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Comparison between the results of a new version of the AVACTA II atmospheric diffusion model and tracer experiments(*)(**)

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Summary. — A new version of the AVACTA II code (a code recommended by EPA) has been implemented and evaluated. AVACTA II is a code based on a mixed segment-puff approach, which allows numerical simulations of both non-stationary and non-homogeneous conditions. In our version, the wind field is calculated through the 3D mass-consistent code $\mathcal{WINDS}$ developed at the Department of Physics of the University of Genoa, Italy. The model evaluation of this new version of the AVACTA II code has been performed using field experiment data on flat, but rough, terrain (Karlsruhe Nuclear Research Center (KNRC) tracer experiments) and wind tunnel measurements (EPA Rushil experiments) both in flat and complex terrain. A comparison is made between simulated and measured concentration distributions. The results of these evaluations are very encouraging.

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1. – Introduction

The purpose of this paper is the presentation of a new version of the air quality model AVACTA II and of a validation of some parts of it, against both field and wind tunnel measurements. Presentation and validation of the code are more extensively described by Canepa [1] and by Canepa and Ratto [2].

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AVACTA II [3–5] is a code able to handle non-stationary and non-homogeneous meteorological conditions, simulating transport, diffusion, linear chemistry transformation and deposition of air pollutants above complex terrain. This code has been accepted by the U.S. Environmental Protection Agency (EPA) and is currently listed as an "alternative" model.

AVACTA II is a mixed segment-puff dispersion model based on the traditional Gaussian approach. The plume is considered as a "chain" of independent elements (segments or puffs) whose initial features and dynamics are function of local time-varying emissions and meteorological conditions. Since meteorological parameters can change both in space and time, every element develops according to different conditions found along its trajectory.

In fact, the commercially available version of AVACTA II model is essentially composed of two parts:
1) subroutine WEST creating a 3D non-divergent wind field [6];
2) the dispersive part of the code, *i.e.* the ensemble of subroutines simulating generation, transport and diffusion of plume elements and all processes related to such dynamics.

In the proposed new version of AVACTA II (more extensively described by Canepa [1] and Canepa and Ratto [2]) the WEST wind field module is replaced by the more sophisticated $\mathcal{WINDS}$ ($\mathcal{W}$ind-field $\mathcal{I}$nterpolation by \on-$\mathcal{D}$ivergent $\mathcal{S}$chemes) [7,8].

Furthermore, the dispersive part of the code was improved by us mainly in its software architecture, without substantial changes to its physics. Many improvements were related to the revision of plume rise algorithms. To the standard options for calculating the plume rise, we added a new algorithm for describing the stack tip downwash effect (aerodynamical stack effects on the emitted plume) in the Briggs formulae [9–11], following the Bjorklund and Bowers approach [12]. The improvements related to the plume rise were not used for the present work and, thus, are not here explicitely discussed. The resulting dispersive part of the code was named P6 (Path Plotting Program for Polluting Puffs and Plumes).

2. – Our version of AVACTA II

$\mathcal{WINDS}$, which in our version takes the place of the module WEST (present in the previous version), belongs to the "family" of "mass-consistent" models (for a review, see [13] and [14]). The model builds a three-dimensional wind field by the following two steps: first, an initial wind field is constructed, through an interpolation procedure, starting from available wind data at given points, then an adjustment, based on the variational method proposed by Sasaki [15, 16], is made to achieve a non-divergent flow field.

The WEST module uses Cartesian coordinates, while $\mathcal{WINDS}$ is written in conformal coordinates, which are terrain-following just above the terrain and usually flat at the top of simulation domain. The conformal coordinates have several advantages: the terrain surface is more accurately represented, imply simpler boundary conditions and allow higher resolution near the terrain surface.

While WEST module can only use vertical wind profiles to build the initial wind field, $\mathcal{WINDS}$ can use different initialization possibilities: ground station data and/or geostrophic wind, observed vertical profiles (sodar, etc.), profiles coming from larger scale meteorological models (*e.g.* Limited Area Models), etc. In $\mathcal{WINDS}$ model, atmospheric stability effects are taken into account through both wind velocity profile in the Planetary Boundary Layer (PBL) [17–20] and weighting coefficients for horizontal and vertical adjustment of the wind field in the presence of orography.

P6, the dispersive part of AVACTA II code [4,21], contains a computationally efficient mixed segment-puff numerical technique aiming at the joint utilization of both segmented plume and puff approaches, respectively, according with two Gaussian formulae

$$C(\vec{r}) = \frac{Q}{2\pi U \sigma_h \sigma_z} e^{-y_r^2/2\sigma_h^2} e^{-(z_s+\Delta h - z_r)^2/2\sigma_z^2}, \tag{1}$$

where C is the average steady-state concentration produced at the receptor $\vec{r} = (x_r, y_r, z_r)$ by a single point source at $\vec{s} = (0, 0, z_s)$, Q is the pollutant emission rate, Δh is the plume rise, U is the average wind speed and σ_h and σ_z are the horizontal and vertical plume standard deviations at the downwind distance x_r;

$$\Delta C(\vec{r}) = \frac{\Delta M}{(2\pi)^{3/2}\sigma_h^2 \sigma_z} e^{-(x_p - x_r)^2/2\sigma_h^2} e^{-(y_p - y_r)^2/2\sigma_h^2} e^{-(z_p - z_r)^2/2\sigma_z^2}, \tag{2}$$

where $\Delta C(\vec{r})$ is the concentration at the receptor $\vec{r} = (x_r, y_r, z_r)$, due to the puff whose center is located at $\vec{p}(t) = (x_p, y_p, z_p)$, ΔM is the mass of the puff.

Both formulae are analytical solutions of a simplified transport and diffusion equation. Nevertheless, they are consistent with the physics of the atmospheric dispersion phenomena.

The most important time steps to be defined by the users of AVACTA II are:
1) the "meteorological" time step, Δt_{m}, an arbitrary interval (typically, 30-60 minutes) of the simulation time; at each time step Δt_{m} the meteorological conditions are possibly adjourned, in order to describe unstationary conditions;
2) the "dispersion" time step, Δt, a fraction of Δt_{m}; during each Δt a new element is added to the element "chain" from each source at each stack tip. For each element, a complete dynamic cycle is performed (transport and diffusion, chemical transformation, deposition, concentration calculation), so that the parameters relative to each element are adjourned to the local situation. Choosing this time step, the user can roughly determine the total number of elements contained in the computational domain; the number of elements constituting the plume can be a critical parameter as far as the performance of the simulation is concerned.

The criterion for identifying the type of element is based on the ratio between the element length, L_{e}, and the horizontal plume standard deviation, σ_{h}, of the element itself. If $L_{\mathrm{e}}/\sigma_{\mathrm{h}} > 2$, the element is described as a "plume segment" and if $L_{\mathrm{e}}/\sigma_{\mathrm{h}} \leq 2$, the element is treated as a "puff". Note that the type of element (segment or puff) does not affect its dynamics, but only the computation of the concentration field.

At each receptor point, the concentration is the sum of the contributions of all existing puffs plus the contribution of the closest segment. This allows a proper dynamic representation of both calm and transport conditions, including the situations in which, due to a 180° change in wind direction, two sections of the same plume may affect the same receptor.

3. – Evaluation of P6 against KNRC experiments

3·1. *The experiments and their simulation.* – The experiments at the Karlsruhe Nuclear Research Center (KNRC), Germany, were performed on flat but rough terrain with an average roughness $z_0 \simeq 1.5$ m, during different meteorological conditions. For a more detailed description of these experiments, see Thomas *et al.* [22,23].

In order to allow a comparison with the results by Brusasca *et al.* [24], we considered the same experiments discussed by them: "72" (neutral atmospheric conditions) and "64" (unstable conditions). During each experiment, two non-buoyant and non-reacting tracers were continuously emitted from two different heights (160 m and 195 m above ground level); the measurements were performed during two different sampling periods, starting about 1 h after the beginning of the emission.

Since the terrain is flat, we constructed the three-dimensional mean wind field by direct interpolation of measured values: using the power law for the wind speed and linear interpolation for the wind direction between 40 and 200 m a.g.l. We used P6 with four different dispersion functions: 1) Briggs open country (BC) [25], 2) Brookhaven (BR) [26], 3) Briggs urban (BU) [25], 4) Pasquill-Gifford-Turner (PG) [27].

Following Brusasca *et al.* [24], we assumed the mixing height, h_{m}, to be 1550 m during experiment "72", and 1500 m during experiment "64". The grid consisted of $50\times40\times40$ nodes (experiment "72") and $31\times31\times40$ nodes (experiment "64") with a grid step of 200 m along the horizontal and 20 m along the vertical. Furthermore, we chose dispersion time steps, Δt, equal to 100 s (experiment "72") and 30 s (experiment "64"), which correspond to about 9 and 45 elements, respectively. Later on, we will discuss the sensitivity of results to the change of the number of plume elements utilized: see subsect. 3˙2.

3˙2. *Comparison of models.* – We compared the performances of the P6 model applied to the KNRC experiments, using four different σ dispersion functions, with the results of models selected by Brusasca *et al.* [24], when applied to the same experiments. Brusasca utilized one particle model and eight Gaussian models; the Gaussian models differed from one another on the choice of the dispersion σ functions (the same utilized by us) and on the way to provide the wind velocity in the code input.

Brusasca made two choices: with the first one, he considered the wind speed and direction measured at the emission height (letter "e" in figures), while in the second case he averaged the values measured from ground to emission height (letter "a").

The analysis presented below was based, for each experiment, on the "entire sample" of concentrations (*i.e.* taking together all data relative to the two emission heights and the two sampling periods). Every "entire sample" is composed of 147 (166) pairs of simulated *vs.* measured concentrations for experiment "72" ("64"), respectively.

Our evaluation was based on the statistical indices NBIAS, NMSE (also used in [24]) and, furthermore, on WNNR and NNR (proposed by Poli and Cirillo [28]). The NBIAS, NMSE, WNNR and NNR values for experiment "72" and "64" are presented in figs. 1 and 2, respectively.

As can be seen from figs. 1 and 2, the P6 code provides the best results when Brookhaven dispersion function (BR) is used for experiment "72" and the Briggs urban (BU) dispersion function is used for experiment "64". Similar results can be obtained considering a "partial set" of concentrations data (for more details see [1] and [2]).

Figure 3 shows, for experiment "72" and "64", a direct comparison between simulated concentrations (ordinate), to which the background concentration was added, and measured concentrations (abscissa). Note that both scales are logarithmic.

We already said (sect. 2) that the number of elements composing the plume can be a critical parameter as far as the performance of the simulation is concerned. In order to verify this point, we simulated both experiment "72" and experiment "64" with eight different values of the dispersion time step, Δt , in order to obtain plumes composed of a different number of elements.

We chose for this test the cases (emission height, sampling period, and σ function)

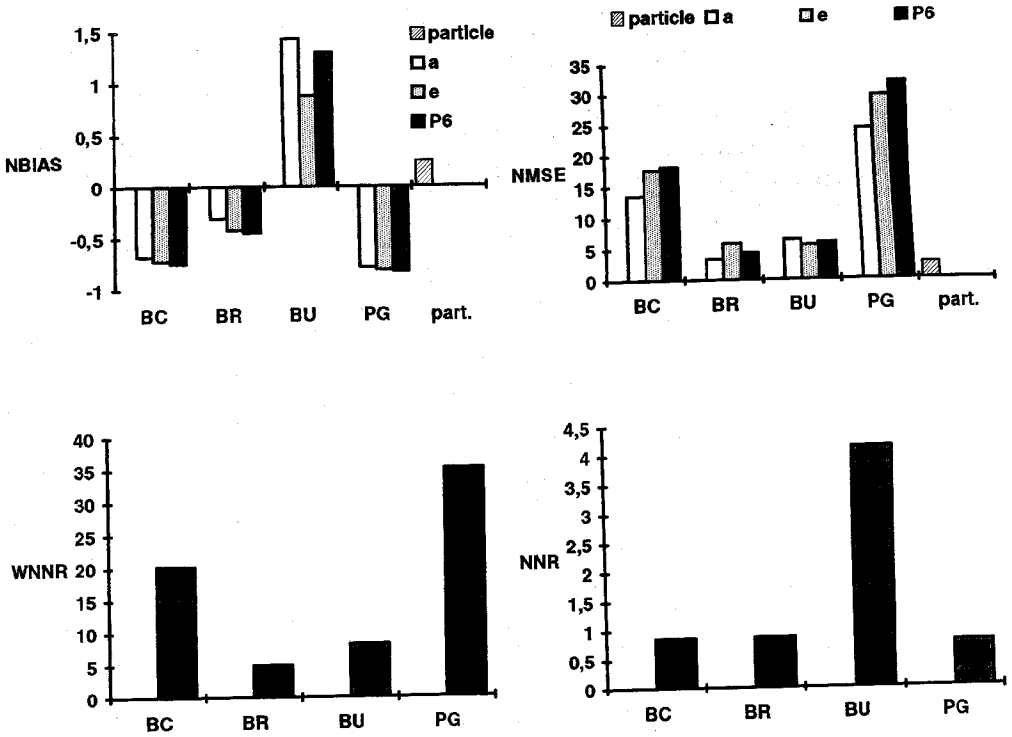

Fig. 1. – KNRC: Experiment "72". Values of indices NBIAS and NMSE, relative to the P6 code, used by us, and to the Gaussian models (for the meaning of "a" and "e", see the text) and to the particle model used by Brusasca *et al.* [24]; and values of indices WNNR and NNR relative to the P6.

which gave the best results, considering "partial set" of concentrations data (see [1, 2]). For experiment "72" we considered: emission at 160 m a.g.l., second sampling period, and the Brookhaven σ function; for experiment "64": emission at 195 m a.g.l., first sampling period, and Briggs urban σ function.

The dependence on the number of elements varies according to the chosen dispersion function. Furthermore, in all cases, the values of the considered statistical indices more or less oscillate when the number of elements is small, becoming constant when the number of elements is greater than 9 (experiment "72") or 45 (experiment "64"). Thus, the number of elements we used to obtain the results previously discussed (about 9 with experiment "72", about 45 with experiment "64") was enough to make the code operate independently of the number of elements. This dependence on the number of elements seems due to the increase in the dispersion function from one element to the next. In fact, in the unstable case the σ function increases much more dramatically with increasing the distance from the source than in the neutral case.

3·3. *Conclusions.* – Considering the "entire sample" of concentrations, the best results both for P6, considered by us, and Gaussian models, considered by Brusasca *et al.* [24], are obtained with the BR σ function for experiment "72", and with the BU σ function for experiment "64". For both experiments, in this case, the low values of WNNR

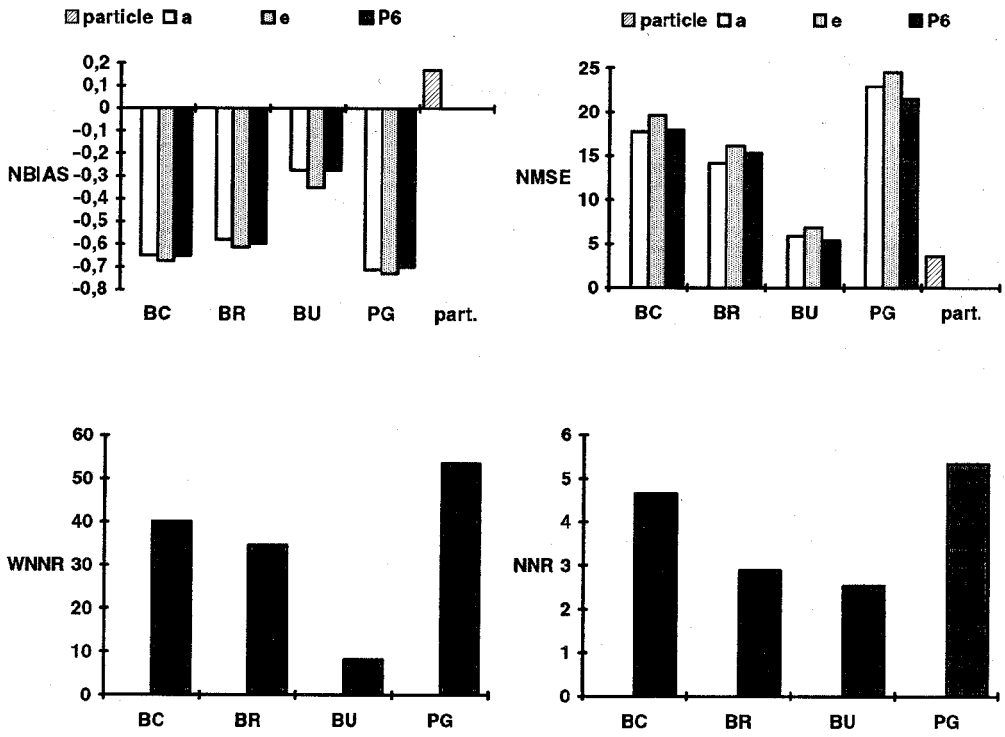

Fig. 2. – KNRC: Experiment "64". Values of indices NBIAS and NMSE, relative to the P6 code, used by us, and to the Gaussian models (for the meaning of "a" and "e", see the text) and to the particle model used by Brusasca *et al.* [24]; and values of indices WNNR and NNR relative to the P6.

index [28] we found indicate the ability of P6 to simulate the highest concentrations.

In all cases, the behaviour of the P6 model was very similar to that of Gaussian models with the same dispersion functions. This is correct, since we were simulating essentially stationary conditions in flat terrain. Minor differences between the performances of the codes (Gaussian models and P6) using the same σ function can be attributed to the differences in the use of the information about the wind field and to the numerical procedure to connect the plume elements in P6.

Only the particle model, considered by Brusasca *et al.* [24], performs systematically better than the P6 code (see figs. 1 and 2). However, the particle model needs much more meteorological information, *e.g.* the turbulence field, than the less sophisticated P6. Furthermore, the computer time to run a particle model is about 100 times that required by the P6 model.

4. – Evaluation of AVACTA II against EPA wind tunnel experiments

4·1. *The experiments and their simulation.* – In this section, we consider the RUSHIL experiments performed in the EPA wind tunnel (by Khurshudyan *et al.* [29] and Snyder [30]). We used some of these experiments in order to evaluate P6 and our versions of AVACTA II. These tracer emission experiments, with different emission heights,

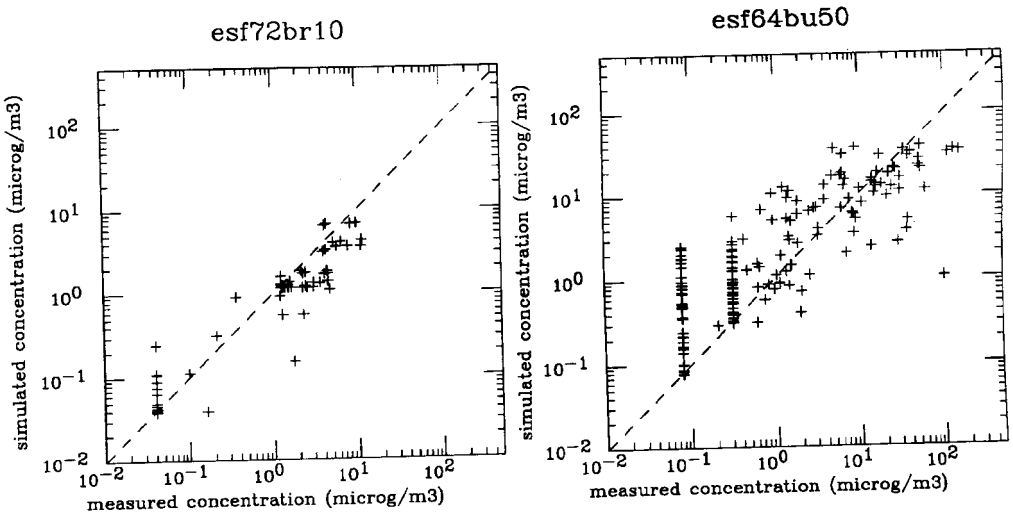

Fig. 3. – KNRC experiments. Direct comparison between simulated (ordinate) and measured (abscissa) concentrations ($\mu g/m^3$). On the left: experiment "72", P6 code with Brookhaven σ-function. On the right: experiment "64", P6 code with Briggs urban σ-function.

were performed in a neutrally stratified flow both on flat terrain and on simple isolated two-dimensional hills with different steepnesses.

Willing to simulate phenomena at the "full" scale, *i.e.* at the scale of real phenomena in terrestrial atmosphere, we chose the PBL height value of the order of 1000 m (as by Finardi *et al.* [31]) and thus (the wind tunnel BL height value being $\sim$ 1 m) the scale factor of lenghts of the order of 1000. We assumed that both the flow speeds and the densities are unchanged with respect to the full scale and so we had for the times and masses scale factors of 1000 and 1000^3, respectively.

In our study, we only considered the case of flat terrain and the less steep hill, named H8. In order to make comparisons with the results by Tinarelli *et al.* [32], we considered the experiments with tracer emissions at 29 m and at 117 m a.g.l. A non-buoyant tracer (C_2H_4) was emitted by a source with a diameter not negligible with respect to the emission heights. Thus, it is not correct to treat such emission as a point-source.

We tried two different approaches: 1) in the first one, indicated with "z" (from Zannetti), following the approach used in AVACTA II, we assumed the three initial dispersion functions (horizontal, vertical above the plume axis, vertical below the plume axis) equal to 0.369 d_s, where d_s is the source diameter; 2) in the second, indicated with "k" (from Khurshudyan), we treated the emission as a point-source placed 35 mm upwind of the real source position, following a suggestion by Khurshudyan.

The computational domain consists of $101 \times 31 \times 100$ nodes with a horizontal grid step of 117 m and a vertical one of 10 m.

We applied the code with the following dispersion functions: 1) Briggs open country (BC); 2) Brookhaven (BR); 3) Pasquill-Gifford-Turner (PG).

We evaluated the performance of our simulations of the experiments made in the EPA wind tunnel with the same statistical indices utilized in subsect. 3·2 and with graphical methods.

TABLE I. – *Flat terrain, source at* 29 m *a.g.l., receptors at the ground: statistical indices relative to our simulations.*

Model	NBIAS	NMSE	WNNR	NNR
BCk	0.87	0.69	0.68	0.89
BCz	1.09	0.97	0.95	1.06
BRk	1.55	1.40	1.17	1.21
BRz	1.48	1.49	1.25	1.18
PGk	0.34	0.50	0.34	0.38
PGz	0.80	0.63	0.62	0.82

4˙2. *The simulation of flow above flat terrain.* – We located the source at the center of the grid cell (16, 16). Here we discuss the simulation results obtained with P6 for the following two cases:
1) receptors at the ground along the axis of the wind tunnel;
2) receptors along the vertical above the receptor at the ground which measured the maximum concentration.

The time step, Δt, was set equal to 120 s, which was enough to guarantee the independence of the code of the number of elements. The two-dimensional flow field, above a flat surface, was obtained directly from the smoothed wind profiles provided by Trombetti *et al.* [33].

The statistical indices for the simulation results relative to the source at 29 m and receptors on the ground are reported in table I. Independently of the parametrization of the source, the PG dispersion function gave the best performance of P6. With respect to the parametrization of the source, the "k" parametrization gave better performances than the "z" one, at least for the PG and the BC dispersion functions.

With the PGk model, giving the best result at the ground, we simulated the corresponding experiments with receptors along the vertical. The resulting statistical indices had higher values than those with receptors on the ground.

As we can see in table II, the performance of P6 simulating the case of emission at 117 m and receptors at the ground was slightly better than that with emission at 29 m a.g.l.

With the BCz, BRk and BRz models, giving the best results at the ground, we simulated the corresponding experiment with receptors along the vertical. The performance for such experiments seems practically unchanged with respect to the experiments with

TABLE II. – *Flat terrain, source at* 117 m *a.g.l., receptors at the ground: statistical indices relative to our simulations.*

Model	NBIAS	NMSE	WNNR	NNR
BCk	−0.19	0.30	0.36	0.74
BCz	−0.17	0.24	0.29	0.62
BRk	0.46	0.28	0.24	0.28
BRz	0.49	0.29	0.25	0.21
PGk	−0.34	0.80	1.05	1.23
PGz	−0.32	0.68	0.88	1.12

the receptors at the ground. P6 with the BRz dispersion function can be considered the code that, on the whole, has a better performance in simulating both experiments with receptors at 117 m a.g.l.

4·3. *The simulation of flow above a model hill.* – We again considered emissions at 29 m and at 117 m a.g.l. and, for each emission height, three positions of the source: position "1" at the upwind hill base, position "2" at the top of the hill and position "3" at the downwind base of the hill.

The wind field was constructed by the two-dimensional version of the $\mathcal{WINDS}$ code, utilizing 15 out of 16 wind profiles provided by Trombetti *et al.* [33]. We simulated the flow only with the approaches which had given the best results on flat terrain, *i.e.* with PGk (emissions at 29 m a.g.l.) and BRz (emission at 117 m a.g.l.).

Instead of indicating either the dispersion time step or the number of elements, we preferred to make reference to a new parameter:

$$r = \frac{\text{number of cells overlapped by the plume axis}}{\text{number of elements}}, \tag{3}$$

which is an indication of the average number of cells interested by a plume element.

The performance of the code was better in cases of elevated sources (117 m a.g.l.) than in the cases of emissions near the ground (29 m a.g.l.).

The results obtained with the emissions at 117 m in position "1", "2" and "3" are given in fig. 4. In case "1" we can observe that the code overestimates the peak concentration and finds it near the top of the hill, while the maximum observed concentration is in the lee of the model hill. It is interesting to observe that the model correctly gives a minimum concentration at the downwind base of the hill. Again, the code correctly describes the experimental concentrations far from the source, while the discrepancies are highest above the hill.

Observing the results obtained with the emission in position "2", the performance improvement is evident with respect to results obtained with the emission in position "1". This improvement was even better in the case of emission position "3".

From the values of the statistical indices and from the graphic comparison between simulated and measured concentrations, it can be seen that, for different values of r:
1) when the source is in position "1" (position "2") the model overestimates (underestimates) the measured peak concentrations; when the source is in position "3" the model overestimates the measured peak concentration in the case of emission at 29 m, but there is a fairly good agreement in the the case of emission at 117 m;
2) the code is able to correctly simulate concentrations far from the source;
3) due to the strong advective wind component, the code is not able to give the (small) measured concentrations upwind of the sources in position "3" (nevertheless, in low wind conditions, AVACTA II would be able to simulate such concentrations).

In all the considered cases, we calculated the number of times a value of r provided the best performance of AVACTA II with respect to each of the considered statistical indices. About 70% of best performances occurs for $r \leq 2.0$. Thus, it is possible to recommend the use of a diffusion time step which gives a plume element length roughly equal to that of the grid step.

4·4. *Conclusions.* – The performance of the code on flat terrain was better in case of elevated source (117 m a.g.l.) than in case of an emission near the ground (29 m). This is

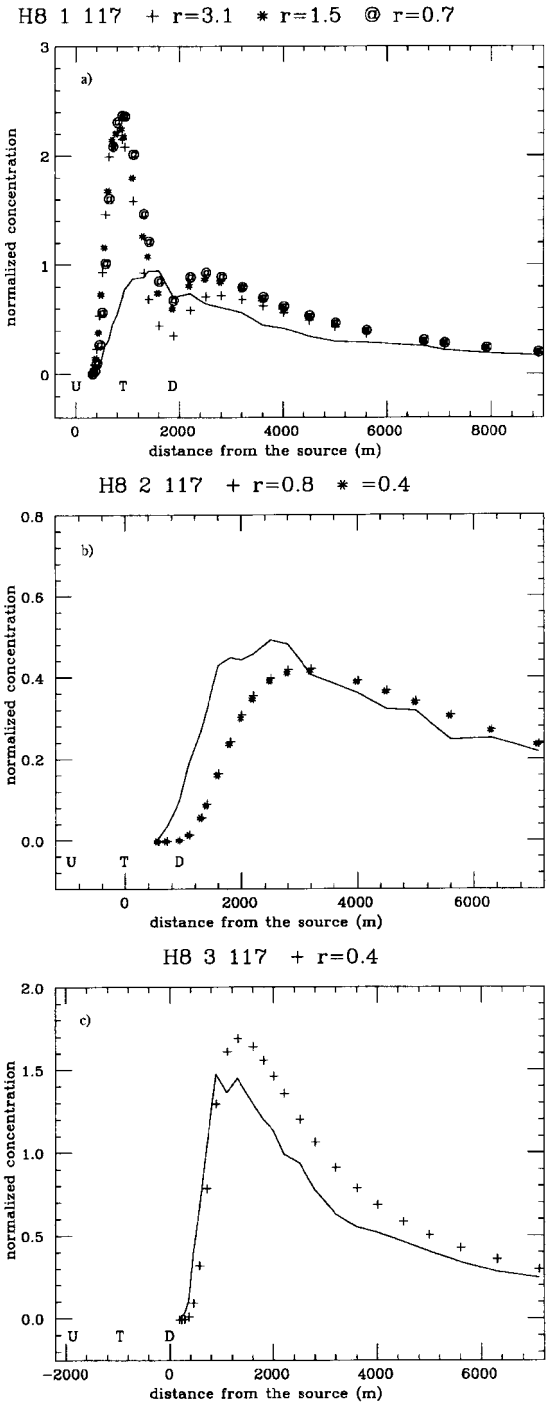

Fig. 4. – H8 model hill, source at 117 m a.g.l., measured (continuous line) and simulated normalized concentrations (symbols indicating the value assumed by the parameter r) as a function of the distance from the source. U, T, D represent the position of the Upwind base, the Top and the Downwind base of the hill, respectively. a) position "1", b) position "2", c) position "3".

not surprising, since, as is well known, Gaussian dispersion functions are based on the assumption of vertically uniform wind speed and homogeneous turbulence, conditions which do not occur near the ground.

Furthermore, we verified that the code more correctly predicts the horizontal concentration profiles near the ground than the vertical concentration profiles (we took the vertical profiles above the maximum concentration at ground). Neither this result is surprising, since the parameters entering the Gaussian dispersion functions are set in order to give correct concentrations at the ground level.

In the presence of the hill, the agreement between the calculated concentrations and the observed ones was on the whole worse than in the case with flat terrain. These discrepancies can be attributed: 1) to the difficulty of the mass-consistent model to correctly construct the average wind field, at least in the lee of the model hill; 2) to the approximation in the description of vertical turbulence: the Gaussian models assume a vertical turbulent diffusion coefficient independent of elevation, but in reality (and in particular with hilly terrain) the turbulence is not vertically homogeneous.

Finally, we were able to suggest to the user of AVACTA II, in cases of complex orography, a choice of the diffusion time step which makes the plume element length of the same order as the horizontal spatial discretization of the computational domain.

5. – Final considerations

The aim of this text has been the presentation of a new version of AVACTA II and of a validation of some parts of it, against both field and wind tunnel measurements.

We have described an evaluation of the dispersion module P6 against some of the experiments performed at the Karlsruhe Nuclear Research Center (KNRC) (flat terrain, neutral and unstable stratifications) and an evaluation of our version of the AVACTA II code against some experiments performed in the EPA wind tunnel (both on flat terrain and on simple 2D hill and in neutral stratification).

We applied P6 with four different dispersion functions to KNRC experiments. In all cases, the behaviour of the P6 model was very similar to that of Gaussian models, with the same dispersion functions, applied by Brusasca *et al.* [24]. Only the particle model utilized by these authors performed systematically better than the P6 code, but the computer time to run a particle model is about 100 times that required by the P6 model.

The performance of P6 for EPA "flat terrain" experiments was better in the case of elevated source than in case of emission near the ground. This behaviour has been explained remembering that Gaussian dispersion functions assume vertically uniform wind speed and homogeneous turbulence, conditions which do not occur near the bottom of the wind tunnel.

We have also shown that, above flat terrain, the code more correctly predicts the concentrations near the ground than the concentration along a vertical above the maximum concentration at ground: this result can be explained remembering that the parameters entering the Gaussian dispersion functions are set in order to give correct concentrations at the ground level. We have also recalled that the dependence of the measured concentration on the distance from the ground reveals the lack of vertical homogeneity of turbulence, lack existing both in the wind tunnel and in the real atmosphere, but not in the model assumption.

For EPA experiments with a model hill, the agreement between the simulated concentrations near the ground and the observed ones is on the whole worse than in the

case with flat terrain for same emission elevation above the ground. As in case with flat terrain, the simulations with the more elevated source gave a better performance than simulations with the emission near the ground. The performance of the code was best when the source was downwind of the hill as a consequence of the fact that, in this case, the dispersion mostly occurs where the flow is less affected by the presence of the model hill.

We also have been able to suggest to the user of AVACTA II, in cases of complex orography, a choice of the diffusion time step making the plume element length of the same order as the horizontal spatial discretization of the computational domain.

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