synthesized in Tab. 4.

Tab. 4. *Limit conditions*

Area	**Name**	**Condition type at the limit**
Inferior surface	Ground	WALL
Superior surface	Exterior	SYMMETRY
Lateral surfaces	North	VELOCITY INLET, SYMMETRY, OUTLET (based on the simulated condition)
	South	Idem
	West	Idem
	East	Idem
Additional surfaces	Coke-oven plant	MASS FLOW INLET
	Blast furnace	Idem

The numeric grid was exported in the compatible format (.mh) with the FLUENT® numerical simulation and modelling program.

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