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

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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. Numerical simulation and modelling using FLUENT® 6.3

1.1. Numerical modelling

The usual programs for numerical simulation of the pollutants factor dispersion in the atmosphere use relative simple dispersion mathematical models. This models use as entry data the meteorological parameters (wind speed and direction, air temperature, solar radiation level by the ground, etc.), but these are usually a priori imposed model, not calculated. The incapacity to simulate the flow phenomena themselves puts under question the utility of these programs in case of a hypothetical situation simulation and modelling (the results precision is strictly dependent on the accuracy of turbulence and speed fields, which can only be estimated in this case). FLUENT® uses the most advanced mathematical models for the chemical substances mixtures calculus, in any aggregation phase (gas, liquid - drops or solid –particles). But in the same time, FLUENT® allows the flow phenomena simulation and modelling with help from the most complex and complete mathematical model that describes fluids behaviour: the Navier – Stokes model.

This thing, although it significantly complicates the simulation process, brings to the user an enormous advantage: the possibility to numerically simulate situations that need a maximum detail and precision degree, vital situations (ecological accidents, natural catastrophes, etc.), pollutants dispersion in the air, water and even soil, etc. For the actual study there was chosen three different calculus situations. These are presented in Tab. 1. Their selection was made taking into account the annual meteorological conditions in the statistic Galaţi area (for the first two) and the risk degree (the third situation).

Tab. 1. *Calculus situation*

Situation	Wind direction	Wind speed	Probability/risk degree
1	N	7.5 m/s*	43.4% / minimum
2	S-E	Idem	9.02% / medium
3	V	Idem	- / big

* The value was chosen so it can be obtained the annual medium speed value of the wind at the normal measuring altitude (~10 m), v_{med} = 4.7 m/s

Fig.1. *Wind direction correspondent to each calculus situation.*

1.2. Determination of the limit conditions

As mentioned in chapter 4.1, the air flow near the soil surface is not uniform, the friction forces and the obstacles from the ground level determining the forming of so called the atmospheric layer limit.

For the numerical simulations to be very realistic and very correct, the limit conditions for the entry borders must be imposed so it can reproduce in the most truthful way this effect.

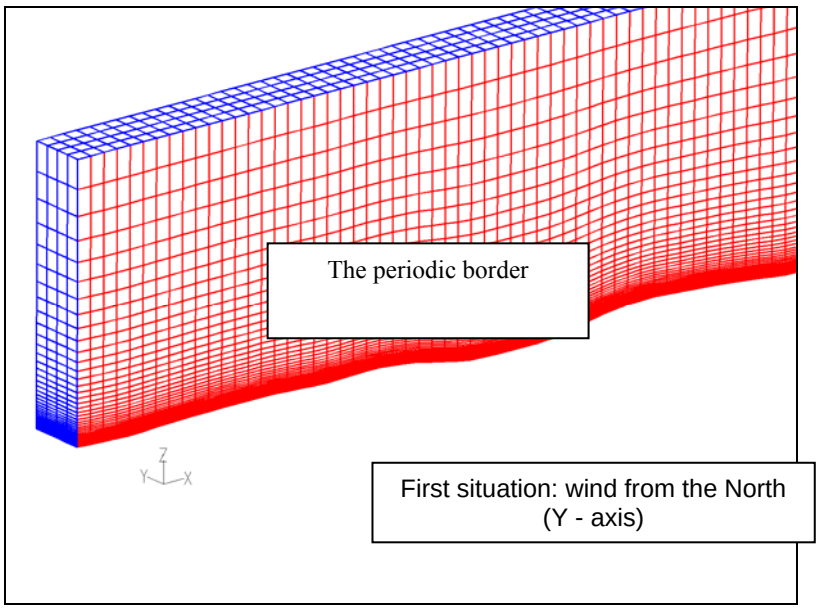

Fig. 2. *Calculus domain for determining the turbulence and speed profiles.*

To this purpose, there were made a series of supplementary simulations for each calculus situation. The FLUENT® program allows the user to obtain through calculus the dimensions that have to be provided in the limit conditions definition and imposing them through text files named „profiles". The quickest and the most elegant way to generate these files is the making of some simulations using the PERIODIC type at the limit conditions on the calculus domains with very much reduced dimensions in the flow direction (this type of what the limit condition permits the emulation of a length domain theoretically infinite).

In Fig. 2 is presented an implementation example, the case in which the wind blows from the North (the negative direction of the Y axis on the adopted coordinating system).

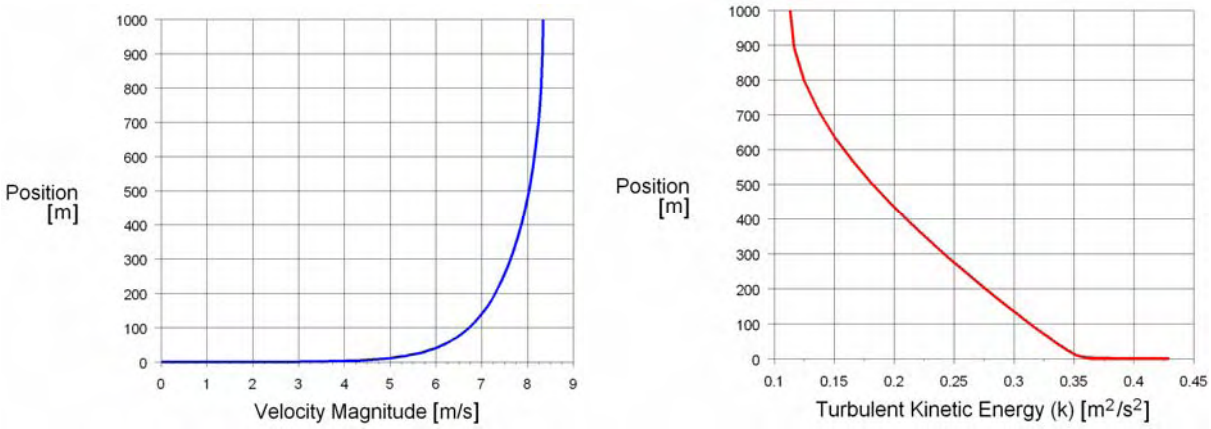

Fig. 3. *Wind speed value variation and atmospheric turbulence with the altitude.*

In Fig. 3 are represented the wind speed and atmospheric turbulences variations with the altitude, calculated for a medium speed of 7.5 m/s. It can be seen the very important effect that the friction with the ground has upon the speeds profiles, the wind speed value growing fast in the first 100 m.

Also it is interesting to point out the fact that the atmospheric turbulence, the most important factor of the pollutants dispersion, has the maximum value on the ground vicinity, but this value decreases pretty slowly with the height. The medium wind speed of 7.5 m/s corresponds to a speed of 4.7 m/s at a height of 10 m (pursuant to the meteorological standards, the wind speed is measured at 10 – 30 m height from the ground), which corresponds to the medium annual speed in the Galați region.

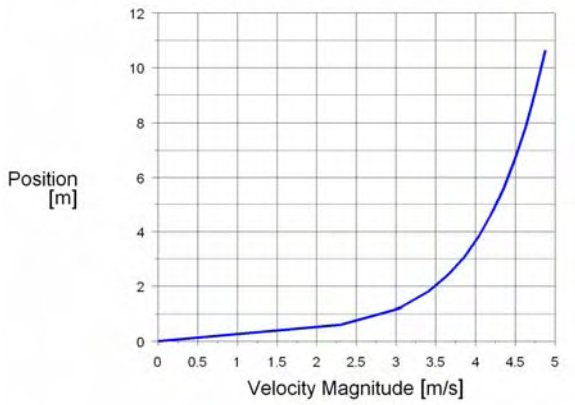

Fig. 4. *Wind speed variation on the ground immediate vicinity.*

The speed and turbulence profiles were extracted for all the study situations from numerical simulations made in the way previously described.

1.3. Physical models selection

The turbulence model selected for all the numerical simulations is SST k-omega. FLUENT® offers the user the possibility to choose no less than 14 turbulence models. Between these, the most adapted simulation model to the atmospheric limit layer flow from the offered precision and the calculus effort/performance proportion point of view is SST k-omega. There were made even some 2D numerical simulations so it can be determined the turbulence model influence on the obtained results. The comparison revealed that the models performances are very close, for this kind of flow, to those of more complex models, such as Reynolds Stress Model, performances obtained with a significantly less calculus effort.

Dispersion modelling was made with the chemical species transport model help available in FLUENT®. This model uses the Fick's law for the chemical species diffusion in laminar or turbulent regime

For species transport calculations, there are two ways to model the diffusion of chemical species. For most applications the Fick's law approximation is adequate, but for some applications (e.g., diffusion-dominated laminar flows such as chemical vapour deposition), the full multi-component diffusion model is recommended.

Mass diffusion coefficients are required whenever there are solved species transport equations in multi-component flows. Mass diffusion coefficients are used to compute the diffusion flux of a chemical species in a laminar flow using (by default) Fick's law:

$$J_i = -\rho D_{i,m} \nabla Y_i - D_{T,i} \frac{\nabla T}{T} \quad (1)$$

where $D_{i,m}$ is the mass diffusion coefficient for species I in the mixture and $D_{T,i}$ is the thermal (Soret) diffusion coefficient.

Equation (1) is strictly valid when the mixture composition is not changing, or when $D_{i,m}$ is independent of composition.

This is an acceptable approximation in dilute mixtures when $Y_i << 1$, for all i except the carrier gas. FLUENT® can also compute the transport of non-dilute mixtures in laminar flows by treating such mixtures as multi-component systems. Within FLUENT®, $D_{i,m}$ can be specified in a variety of ways , including by specifying D_{ij}, the binary mass diffusion coefficient of component i in the component j. D_{ij} is not used directly, however; instead, the diffusion coefficient in the mixture, $D_{i,m}$, is computed as:

$$D_{i,m} = \frac{1 - X_i}{\sum_{j, j \neq i} \left(X_j / D_{ij} \right)} \quad (2)$$

where X_i is the mole fraction of species i. There is the possibility to input $D_{i,m}$ or D_{ij} for each chemical species.

In turbulent flows, equation (1) is replaced with the following form:

$$J_i = -\left(\rho D_{i,m} + \frac{\mu_t}{Sc_t} \right) \nabla Y_i - D_{T,i} \frac{\nabla T}{T} \quad (3)$$

where: - J_i is the diffusive flux for the *"i"* species;
- Y_i is *"i"* species concentration;
- $D_{i,m}$ is the *"i"* species mass diffusion coefficient in the *"m"* mixture;
- μ_t is turbulent viscosity;
- $D_{T,i}$ is thermal diffusion coefficient of the *"i"* species;
- ρ is density;
- T is temperature;
- Sc_t is the turbulent Schmidt number for the turbulent flow:

$$Sc_t = \frac{\mu_t}{\rho D_t} \quad (4)$$

where D_t is the effective mass diffusion coefficient due to turbulence.

In turbulent flows the mass diffusion coefficient inputs consist of defining the molecular contribution to diffusion $D_{i,m}$ using the same methods available for the laminar case, with the added option to alter the default settings for the turbulent Schmidt number. This parameter relates the effective mass diffusion coefficient due to turbulence with the eddy viscosity μ_t. The turbulent diffusion coefficient normally overwhelms the laminar diffusion coefficient, so the default constant value for the laminar diffusion coefficient is usually acceptable.

2. Conclusions

This paper has reported on the development and evaluation of a new modelling system for air pollutants based on FLUENT® 6.3 software.

This software uses the most advanced mathematical models to calculate the chemical substances mixture situated in any state of aggregation (gaseous, liquid – droplets or solid - particles) and also permits the modelling and simulations of the flowing phenomena using a complete and complex mathematical model which describes the fluids behaviour namely the Navier-Stokes.

This fact, although it is making the simulation process significantly complicated, brings an enormous advantage to the user namely the possibility to simulate numerical situations that require a maximum degree of precision and detail, virtual situations (ecologic accidents, natural disasters, etc.), dispersion of pollutants in air, water and even soil.

FLUENT® 6.3 offers the user 4 different numerical solvers, every one of them being better fit to a particular class of numerical simulations.

In the analysed situations the PBCS solver ("Pressure - Based Coupled Solver") was used, due to the optimum precision and it is converging speed.

Qualitative simulations were realised, the fluxes values being considered identical for all pollutants and the same in all studied situations.

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