Validation study of Windtrax reverse dispersion model coupled with a sensitivity analysis of model-specific settings

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HIGHLIGHTS

- Windtrax can be used to quantify Emission Rates from complex sources;
- Windtrax has been investigated in terms of validation and sensitivity to model specific parameters;
- The model appears to be reliable under neutral conditions;
- Model specific parameters slightly influence the results.

ABSTRACT: In last years, atmospheric dispersion models have reached considerable popularity in environmental research field. In this regard, given the difficulties associated to the estimation of emission rate for some kind of sources, and due to the importance of this parameter for the reliability of the results, backward dispersion models may represent promising tools. In particular, by knowing a measured downwind concentration in ambient air, they provide a numerical value for the emission rate. This paper discusses a critical validation of the Windtrax backward model: the investigation does not only deal with the strict reliability of the model but also assesses under which conditions (i.e. stability class, number, and location of the sensors) the model shows the greatest accuracy. For this purpose, Windtrax results have been compared to observed values obtained from available experimental datasets. In addition, a sensitivity study regarding model-specific parameters required by Windtrax to replicate the physics and the random nature of atmospheric dispersion processes is discussed. This is a crucial point, since, for these settings, indications on the numerical values to be adopted are not available. From this study, it turns out that the investigated model specific settings do not lead to a significant output variation. Concerning the validation study, a general tendency of the model to predict the observed values with a good level of accuracy has been observed, especially under neutral atmospheric conditions. In addition, it seems that Windtrax underestimates the emission rate during unstable stratification and overestimates during stable conditions. Finally, by the definition of alternative scenarios, in which only a portion of the concentration sensors was considered, Windtrax performance appears better than acceptable even with a small number of concentration sensors, as long as the positioning is in the middle of the plume and not in the strict vicinity of the source.

Keywords: Dispersion Modelling; Backward Lagrangian Stochastic Model; Inverse Modelling; Sensitivity Analysis; Validation; Complex Sources

1. Introduction

In last years, urbanization and industrialization have been major contributing factors to poor air quality. As the air quality deteriorates, exposure to air pollution remains a fundamental concern to public health: chemical species in the atmosphere, such as NO_2, SO_2, CO, PM_{10}, $PM_{2.5}$, C_6H_6, could severely damage the health of the population (Breton et al., 2021; Haga et al., 2021).

Information on atmospheric pollution and its environmental impact on citizens is the starting point for improving air quality: the evaluation of the extent of exposure to chemicals becomes a key issue

(Piccardo et al., 2022). In this regard, dispersion modelling represents a useful tool for reproducing spatio-temporal distribution of contaminants emitted by a specific source thereby quantifying the areas of population exposure as well as the ground level concentrations of contaminants (Mangia et al., 2014).

There are several types of atmospheric dispersion models, Gaussian (Gifford, 1959), Eulerian (Jacobson, 2005; Seinfeld and Pandis, 1998), Lagrangian (Rodean, 1996), and fluid dynamics models (Moon et al., 1997). The aim of these tools is the calculation of the ambient air concentration of a species, given the meteorological and emissive conditions of the source (Capelli et al., 2012; Leelőssy et al., 2014; Tagliaferri et al., 2020).

In recent years, while the calculation of dispersion in atmospheric models has advanced (Herring and Huq, 2018; Yudego et al., 2018), model accuracy also depends on the quality of the input dataset: particularly the mass flux rate from the source (Tagliaferri et al., 2022). For point sources, such as stacks and chimneys, emission rates can be measured rapidly. On the other hand, when dealing with non-point sources, the estimation of the emission rate is a particularly challenging task due to the difficulties of direct sampling and the possible influence of different external variables, such as temperature and wind speed, on the emission rate of this kind of source (Invernizzi et al., 2019; Tagliaferri et al., 2021). Also, management and logistical practices may influence the emission from aerated basins and storage tanks (Invernizzi et al., 2020; Invernizzi and Sironi, 2021).

To this end, it would be useful to have a continuous and indirect method to estimate the emission rate. The use of an inverse dispersion model would be very fit for this purpose: this tool, by knowing a concentration value in ambient air, is able to quantify the emission rate of the source (Flesch et al., 2007).

Windtrax software (Crenna, 2006) is a backward Lagrangian stochastic model, based on the principles of Monin-Obukhov Similarity Theory (MOST) that computes an ensemble of random paths thus quantifying the unknown emission rates from measured downwind concentrations (Flesch and Wilson, 2005, 1995).

Windtrax is widely used for the evaluation of emission rates in the agro-meteorology field, where emissions of greenhouse gases, methane, or ammonia are typically measured (Gao et al., 2009; Lin et al., 2015; McBain and Desjardins, 2005; Thomas B. McKee, 1993; Yang et al., 2016). The papers published in the literature about Windtrax are generally focused on the evaluation of how well it predicts the emission of pollutants from area sources (Gao et al., 2009; McBain and Desjardins, 2005; Ro et al., 2014; Thomas B. McKee, 1993; Wang et al., 2013; Yang et al., 2016).

On the contrary, the present paper focuses on the application of Windrax for a different type of source. In fact, before tackling datasets with complex sources, it was decided to initially test the model by considering sources, such as stacks, which, to the best knowledge of the authors, were rarely discussed in the literature in similar studies.

In addition, when dealing with point sources, thanks to their easy measurement and characterisation, the observed emission rate to be compared with the model output is more reliable: consequently, the model validation is more robust. In this study, two experimental campaigns with a point source (i.e. stack) will be considered.

Windtrax model was chosen mainly because it is freely downloadable, easy-to-use thanks to a user-friendly interface, and widespread mentioned in the literature.

Initially, a critical validation of the model is carried out: the investigation does not only deal with the strict reliability of the model but also assesses under which conditions (i.e. stability class, number, and location of the sensors) the model shows the greatest accuracy. In this regard, a further aspect of novelty of this paper, in addition to the investigated type of source, concerns the validation study. More in detail, it is not limited to evaluating the impact of the measurement fetch (i.e. distance from the source and the concentration sensor) and the atmospheric stability conditions, previously discussed in the literature in case of agricultural area sources. It also focuses on the influence of the number of available detectors: it investigates if high model performance can be achieved with a single concentration sensor or if the model response may be improved by increasing the number of detectors. In addition, to improve the current state of the art, a sensitivity study regarding some model-specific parameters required by Windtrax to replicate the physics and the random nature of atmospheric dispersion processes, is discussed. This is a crucial point, since, for these settings, indications on the numerical values to be adopted are not available, neither in the literature nor in the model user's guides.

In summary, the present work aims to validate the Windtrax model by comparing the model results with observed values obtained from experimental datasets available in the literature, to perform a sensitivity analysis in order to quantify the influence of the model-specific parameters and to identify optimal values of these variables. Moreover, a specific analysis, to provide information on the optimal positioning of the sensor concentration, has been conducted.

The structure of the paper includes a brief summary of the theory of the model, the experimental campaigns, the elaborated statistics and an insight on sensitivity (Section 2). Section 3 reports the results and a critical discussion. Finally, Section 4 summarizes the conclusions and possible improvements to optimize the performance of the software.

2. Methods and Materials

2.1 Windtrax model

WindTrax 2.0.9.7 (Crenna, 2021) is a software that simulates the transport of gaseous substances in the atmosphere. It is based on the theory of the Lagrangian Particle Model (Crenna, 2006): the dispersion of pollutants is considered as a flow of dimensionless particles whose trajectory is described in a stochastic way.

It can be used either to calculate the concentration of a gaseous substance at a given point if the Emission Rate is known, or to calculate the Emission Rate if the concentration of the pollutant at a given point is known. The generic equations on which the model is based are:

$$a_{11}Q_1 + a_{12}Q_2 + \cdots + a_{1n}Q_n + C_b = C_1$$

$$a_{m1}Q_1 + a_{m2}Q_2 + \cdots + a_{mn}Q_n + C_b = C_m \quad [1]$$

Where C_b is the background concentration, Q_j are the emission rates, a_{ij} are the coefficients, computed by the model, relating the emission rate to the measured concentration C_i.

In order to solve the system of equations, there must be at least as many known concentration measurements as there are unknown emission rates. If the number of known concentrations C_i is greater than the number of unknown sources Q_j, the solution will be the best fit in the least-squares sense (Crenna, 2006).

A full description of the Windtrax model is not presented here, since it has been widely discussed in the literature (Crenna, 2006; Flesch and Wilson, 2005, 1995).

2.2 Uttenweiler and Round Hill campaigns

In this paragraph, a very brief description of the field experiments used in the present study to validate the model is provided. For further details, the authors resend to the field test reports (Bachlin et al., 2002; Cramer et al., 1958).

The Uttenweiler campaign was conducted in a pre-existing pig farm on 12 and 13 December 2000 and 31 October 2001. The farm is situated outside the small village Uttenweiler, 20 km west of the city of Bielberach (5331621 m N, 548508 m E, UTM zone 32U) in Germany. The surrounding area is mostly flat. This farm consists of the pig barn and the feed processing room. The gas tracer, sulphur hexafluoride (SF_6), was continuously emitted by a single point source located on a building and measured with a sampling rate of 0.1 Hz. The stack was at 8.5 m above the ground level, and it was connected to the internal ventilation system. 14 trials were performed, named in alphabetical order from B to O: experiment A was an attempt. Concentration sensors were located on two parallel transects, one at 140 m from the source, the other at 280 m.

During the field tests, meteorological measurements were carried out using different devices (i.e. an ultrasonic anemometer and a cup anemometer). To set the simulations, meteorological data from ultrasonic anemometer (with a sampling frequency of 10 Hz) were taken into account, since it provides atmospheric turbulence parameters from which to derive the stability conditions. This instrument was located downwind at z = 3.5 m near the first transect at which concentration measurements were undertaken.

The second campaign is the Round Hill experiment (Cramer et al., 1958). The site area, with flat terrain, is close to the Round Hill Field Station of the Massachusetts Institute of Technology (338022 E, 4600793 N, UTM zone 19T). The vertical emission consisted of a stack at 30 cm from the ground releasing SO_2. The dataset from the Round Hill campaign provides several concentration values measured from sensors positioned along arcs at different distances downwind of the release (i.e 50 m, 100 m and 200 m). Each arc is composed of receptors spaced at 3-degrees covering 180 degrees. A large number of experiments were conducted, some of which have been considered in the present study. In particular, eight experiments characterized by different stability classes, were chosen to be tested: three of them are conducted under Moderately Unstable (MU) conditions, two in Neutral (NN) conditions, two in Moderately Stable (MS) conditions and only one in Extremely Stable (ES) conditions. The data set was obtained by means of the website http://www.harmo.org/jsirwin. Meteorological data were obtained by means of a system composed by cup anemometers and ventilated thermocouples, installed at four levels (1.5, 3, 6 and 12m) on a portable tower, for measuring vertical gradients of mean wind speed and air temperature. In addition, a cup anemometer located at a height of 2 m near the release point, was installed to estimate mean wind speeds and frequency distributions of azimuth wind direction.

2.3 Model Validation

The first objective of this work was to estimate the performance of Windtrax in predicting the experimental data of emission rate from the source, by using as input the measured ambient air concentrations. For this purpose, some statistical indicators were used (Chang and Hanna, 2004; Gustafson and Yu, 2012; Hanna and Chang, 2015; Willmott, 1981): Mean Bias (MB), Normalized Mean Bias (NMB), Root Mean Squared Error (RMSE), Normalized Mean Squared Error (NMSE), Index of Agreement (IOA) and FAC2.

The equations of each indicator are reported below:

$$MB = \frac{1}{N}\sum_{i=1}^{N} E_i = \bar{M} - \bar{O} \qquad [2]$$

$$NMB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i} = \frac{\bar{M}}{\bar{O}} - 1 \qquad [3]$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2} \qquad [4]$$

$$NMSE = \frac{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2}{\overline{MO}} \qquad [5]$$

$$IOA = 1 - \frac{\sum_{i=1}^{N}(M_i - O_i)^2}{\sum_{i=1}^{N}(|(M_i - \bar{O}| + |(O_i - \bar{O}|)^2} \qquad [6]$$

$$FAC2: 0.5 \leq \frac{M_i}{O_i} \leq 2 \qquad [7]$$

Where M_i is the single modelled emission rate and O_i is the single observed value. The optimal values of these parameters indicating the best fit between the model results and the experimental data are: $MB = 0$, $NMB = 0$, $RMSE = 0$, $NMSE = 0$, $IOA = 1$. Regarding the last index, FAC2, the percentage of values within the factor 2 range will be expressed.

The percentage (%) error of the modelled value with respect to the observed one has also been calculated. The latter is computed by means of the following formula:

$$ER\% = \frac{M_i - O_i}{O_i} \qquad [8]$$

2.4 Sensitivity of model to specific parameters

A further target of this study is to assess the sensitivity of Windtrax to some model-specific parameters and settings. They might represent a significant source of uncertainty because clear indications on the numerical values to be adopted are not available. As a result, their definition is left to the professional judgment of the modelist. The sensitivity study allows to evaluate the effect on the estimated emission rate caused by a variation of an input datum, thereby identifying the most influential variables.

In particular, the investigated parameters are:

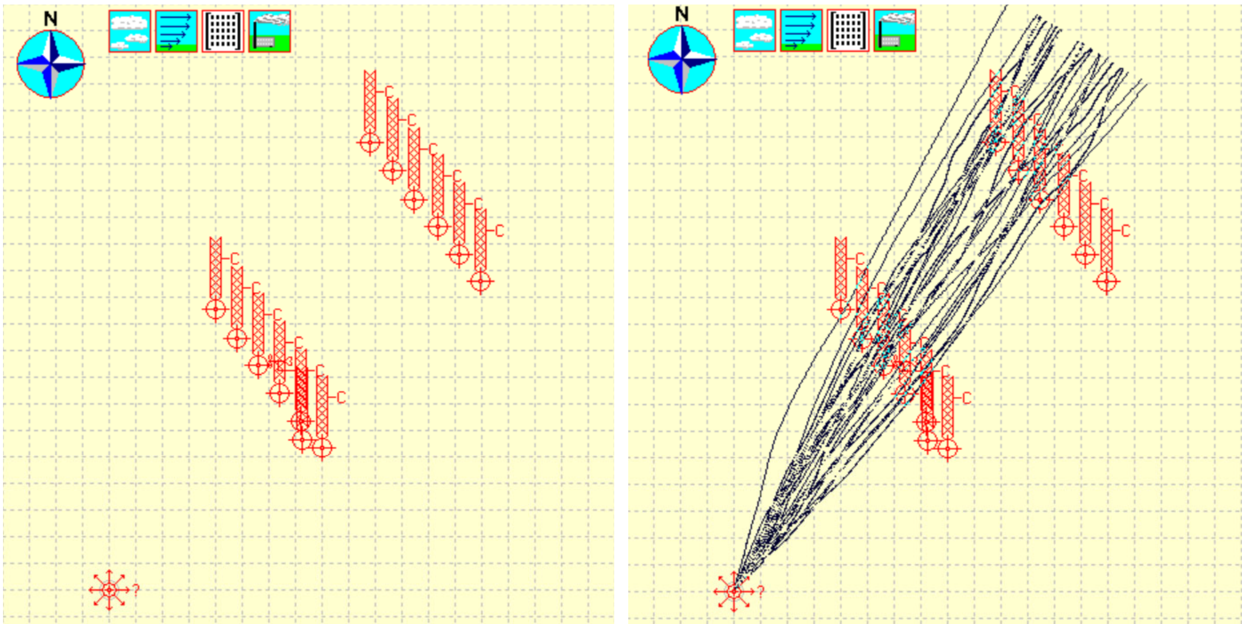
- concentration-sensor box dimension: the particles released from the source are collected within a volume surrounding the sensor. In the graphical interface of the software, it is necessary to set the box size to identify how many particles pass through the sensor. Ideally, it should be as small as possible. The drawback of making it too small is that huge numbers of particles need to be released to get a reasonable particle sample passing through the sensor's collection box.
- numerical approach generating the random stochastic trajectory of the particles. In particular, two different options are available:
    - "*Just-in-time*" mode, which generates new random numbers for each calculation,
    - "*Precalculated*" mode, a set of one million random numbers is pre-generated and stored in an array. They are then selected from the array by indicating a random array index.

To evaluate the sensitivity of the model to these parameters, the percentage error of the modelled value with respect to the observed one was computed for different values of the investigated parameters (Equation [8]).

3. Results and Critical discussions

3.1 Uttenweiler campaign

The Uttenweiler campaign was carried out in 14 experiments (B-O) lasting ten minutes each.
All these experiments had their own characteristics, such as weather data (wind velocity, wind direction, stability class) and instrument placements (sonic anemometer and concentration sensors). Therefore, each experiment was implemented separately in the software, in order to obtain as many calculated Emission Rate values as the number of experiments. As an example, a picture of the spatial configuration of experiment B is given in Figure 1a. In detail, the star with outgoing arrows next to a question mark represents the point source having unknown emission rate; the columns having the symbol "C" are the concentration sensors (which need concentration values as input); finally, the remaining column represents the anemometer. In Figure 1b, an example of the Windtrax interface is shown while the simulation is running, with particles emitted from the point source.



(a) *(b)*

Figure 1. Experiment B spatial configuration on Windtrax on the left (a); Windtrax simulation, in which the trajectories traced by the emitted particles are visible, on the right (b) (Crenna, 2006).

In this section, the sensitivity study and the validation of the model with the Uttenweiler experimental campaign will be discussed (Bachlin et al., 2002).

3.1.1 Sensitivity to model specific parameters

First of all, the sensitivity of the model to the parameters previously described (concentration sensor box dimension and random sequence generation mode) is tested. In the following figure (Figure 2), the percentage error between the modelled and the observed value, obtained for all the experiments considered when changing the concentration sensor box, is reported.

The dimensions (for both height and width) tested are: 0.5 m, 0.8 m and 1 m. From this plot, it can be inferred that the box dimension seems to have a negligible influence on the model output.

The other parameter considered is the Random Number Generation Mode, for which Windtrax offers the "*Precalculated*" and the "*Just in time*" options. In Figure 3, the percentage errors in twenty runs are reported: first, ten simulations of experiment B were performed with “*Just in time*” options and the same input data, no variables were changed. Then, ten simulations of the same experiment with “*Precalculated*” option were run. From the results of this test, a maximum error of about 10% is highlighted, regardless of the option selected. Thus, it can be concluded that there is not a remarkable difference between “*Precalculated*” and “*Just in time*” modes and that the random generation option does not produce significant differences in the results.

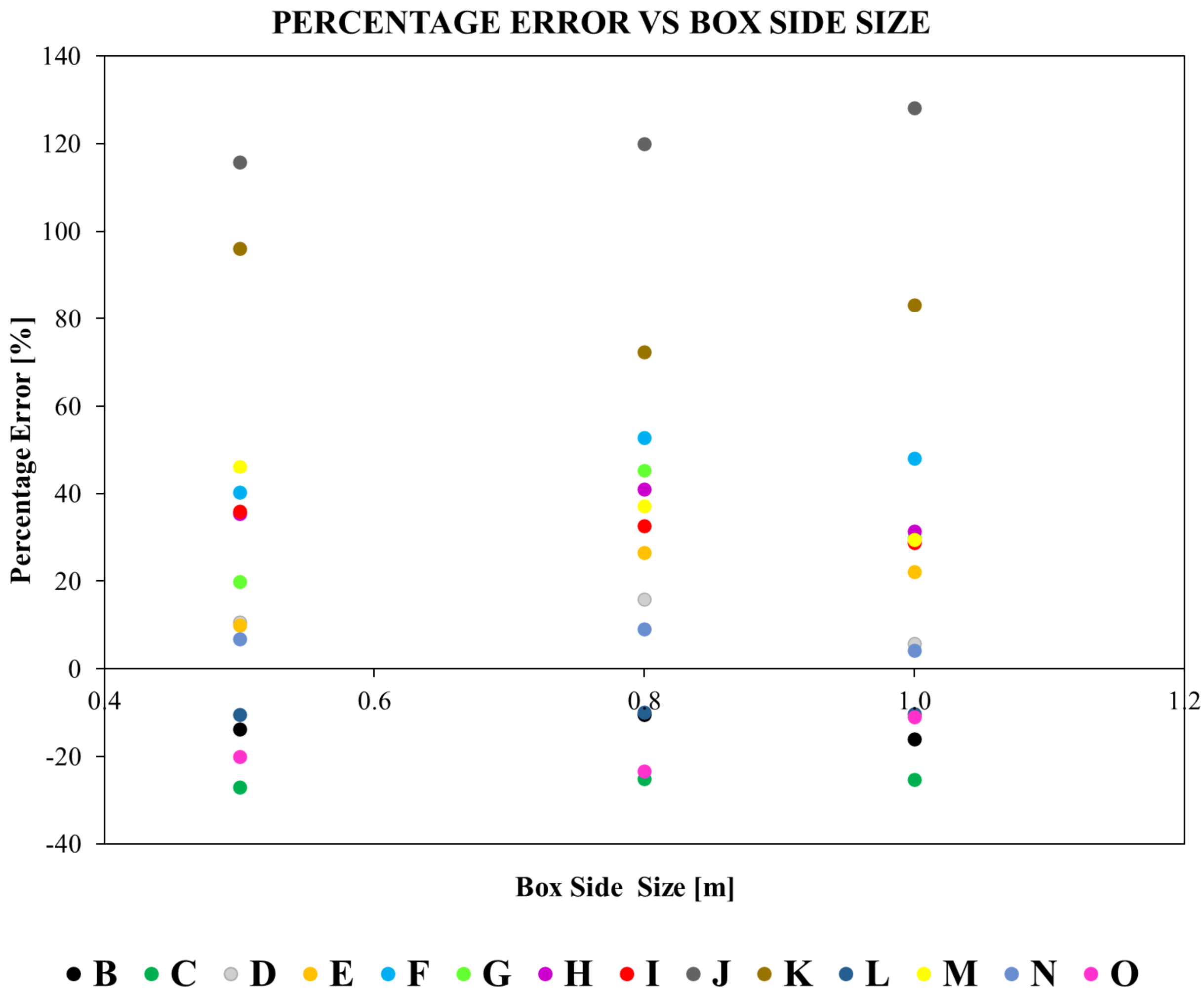


Figure 2. Percentage Error of all experiments considered in function of the Box Side Dimensions.

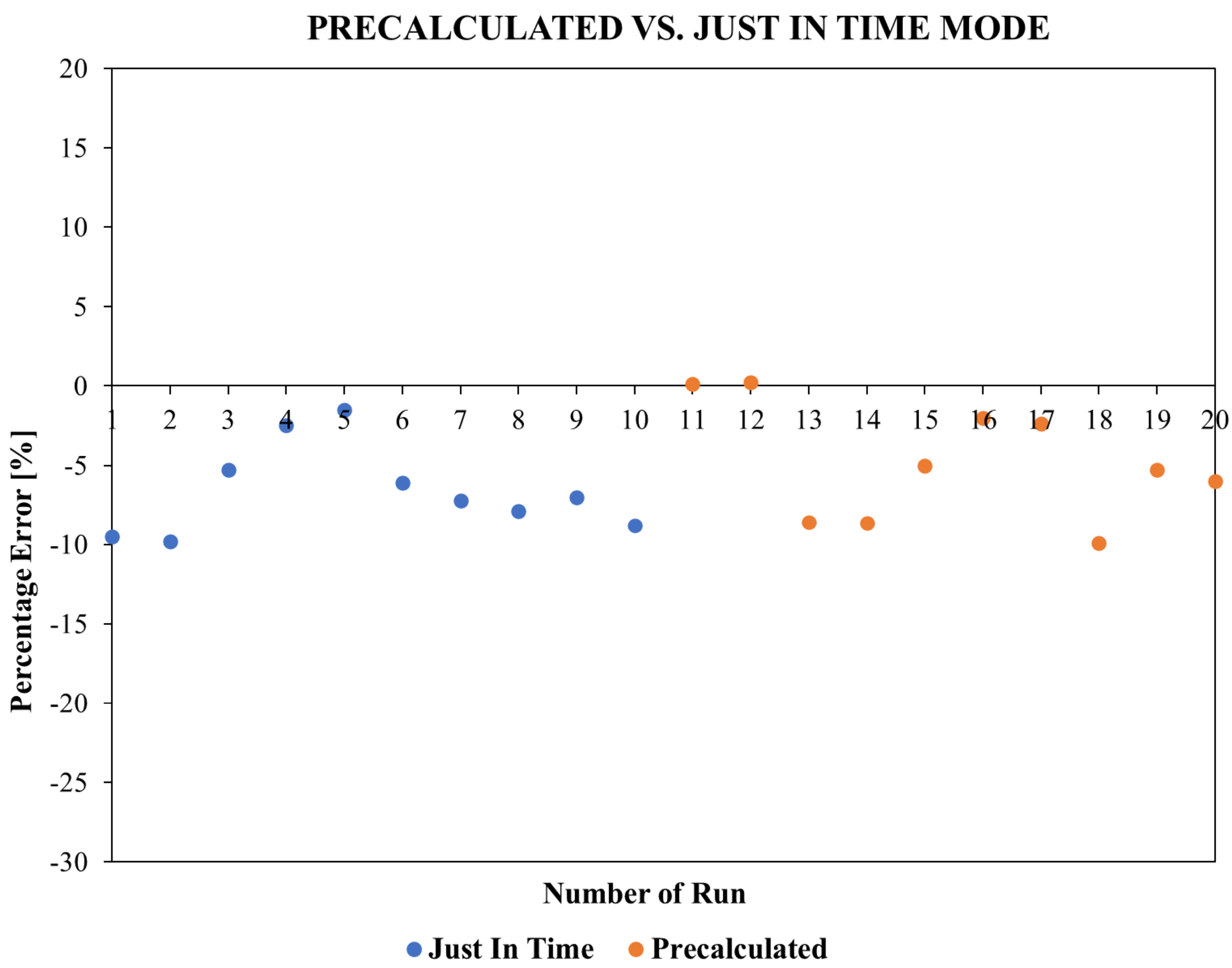


Figure 3. "Precalculated" and "just in time" methods for the calculation of Random Number Generation. Percentage errors resulting from 20 different runs are reported for experiment B.

3.1.2 Model validation

Before starting the validation study, based on the results obtained from the sensitivity analysis, the model-specific parameters were defined. In particular, it was decided to adopt "*Just in time*" method for the generation of stochastic trajectories and the dimension of concentration sensors was selected as default (0.2 m as height, 2 m as width). These parameters were fixed for all the runs.

As first test, all the possible ambient air concentration data (12 measurement points) of the Uttenweiler campaign were entered as input data. In Table 1 the statistical indicators, computed by considering all the 12 sensors of all the 14 experiments (B-O), are reported.

MB [g/h]	NMB [-]	RMSE [g/h]	NMSE [-]	IOA [-]	FAC2 [%]
46.3	0.3	94.1	0.21	0.7	100

Table 1. Statistical indicators computed by considering all the experiments; from the left: Mean Bias, Normalized Mean Bias, Root Mean Square Error, Normalized Mean Square Error and Index of Agreement.

Focusing on the statistical indicators NMB, NMSE and IOA, the values predicted by the Windtrax model (Crenna, 2006) appear quite good. To confirm this, it is emphasized that the totality of the values obtained belong to the FAC2 range.

From Equation [1], it is possible to deduce the number of the unknown emission rates should be at least equal to the number of the ambient air concentration data. In the present experimental campaign the situation is someway fanciful: 12 ambient air concentration measurements are available, whereas only one emission rate should be estimated. Thanks to this amount of data, an analysis has been conducted in order to evaluate the performance of the model by reducing the number of the available air concentration data. This assessment is intended to reflect a more realistic condition for measurement campaigns and estimation of emission fluxes using inverse modelling, where the number of concentration sensors is smaller. As discussed in the previous paragraph, the Uttenweiler campaign is characterized by a particular positioning of the concentration sensors: it develops in one or two transects (depending on the specific experiment) placed approximately perpendicular to the direction of the wind. In experiments with two transects, these are placed parallel to each other and downwind to the emission source, one at 140 from the stack, the other at 280 m, as for example reported in Figure 1.

Besides the assessment of the influence of the number of sensors, to obtain useful information about the placement of concentration detectors and the optimal distance from the emission source, only experiments that have two parallel transects of receptors (B-H, M-O), have been considered in the following analysis. Therefore, trials I, J, K, L, with a single transect, are neglected. In this way it was also possible to test the influence of the distance of the receptor from the source on the accuracy of the results, i.e. to highlight if there is a significant difference when considering receptors closer or farther from the emission.

The different configurations implemented into the model are:

1) Two transects of concentration sensors, placed parallel to each other (as in the Uttenweiler experimental campaign),
2) The entire transect of concentration sensors closest to the source,
3) The entire transect of concentration sensors farthest from the source,
4) Two downwind sensors on the transect closest to the source,
5) Two downwind sensors on the transect farthest from the source,
6) One downwind sensor on the transect closest to the source,
7) One downwind sensor on the transect farthest from the source,
8) Two downwind sensors, one on the transect closest to the source and one farthest from the source.

The choice of receptors to be considered, when reducing the number of detectors (conf. 1-7), has been made according to the position of sensors with respect to the plume direction: detectors located closest to the plume axis have been preferably considered. This is because Windtrax, in some cases, does not provide the estimation of the emission rate whether the concentration sensors are positioned far from the plume centerline.

To show the results of this test, the percentage errors between the modelled and the observed value (calculated with Equation [8]) for experimental trials conducted in neutral/stable conditions (B, C, E, F, G) and very stable (D, H, M, N, O) atmospheric conditions are shown (Figure 4). In doing so, the way in which the stability class affects the performance of the model can be easily recognized in order to identify the optimal meteorological conditions to run the model.

In particular, for each experiment, the eight different configurations (1-8) of receptors discussed above are considered. Therefore, in each plot, 40 points are shown, obtained by the combination of the 5 experimental trials (B, C, E, F, G for neutral/stable conditions and D, H, M, N, O for stable and very stable conditions) and the 8 receptors configurations (1-8), reported on x-axis. In addition, in order to evaluate the influence of the source distance, different indicators are adopted to distinguish the configurations in which all the receptors are located near (N) from the emission source (configurations 2, 4, 6), far (F) from the source (conf. 3, 5, 7) or some in the vicinity and others far (N&F) from the source (conf. 1, 8).

It is worth noting that values reported on the y-axis in the two plots are different, ranging from -60 % to 100 % in the case of neutral/stable conditions and -100 % to 350 % for unstable conditions.

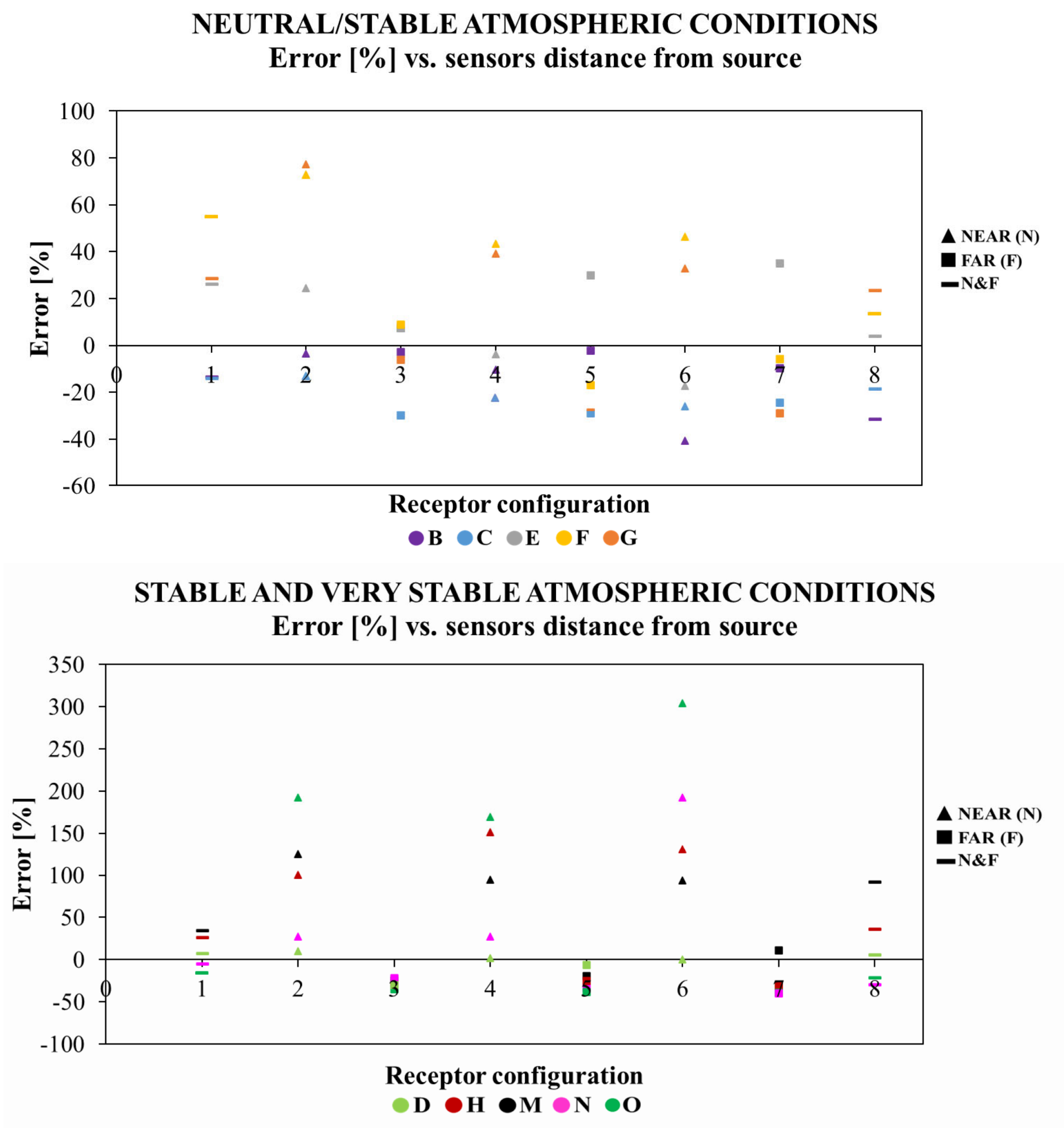


Figure 4. Estimated error (%) for the experiments computed under neutral/stable and stable or very stable atmospheric conditions in different receptors configurations (1-8), near (N) or far (F) from the source.

From these plots, it is possible to observe that the highest values of error occur when considering experiments with stable and very stable conditions. In addition, under stable stratification, high standard deviations are frequently estimated (see Supplementary Material).

The high errors obtained in stable conditions may be related to the fact that the plume emitted from the source under stable conditions is poorly dispersed in both the vertical and horizontal directions. As a result, concentration sensors are less likely to be crossed by the plume.

Moreover, errors estimated in stable and very stable conditions are more pronounced when the concentration sensor is positioned close to the emission source, with a significant overestimation of the observed value. This may be related to the fact that the poor dispersion of the plume is more pronounced in the vicinity of the emission source where the pollutant is less diluted and dispersed.

Another consideration concerns the influence of the number of receptors on the model accuracy. From Figure 5, it turns out that the reduction of the number of sensors does not necessarily improve the model performance. Thus, it can be inferred that the correct downwind placement of the sensor is much more significant than the number of sensors. In other words, the model results show a good accuracy even when considering a single measurement point provided that the sensor is properly located.

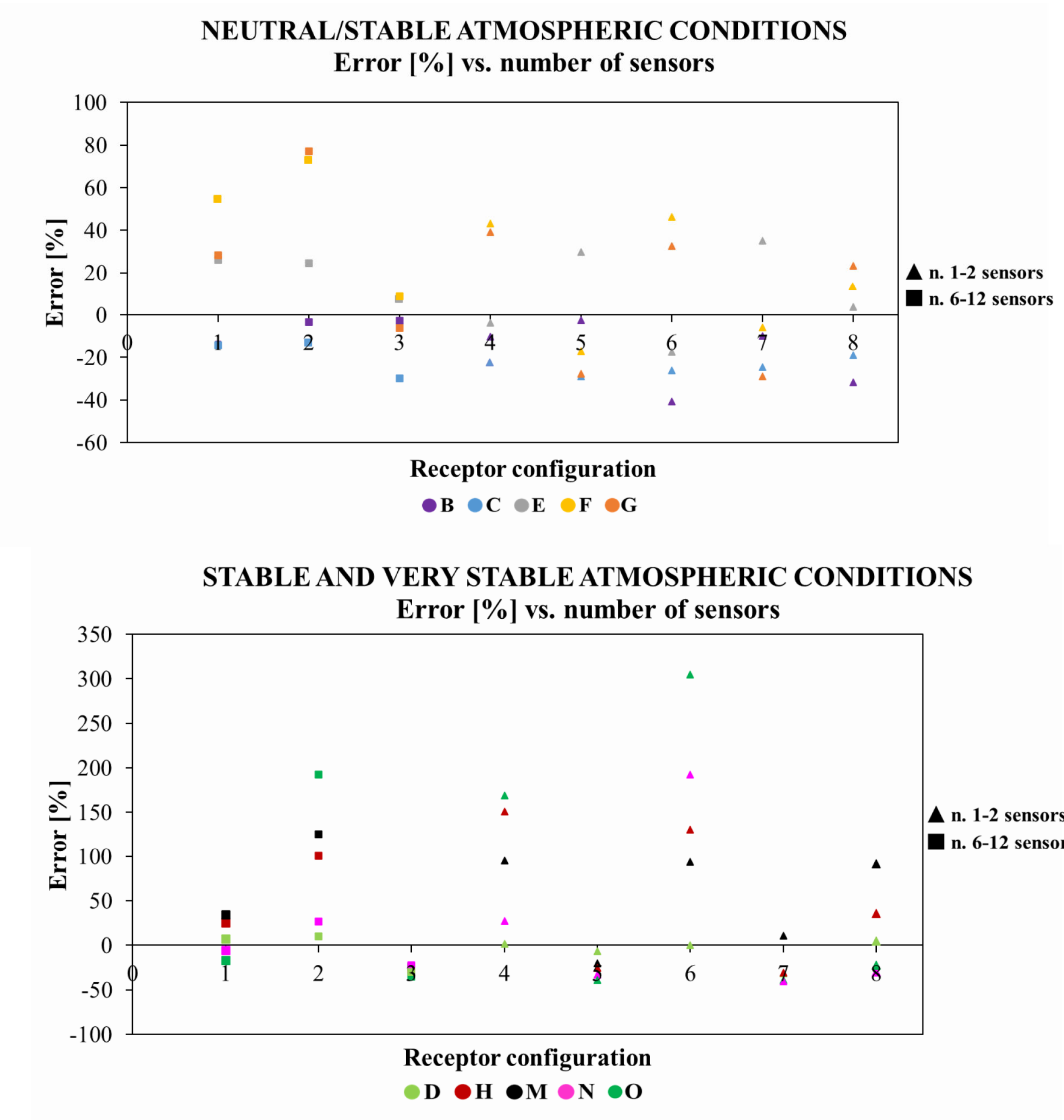


Figure 5. Estimated error (%) for the experiments under neutral/stable and stable or very stable atmospheric conditions when considering receptors configurations involving 1 or 2 sensors (conf. 3-7) or 6 or 12 sensors (conf. 0-2).

To conclude, the implementation of the Uttenweiler dataset shows good performance of the model in predicting the emission rate under neutral/stable condition. Under stable and very stable conditions great care must be taken with the location of the sensor due to the fact that the plume is poorly dispersed. In this sense, a possible solution might be to move the sensor away from the source.

3.2 Round Hill campaign

In this section of the paper the validation of the model with the Round Hill Campaign (Cramer et al., 1958) will be discussed. It is worth highlighting that, due to the low influence associated to the model-specific parameters previously investigated, the sensitivity study was not repeated for the Round Hill dataset.

3.2.1 Model validation

The simulations of Round Hill campaign allow to test the performance of the model in a wide range of stability conditions (i.e. Moderately Unstable, Neutral, Moderately Stable and Extremely Stable). In addition, for each experiment, different configurations of receptors were considered:

1) One arc of six downwind receptors at 50 m from the source;

2) One downwind receptor at 50 m from the source;

3) Two downwind receptors, one at 50 m and one at 100 m from the source;

4) One downwind receptor at 100 m from the source;

5) One downwind concentration at 200 m from the source.

The choice of receptors to be considered has been made following the same approach discussed for the Uttenweiler campaign, i.e. according to the position of sensors with respect to the plume axis.

In Figure 6 the % errors obtained for the different configurations of receptors (1-5) for the eight experiments are reported. It should be noted that for configuration 5 two points are missing (experiments n.1 and n.3), due to the failure to obtain a model result for the specific experiments.

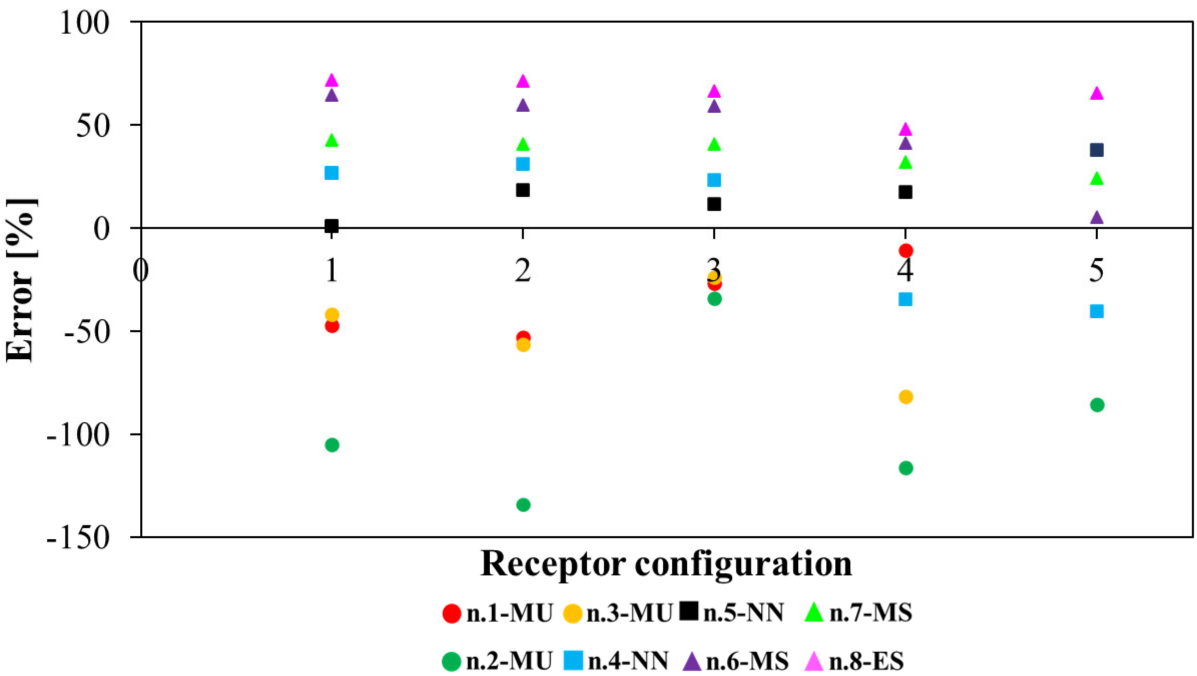


Figure 6. Percentage Error for the eight experiments with different stability classes (MU=Moderately Unstable, NN=Neutral, MS=Moderately Stable and ES=Extremely Stable), in five different spatial configurations of concentration sensors (1-5). The absence of two indicators in configuration 5 means that there were no results provided by the model.

From Figure 6 a general tendency of the model to overestimate in stable atmospheric conditions, as for the Uttenweiler dataset, and to underestimate in unstable conditions may be observed.

In addition, the best fit between the modelled value and the observed emission rate is shown in neutral stability conditions: in this situation, the percentage errors range between ±40% with an average value of about 10 %.

Conversely, the mean % error for experiments in unstable conditions is about -60%; while the mean error for trials in stable conditions is about 50%. Although the absolute values of the percentage errors obtained under stable and unstable stratification are comparable (50% vs 60%), it seems that, in unstable conditions, the model shows a general tendency to underestimate the observed values, whereas in stable conditions it generally overestimates the emission rate, as confirmed by the Uttenweiler dataset.

Moreover, in unstable situations, a more scattered error pattern (i.e. very low errors in some experiments, very high in others and eventually no results provided by the model) is shown. This behaviour is probably attributable to the high level of turbulence in unstable conditions. For this reason, it might be concluded that the model is more reliable in stable than in unstable conditions, even because the positioning of the sensor not too close to the emission source might help in the improvement of the model predictions. In fact, in stable conditions, the average percentage error seems to decrease as the distance of the sensors from the source increases: in particular, when considering the three experiments under stable stratification (n.6, n.7, n.8), in configuration 2 (receptor at 50 m from the source) the resulting error is about 60%, in configuration 4 (receptor at 100 m from the source) it decreases up to 40% and in configuration 5 (receptor at 200 m from the source) the error is 32%. This outcome confirms what previously discussed for the Uttenweiler campaign: in stable conditions the slow dispersion of the plume may lead to incorrect estimation in near-field assessments.

By reducing the number of concentration sensors, for instance by comparing (Figure 6) the errors obtained for configuration 1 (6 receptors at 50 m) and configuration 2 (1 receptor at 50 m), it turns out what previously verified with the Uttenweiler dataset: even considering a single concentration value, provided that the sensor is crossed by the plume, it seems that the model still responds well. Thus, it can be concluded that the number of sensors is not so limiting, but rather their correct placement.

In Table 2, the statistical indicators presented in section 2.3 are shown, taking into account all the simulated experiments of the Round Hill campaign. Overall, considering the absolute values of these statistical indicators, it seems that the model predicts the experimental data with a quite high level of accuracy: for example, FAC2 is 74%.

MB [g/s]	**NMB [-]**	**RMSE [g/s]**	**NMSE [-]**	**IOA [-]**	**FAC2 [%]**
-1.1	-0.14	5.0	0.32	0.11	74

Table 2. Statistical indicators for all the considered experiments; from the left: Mean Bias, Normalized Mean Bias, Root Mean Square Error, Normalized Mean Square Error and Index of Agreement

Moreover, given the wide range of atmospheric stability conditions available, for the Round Hill campaign, the performance parameters are computed (Figure 7) even distinguishing between the experiments conducted in neutral, stable and unstable conditions.

As for the Uttenweiler dataset, the best response is obtained when considering neutral conditions: in this situation, a FAC2 value of 100% is computed. Also, the other performance indicators are very close to the optimal values.

Therefore, from this study, it appears that the model is more reliable for neutral conditions, where a good agreement between the experimental data and the simulated values is observed.

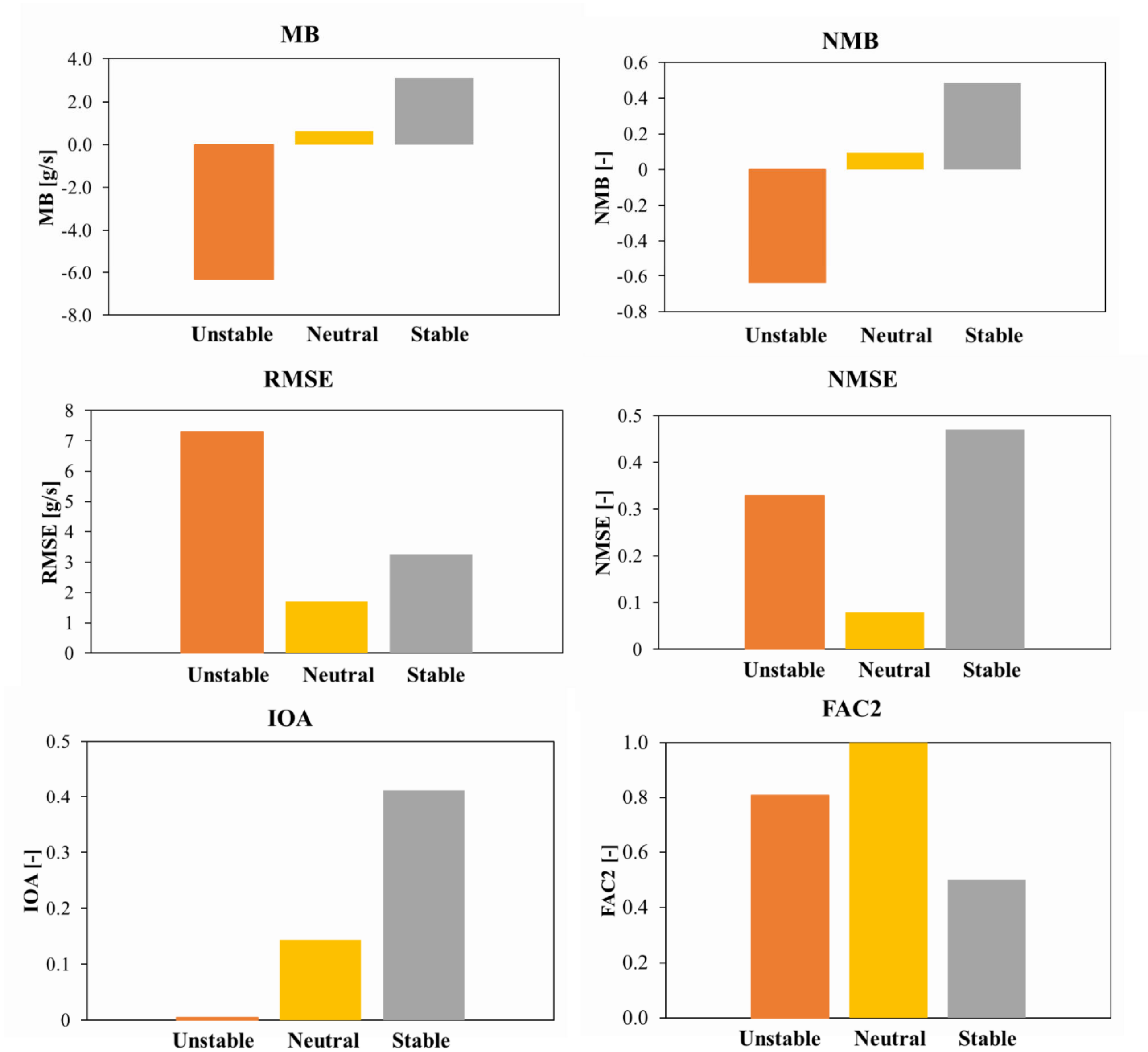


Figure 7. Statistical indicators for all the simulated experiments (Round Hill dataset) by distinguishing between unstable, neutral and stable conditions.

4. Conclusions

Due to the high complexity associated with the quantitative characterization of some kind of emission sources, the availability of a reliable tool to estimate the source emission rate starting from a downwind measured concentration would be of great interest.

This work arises from this intent. It aims to test the performance and the potential usability of the backward Lagrangian model Windtrax, widespread mentioned in agrometeorological literature.

In particular, this validation study is not limited to investigating the reliability of the model in predicting the observed emission rate, but it also tries to understand under which conditions the performance of the model are expected to be higher. In addition, the present paper discusses a sensitivity analysis of Windtrax to some model-specific parameters since the definition of these variables is mandatory, but no clear indications are available.

First of all, a sensitivity analysis was carried out on model specific parameters (i.e. concentration sensor box dimension and random number generation mode). It was found that these variables do not lead to a significant output variation.

Concerning the validation, from the results of this study, it turns out a general tendency of the model to predict the observed values with a good level of accuracy. In particular, for the Uttenweiler and the Round Hill campaigns, acceptable values of the performance indicators are obtained. For the Uttenweiler dataset, it turns out that all the values obtained belong to the FAC2 range. The estimated FAC2 indicator for the second campaign is satisfactory, corresponding to 74%. By the definition of alternative testing scenarios, where only a portion of the concentration measurement sensors were considered, further information have been obtained: the performance of the software is better than acceptable even with a small number (1 or 2) of concentration sensors, as long as the positioning is in the middle of the plume and not in the strict vicinity of the source. This appears particularly strengthened in stable conditions.

In addition, from this evaluation, the performance of the model in different stability conditions were investigated. In this regard, it appears that the model is more reliable in neutral conditions, where a good agreement between the experimental data and the simulated values is observed. Accordingly, studies available in the literature revealed lower emission calculation errors under neutral atmospheric conditions (Gao et al., 2009; Wang et al., 2013) even though, as discussed in the introduction, they focus on a different source configuration with respect to the point source implemented in this study. In addition, Gao et al., (2009) confirmed the general tendency, observed in this study, of Windtrax to underestimate the emission rate during unstable stratification and overestimate during stable conditions, whereas an opposite behaviour is observed by Wang et al., (2013). The latter also showed higher performance in stable conditions when moving the sensor far away from the emission source as long as the distance is not excessively increased.

In conclusion, Windtrax appears to be a very promising tool for the estimation of the emission rates. Its use may be very attractive also for the continuous monitoring of the emission rate, in order to correlate it with external variables (meteorological, operational…).

However, it is worth highlighting that it is not a trivial tool, and therefore, in order to obtain useful results, it requires a preliminary analysis, regarding the position of the concentration sensors and the optimal meteorological conditions.

Finally, to improve and optimize the performance of the model, it could be helpful to implement into the software an algorithm to simulate the plume rise mechanism and elevated (not-ground-level) area sources.

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