On the minimal wind directions required to assess mean annual air pollution concentration based on CFD results

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Abstract: Computational fluid dynamics has shown a great interest among the scientific community to assess air pollutant concentrations in urban areas and, define strategies to limit air pollution and achieve sustainable cities of the future. Recent studies have given methodologies on how to assess mean annual concentrations based on numerical model results to compare with the annual air quality standards. Nonetheless, these methodologies need many wind directions to be modelled and, therefore, lead to high calculation costs. The purpose of this paper is to present two approaches to decrease the calculation costs when calculating annual concentration from computational fluid dynamics results by (1) ignoring uniformly spaced wind direction and (2) considering the predominant wind directions. According to the results, the first approach is on overall better than the second one for any wind rose or building layout considered. With the first approach, the calculation costs can be reduced up to 50% without leading to more than 20% of error, and even less error can be expected for homogeneous wind roses. Finally, a method to finely evaluate errors made when using the first approach versus using the whole wind rose, without computing it, is presented.

Keywords: CFD, air pollution, mean annual concentration, wind rose, computation optimization.

Highlights:

- Calculation costs can be decreased when assessing annual concentrations.
- Evenly spaced wind direction approach works better than the predominant one.
- 50% of calculation cost gain leads to less than 20% of error with the first method.
- The error of not considering the complete wind rose can be finely evaluated.

Acronyms and abbreviations	
CFD	Computational Fluid Dynamics
COST	European Cooperation in Science and Technology
EU	European Union
LES	Large Eddy Simulation
RANS	Reynolds-Averaged Navier-Stokes
RNG	Re-Normalization Group
WHO	World Health Organization

1. Introduction

Air quality is a topical issue since atmospheric pollution has an impact on both environment and human health. Indeed, it has for example a great impact on acid rains (Zhang et al., 2017), but also on agricultural productivity (Wang et al., 2020), and can lead to several diseases (Calderón-Garcidueñas et al., 2020; Z. Yang et al., 2020), thus lowering life expectancy (Balakrishnan et al., 2019; Wu et al., 2020). In the meantime, studies have shown that people living in the vicinity of heavy-traffic roads are more likely to be at risk (Anderson et al., 2012). Additionally, other findings have shown that outdoor nitrogen dioxides (Shaw et al., 2020) and particulate matters (Bai et al., 2020; Ścibor et al., 2019) concentrations have a significant impact on indoor air quality. With more than one in two people living in urban areas nowadays with a related percentage expected to reach 68% worldwide in 2050 (United Nations, 2019), and knowing that urban areas are more polluted than rural ones (Jurado et al., 2020), mitigating outdoor air pollution becomes more and more a global challenge and a key point to achieve sustainable cities of the future for a majority of people (Bibri and Krogstie, 2017).

In order to mitigate air pollution, it is, first of all, necessary to have comparison criteria such as limit or target values. Such values, with daily, hourly and annual discretizations, were issued worldwide by the World Health Organization (WHO) and in Europe by the European Union (EU) in order to give standard values to protect population health (EU, 2008; WHO, 2017). Then, ways to assess air pollutant concentrations are needed and, especially, annual concentrations, since studies have shown that annual standards are harder to reach and more constraining that the other ones (Jenkin, 2004; Mavroidis and Ilia, 2012; Yuan et al., 2019). To assess annual concentrations, two distinct possibilities including on-site monitoring and numerical modelling can be used. While on-site monitoring requires waiting a full year, which could be reduced to one month for nitrogen dioxides using some methodologies (Jurado et al., 2020), numerical modelling allows getting results quickly and considering various scenarios including emission and urban morphology evolution (J. Yang et al., 2020).

Among the numerous numerical models available to model air pollutant dispersion, computational fluid dynamics (CFD) has shown a great potential and a great interest from the scientific community given the many physical phenomena that can be considered. It includes notably the effects of vegetation on both airflow and pollutant deposition (Buccolieri et al., 2018; Lee et al., 2018; Santiago et al., 2017b), the atmospheric chemistry involving nitrogen oxides (Bright et al., 2013; Sanchez et al., 2016) as well as the effects of heat exchanges and solar radiation (Allegrini et al., 2015; Reiminger et al., 2020a; Toparlar et al., 2017; Yumino et al., 2015). CFD models have already been used to assess annual concentrations (Rivas et al., 2019; Vranckx et al., 2015) and, additionally, a recent study has highlighted and discussed the different ways to assess annual concentrations based on numerical results and wind data (Reiminger et al., 2020b). However, these different studies always considered all the wind directions available in the wind rose which lead to a significant number of simulation to be performed. In view of the calculation time and, therefore, the calculation costs of CFD modelling, the question of reducing the number of wind directions to model in order to compute annual air pollutant concentrations is relevant.

The aim of the present work is to assess the possibility of limiting the number of wind directions needed to be modelled in order to compute annual air pollutant concentrations based on CFD results. Particularly, the novelties of this work reside on both quantitative and qualitative results using the methodology to compute mean annual concentrations presented by Reiminger et al. (2020b): questioning the discretization of wind roses which can change the results; allowing computing the mean annual concentration with fewer simulations to reduce the computational cost of a CFD study; challenging different ways of reducing the number of directions to compute annual concentration in an air quality CFD study; determining the order of magnitude of the additional error made by reducing the number of wind directions modelled for several building layouts and wind roses; a methodology to determine the error made once the chosen number of simulations is computed, thus enabling the user to see if the error is within a satisfying range or if it needs more directions to be modelled. To do so, different options are compared considering (1) different discretization steps in the wind directions and (2) the greatest contributions to the total wind frequencies. The meteorological data, the areas modelled, the CFD model used for the purpose of illustration and the methodology to compute the annual concentrations are presented in Section 2. Then, the approaches to limit the number of wind directions needed are described and compared in Section 3. Finally, a discussion is presented in Section 4.

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2. Material and methods

2.1. Meteorological data

The wind data used for the purpose of this work were obtained from five meteorological stations in France in Strasbourg, Brest, Nîmes, Lille and Paris respectively located in the extreme east, west, south, north and in the center of the country. These data were provided by Météo-France, the french official climatology and meteorology service, and correspond to ten years of averaged data for the Strasbourg station (from 1999 to 2008) and twenty years of averaged data for the other stations (from 1999 to 2018). The corresponding wind roses are presented in Figure 1.

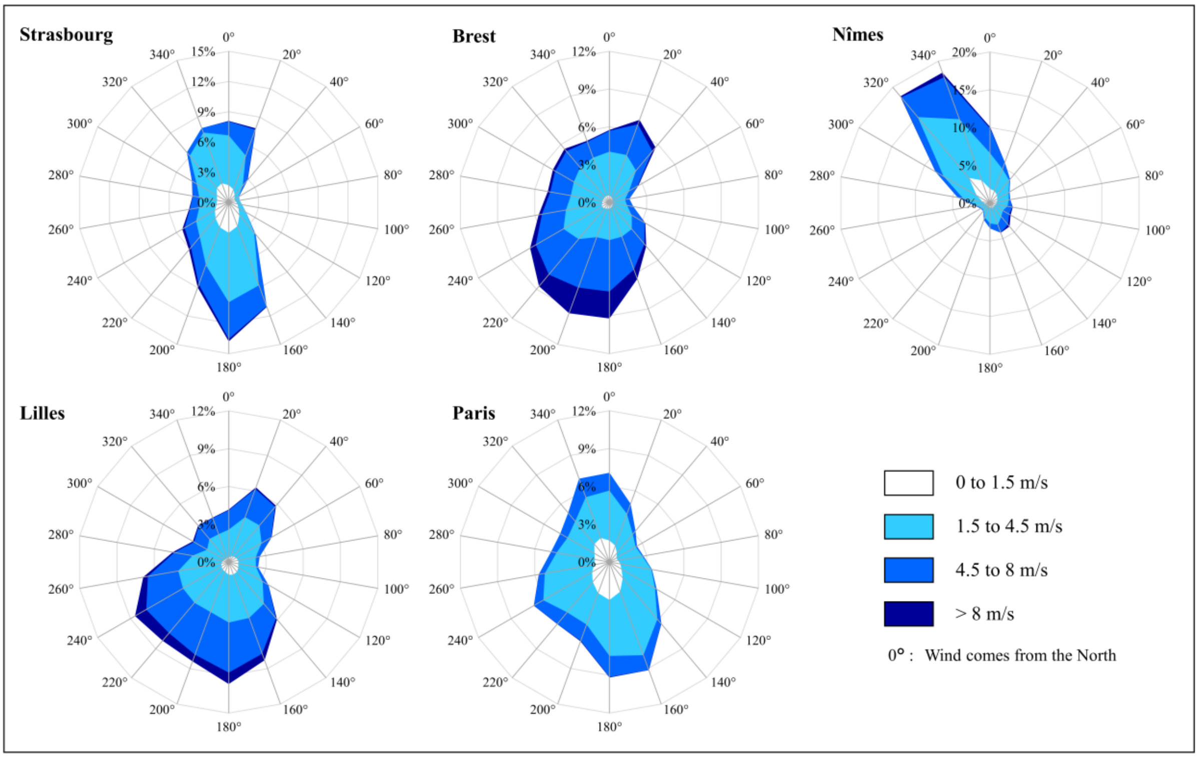

Figure 1. Wind roses for the five meteorological stations considered.

These stations were chosen firstly to cover different wind types throughout France but also because of the differences observed in the wind data to improve the statistical independence of the results. Indeed, according to Figure 1, the five wind roses are complementary with the station of Strasbourg having a preferential wind axis (North-South) with winds distributed in both directions while the station of Nîmes has only a preferential direction from the North-West. The other stations having finally no preferential direction but a greater variation in the share of velocities with the station of Paris having a majority of winds ranging from 1.5 to 4.5 m/s and the Brest Station having the greater frequency of winds higher than 8 m/s.

2.2. Numerical model

All the simulations were performed using the unsteady and incompressible *pimpleFoam* solver taken from the OpenFOAM 6.0 library, since unsteady simulations can improve the results for the concentration field over a steady state calculation (Tominaga and Stathopoulos, 2017). This solver was modified to include an Eulerian passive scalar transport equation to account for pollutant dispersion, which is commonly used to model gaseous (Santiago et al., 2017a) or particulate matter (Pospisil and Jicha, 2010) dispersion. It should be noted that, for some types of pollutants such as pollen, specific phenomenon needs to be considered (Salesky et al., 2019) but is not of interest for the purpose of this work. The partial differential equations were solved using the Reynolds-Averaged Navier-Stokes (RANS) methodology and an RNG k-ε turbulence model (Koutsourakis et al., 2012; Papageorgakis and Assanis, 1999). This solver was previously validated by Reiminger et al. (2020b).

Seven different urban configurations were considered for this study: five real building layouts in Strasbourg city, noted N1 to N5, and seven road layouts (three different road layouts were applied to the N5 building layout). A top view of these different configurations is given in Figure 2 and additional information on building heights are given in Table 1.

Table 1. Minimal, mean and maximal height of the buildings for the five building layouts considered.
(+: homogeneous, -: heterogeneous).

Building layout	N1	N2	N3	N4	N5
Minimal height [m]	2	3	2	2	2
Mean height [m]	9	11	17	14	16
Maximal height [m]	11	14	26	21	22
Homogeneity	+	+	-	-	-

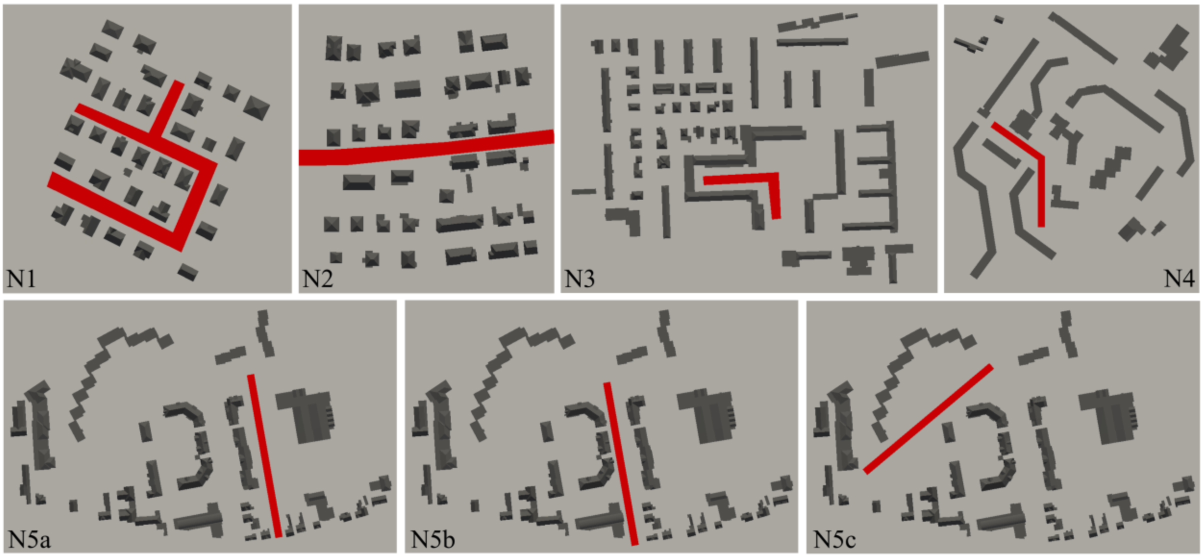

Figure 2. Top view of the five building layouts used in this study (N1 to N5) and the three road layouts used for the N5 case (N5a to N5c) with in red the roads considered as pollutant sources.

For each of these cases, the recommendations of the cost actions 732 guidelines (Franke et al., 2007) were followed. For our computational domains, considering H the highest building height in each area considered, the distance between the inlet and the buildings is at least $5H$, which is also the minimal distance between the outlet boundary and the buildings, as well as between the buildings and the lateral boundaries. Lastly, the height of the computational domain was set to $6H$. After a grid sensitivity check, hexahedral meshes of 1 m in the areas of interest and 0.5 m both near the buildings wall boundaries and emission sources were used which corresponds to a comparable resolution of other studies (Di Sabatino et al., 2007; Sanchez et al., 2017; Vranckx et al., 2015). This resolution leads to a total number of cells ranging from 550,000 to 2.8 million depending on the area considered and an example of the resulting meshes is presented in Figure 3 for the urban configurations and N2.

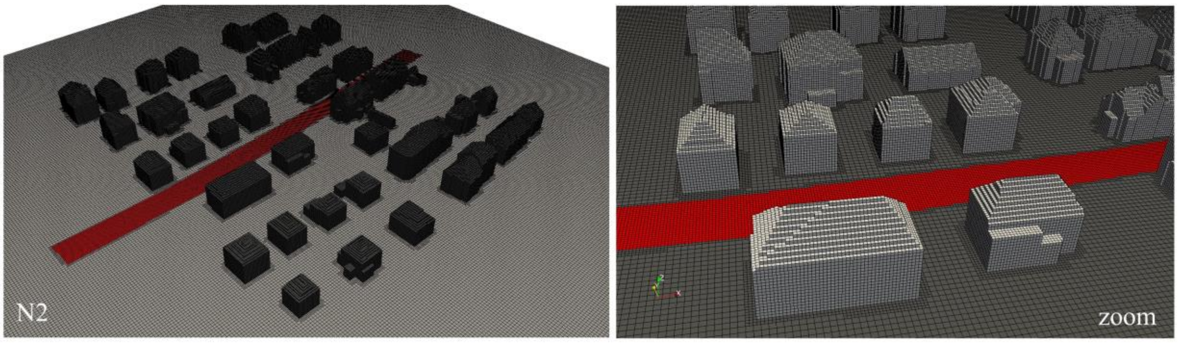

Figure 3. Illustration of the selected meshes for the N2 urban layouts (in red the roads considered as emission sources).

Concerning boundary conditions, symmetry conditions were applied at the top and the lateral boundaries when no-slip conditions were applied to the wall surfaces such as the building's walls or the ground. Neutral velocity, turbulent kinetic energy and turbulent dissipation rates profiles following the log-law profile suggested by Richards and Norris (2011) with a wind velocity of 1.5 m/s at 10 m high were used for the inlet boundary and a free stream condition was set at the outlet.

A total of 126 simulations were performed considering 18 wind directions (20° steps) and 7 urban configurations.

2.3. Annual concentration calculation

The annual air pollutant concentrations were calculated based on the 126 CFD results obtained and the continuous methodology suggested by Reiminger et al. (2020a). This methodology involves four equations which are given hereafter. Particularly, it corresponds to (1) the equation of the optimized sigmoid function used to describe the wind distribution based on the wind rose data, (2) the equation of the evolution of the CFD modelled concentration with the wind velocity for neutral atmospheres, (3) the equation to compute the mean annual concentration for a given wind direction and (4) the equation to compute the mean annual concentration. Further details on how to apply this methodology and these equations can be found in the original paper of Reiminger et al. (2020a).

$$f(v) = \alpha.\left(-1 + \frac{1}{1+\beta_1.e^{-\gamma_1.v}} + \frac{1}{1+\beta_2.e^{\gamma_2.v}}\right) \qquad (1)$$

where $\alpha, \beta_1, \beta_2, \gamma_1$ and γ_2 are positive parameters.

$$C_u = U_{ref}.\frac{C_{ref}}{u} \qquad (2)$$

where C_u is the pollutant concentration for the wind velocity u not simulated and C_{ref} the pollutant concentration for the simulated wind velocity U_{ref} (1.5 m/s at 10 m high).

$$\bar{C_d} = C_{max}.\frac{\int_0^{v_{min}} f(v).dv}{\int_0^{+\infty} f(v).dv} + \frac{\int_{v_{min}}^{+\infty} c(v).f(v).dv}{\int_0^{+\infty} f(v).dv} + C_{bg} \quad (3)$$

$$\bar{C} = \frac{\sum_{d=1}^{n} \bar{C_d}.f_d}{\sum_{d=1}^{n} f_d} \qquad (4)$$

where $\bar{C}_d$ is the mean annual concentration for a given wind direction, C_{max} is the maximal concentration accepted for the calculation, v_{min} is the velocity under which $c(v)$ is considered equal to C_{max}, $f(v)$ is equation (1), $c(v)$ is equation (2), C_{bg} is the background concentration, $\bar{C}$ is the mean annual concentration and f_d the total frequency of a given wind direction.

When using this continuous methodology, it is necessary to define a minimal velocity (v_{min}) for which a constant pollutant concentration (C_{max}) will be applied, considering that the pollutant concentration will not increase indefinitely with the decrease of the wind velocity but reach a threshold due to numerous new phenomena such as vehicle-induced turbulence or natural convection (Reiminger et al. 2020a). For the purpose of this work, v_{min} was set to 1.1 m/s since it corresponds to a low wind speed were additional turbulence due to traffic start to be as important as wind speed turbulence (Vachon et al., 2002). Lastly, C_{max} was calculated according to equation (2), with $u = v_{min}$.

For the purpose of this study, no background concentration was considered.

2.4. Comparison cases considered in this study

The continuous methodology described previously was applied to all wind roses and all areas considered, leading to a total of 5 × 7 = 35 results which are considered as the reference results.

Two approaches were studied to limit the number of wind directions needed to be modelled in order to compute annual air pollutant concentrations based on CFD results: (1) ignoring some wind directions with a regular step (e.g. considering only one wind direction out of two) and (2) considering the predominant wind directions (e.g. considering the first ten wind directions with the greatest contributions to the total wind frequency). The results of these methodologies compared to the reference results are given in Section 3. A comparison between the two methodologies is also provided. The errors discussed in this paper are the error between the CFD reference results considering the whole wind rose (18 directions) and the various presented methods. Thus, it is not a comparison with the error made by CFD compared with real in situ values which is another matter entirely as discussed in (Rivas et al., 2019) in which they reach less than 30% error concentrations without consideration of chemical mechanisms.

3. Results

3.1. Annual concentration calculation when ignoring wind directions with a regular step

The first approach considered to decrease the number of simulations for annual concentration calculation consists in ignoring some wind directions with a regular step. In particular, we try to consider one direction out of two, three, six and nine. By doing so, the annual concentrations are calculated considering 9, 6, 3 and 2 wind directions respectively, as shown in Figure 4. It should be noted that depending on the number of directions considered, a more or less important number of possibilities do exist leading to various starting directions (considering one direction out of two leads to two possible starting directions: 0° and 20°, considering one direction out of three leads to three possible starting directions: 0°, 20° and 40°, etc.). The results were then compared with the reference annual concentrations obtained considering the whole wind rose, thus, 18 wind directions.

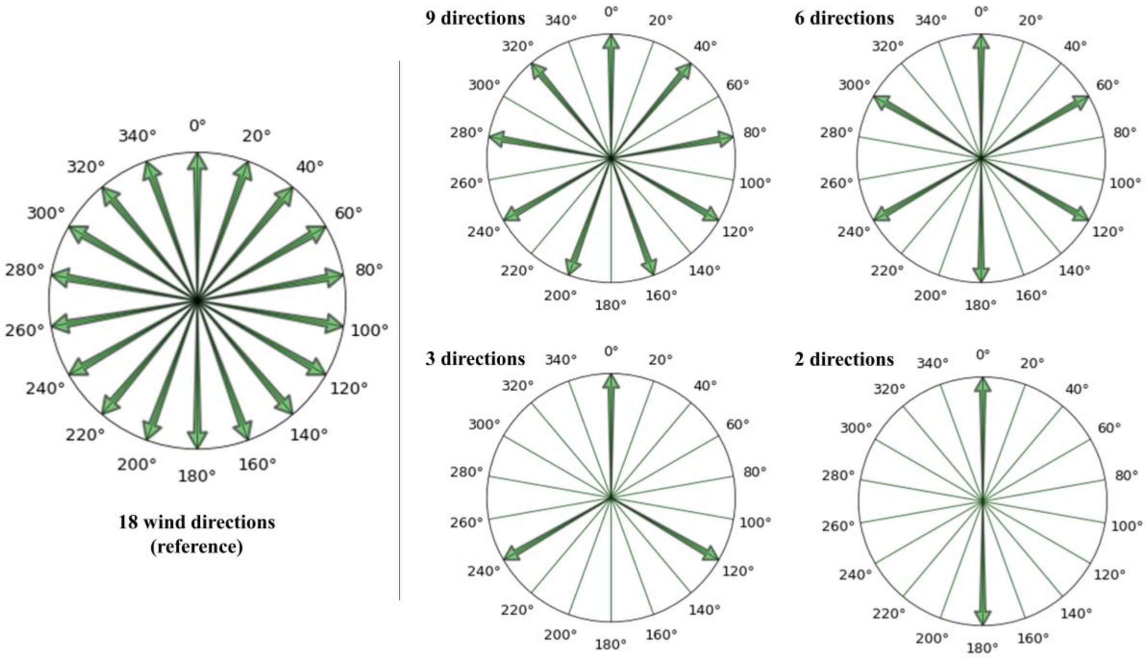

Figure 4. Explanation on what is referred as 18, 9, 6, 3 and 2 wind directions with regular steps for annual concentration calculation.

A first comparison is given in Figure 5 corresponding to the building layout N1 and the wind rose from Paris considering one direction (B1) out of two, (B2) out of three, (B3) out of six and (B4) out of nine. In spite of some local variations, it can be seen that the results obtained using 9 and 6 wind directions, respectively in Figure 5 (B1) and (B2) are close from the reference case which needed 18 wind directions. The results obtained with 2 and 3 wind directions, respectively in Figure 5 (B3) and (B4), seem more different from the reference result.

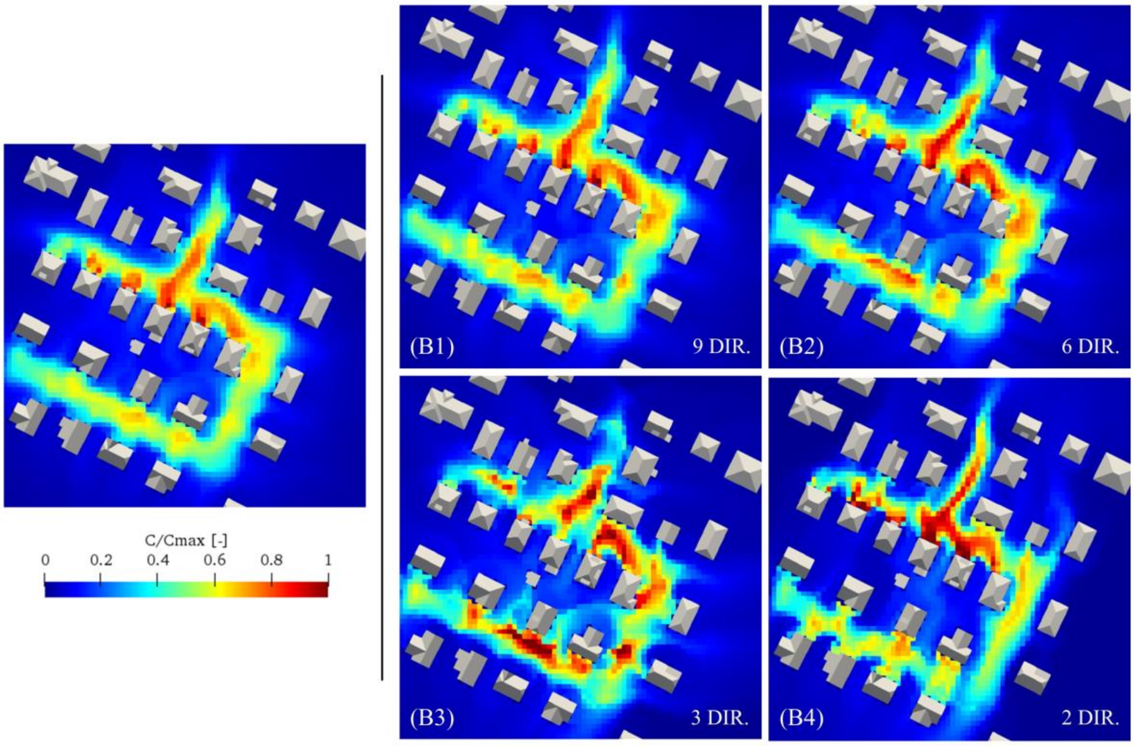

Figure 5. Examples of mean annual concentrations results for the building layout N1 and the wind rose of Paris using (A) the whole wind rose (reference), (B1) 9 directions, (B2) 6 directions, (B3) 3 directions and (B4) 2 directions.

In order to have a global information, global parameters were calculated. The overall results on mean error, mean relative standard deviation, calculation costs gain and the ratio between the gain and the error are given in Table 2 considering all the seven building layouts, the five wind roses, and the different starting directions. As previously observed, the best results compared to the reference are achieved considering one direction out of two which lead to an overall error of 13.8%. Decreasing the number of directions increases the error but considering one direction out of three lead to an error of around 21% on average. Finally, considering only two or three wind directions to compute the annual concentrations lead to high errors of more than 40%. Lastly, the best compromise between the gain in calculation costs and the induced error is obtained considering one direction out of two, with a corresponding ratio of 3.8 and a total gain of 50% with the assumption that all simulations have the same calculation cost.

Table 2. Global results for annual concentration calculation using a regular wind direction step with the mean errors, the standard deviations, the calculation cost gain and the ratio between gain and error.

Directions considered	Mean error (%)	Standard deviation	Cost gain (%)	Gain/Error
9	13.8	6.8	50	3.8
6	20.9	10.3	67	3.2
3	38.8	20.3	83	2.2
2	52.4	30.3	89	1.7

Lastly, the influence of the building layout and the wind rose was assessed. The results are given in Figure 6 for the four cases considered (9, 6, 3 and 2 wind directions) with (A) the mean errors as a function of the wind rose and (B) as a function of the building layout. According to Figure 6 (A), the wind rose has an impact on the mean errors obtained with the four cases considered leading to an overall maximal variation of 1.7. As an example, considering one wind direction out of two (9 directions in total), an error of 10.0% is obtained with the wind rose of Brest and 17.8% with the one of Nîmes. If we consider the overall patterns of the wind roses (see Figure 1), the wind roses of Brest and Lille, homogeneous over wind direction and wind speed, lead to the minimal differences compared to the reference. Inversely, the wind roses of Nîmes and Strasbourg, with a preferential direction and more intermediate velocities (ranging between 1.5 and 4.5 m/s), lead to the maximal differences compared to the reference. Finally, an intermediate result is obtained with the wind rose of Paris, homogeneous but with more intermediate velocities. This observation is valid whether the case considered (9, 6, 3 or 2 wind directions). Such trends are not observed as a function of the building layout and, according to Figure 6 (B), an overall maximal variation of 3.9 is obtained which is higher than previously when making the comparison as a function of the wind roses. The results are thus more sensitive to the building layout than to the wind rose considered.

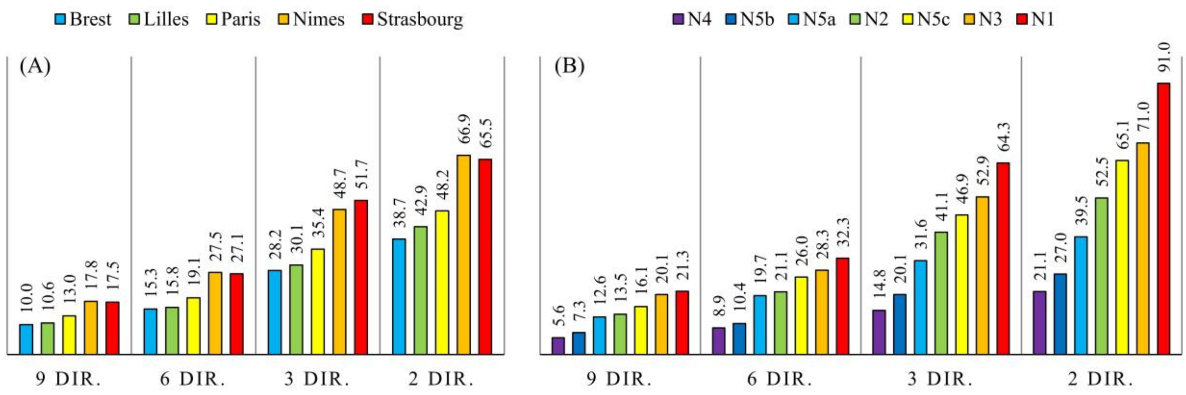

Figure 6. Mean error over the mean annual concentration compared to the reference using a regular wind direction step as a function of (A) the wind rose location and (B) the building layout (DIR: Directions).

According to the previous results, calculating mean annual concentration by ignoring some wind directions with a regular step can lead to significant calculation cost reductions without leading to too much induced errors. It is particularly true when modelling one wind direction out of two, where calculation costs are reduced to 50% and an error of less than 20% can be expected (around 13.8% on average) whatever the wind rose or the building layout considered. Finally, the more a wind rose is homogeneous the smaller the error is.

3.2. Annual concentration calculation when considering the predominant wind directions

The second approach studied to decrease the number of simulations for annual concentration calculation is about considering the predominant wind directions. In particular, the first, the first two, the first three up to the first seventeen wind directions with the most occurrence frequencies were successively considered. The results were then compared again with the reference annual concentrations obtained considering the whole wind rose, thus, 18 wind directions.

A first comparison is given in Figure 7 corresponding to the building layout N1 and the wind rose from Paris and considering (B1) the first fifteen, (B2) the first nine, (B3) the first six and (B4) the first wind direction with the most occurrence frequency. In spite of some local variations, it can be seen that the results obtained using 15 and 9 wind directions, respectively in Figure 7 (B1) and (B2) are close from the reference case which needed 18 wind directions. The results obtained with less wind directions seems more different from the reference result, leading to higher local concentrations.

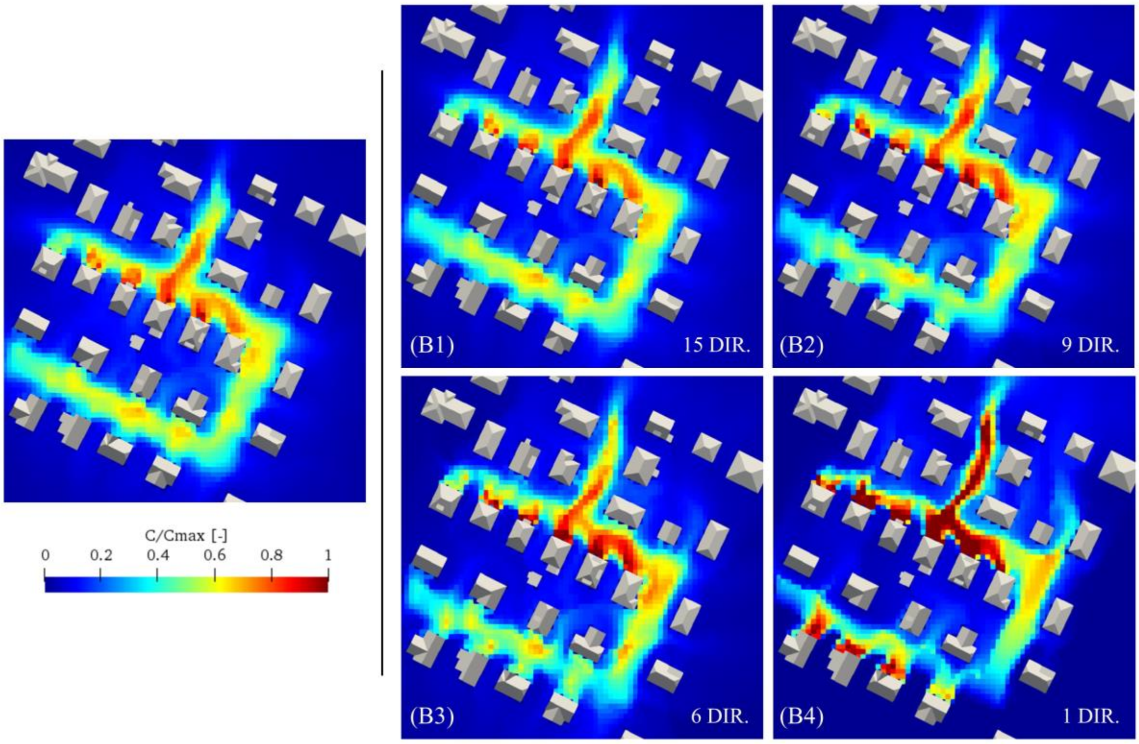

Figure 7. Examples of mean annual concentrations results for the building layout N1 and the wind rose of Paris using (A) whole wind rose (reference), (B1) 15 directions, (B2) 9 directions, (B3) 6 directions and (B4) 4 directions.

The evolution of the global mean error (considering all building layouts and wind roses) with their respective standard deviation is given in Figure 8. The gain in calculation cost and the ratio between gain and error are also plotted. According to this figure, the global evolution of the induced error while ignoring some wind directions seems to be linear between 10 and 18 wind directions considered to compute the mean annual concentration. In this case, around 1.75% of error is generated for each wind directions not considered. For fewer than 10 wind directions considered, the error starts evolving exponentially. The maximal value of the ratio between gain and error is reached for 15 wind directions with an overall value of 3.25 between 12 and 17 wind directions. This ratio starts decreasing linearly for fewer than 12 wind directions considered.

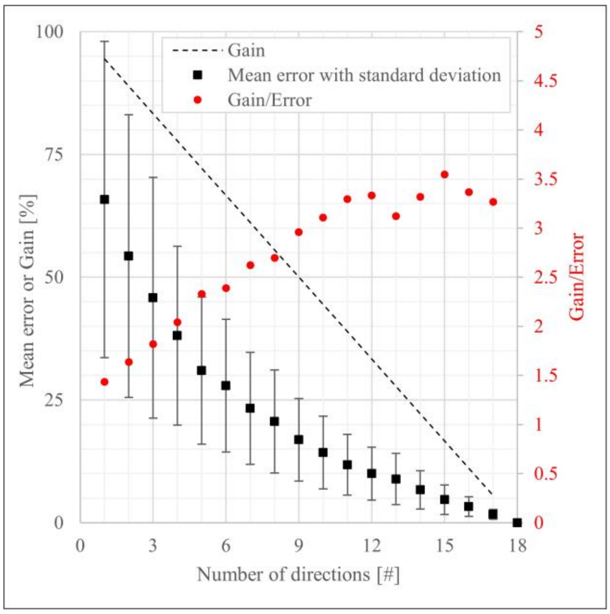

Figure 8. Global results for annual concentration calculation using the predominant wind directions with the mean errors, the calculation cost gain and the ratio between gain and error.

As previously, the influence of the building layout and the wind rose was assessed and the results are presented in Figure 9. According to Figure 9 (A), the wind rose have an impact on the mean errors obtained leading to an overall maximal variation of 1.9. If we consider the overall patterns of the wind roses (see Figure 1), there is no specific trends between the wind rose patterns and the errors using this approach. As an example, the wind rose of Paris and Nîmes are strongly different (the first one being homogeneous and the second one having a preferential direction) but neither of them give systematically less error than the second one. According to Figure 9 (B), it is the same observation when comparing the results as a function of the building layout. In this case, the maximal variation is higher with an overall value of 4.2 which indicates that the error is more sensitive to the building layout than to the wind rose.

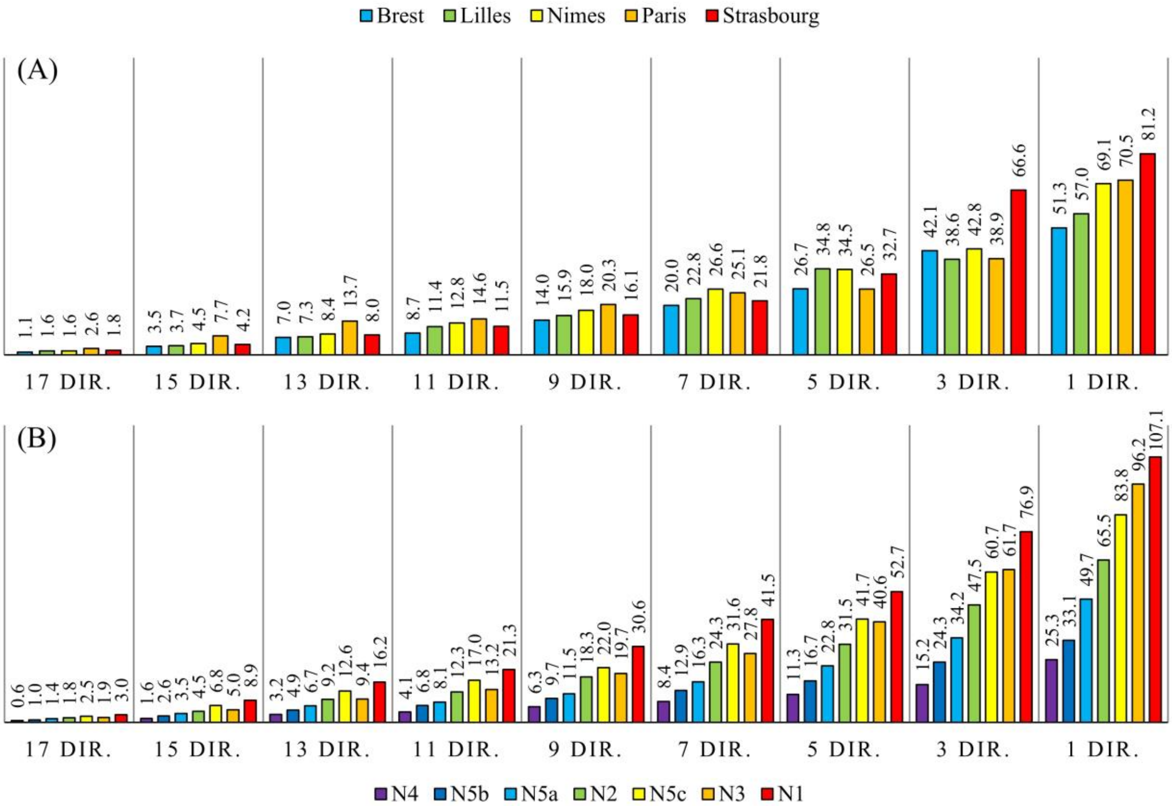

Figure 9. Mean error over the mean annual concentration compared to the reference using the predominant wind directions as a function of (A) the wind rose location and (B) the building layout (DIR: Directions).

3.3. Comparison between both methodologies

The first methodology, which uses a regular step, showed trends in the errors depending on the wind rose pattern: the more the wind rose is homogeneous and the less the error is high. Such a trend was not observed with the second methodology which uses the predominant wind directions. These two methodologies were compared as a function of the wind rose in order to find out which of the two is the best overall and for specific wind rose patterns. The results are given in Figure 10. No comparison was performed according to the building layout since specific trends were not observed for this parameter.

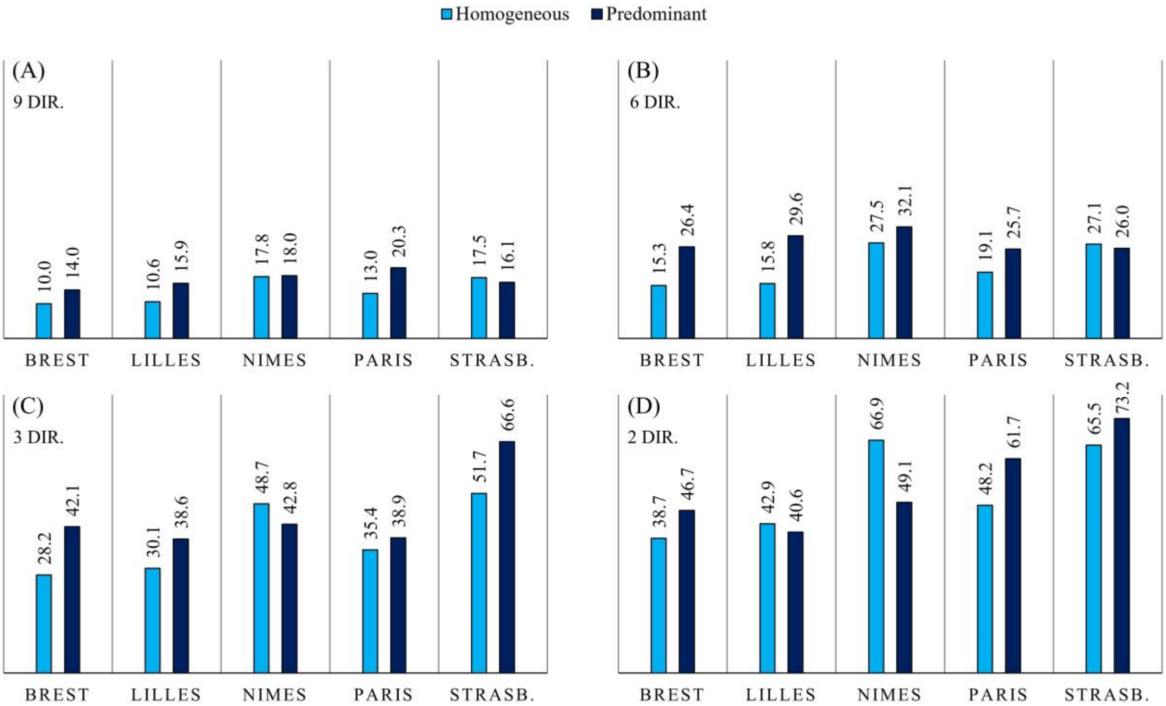

Figure 10. Comparison of the mean error over the mean annual concentration compared to the reference as a function of the wind rose for 9, 6, 3 and 2 wind directions using the first (homogeneous) and the second (predominant) approach.

According to Figure 10 it can be seen that depending on the wind rose and the number of directions considered, one approach can perform better compared to the second and vice versa. As an example, the first approach considering regular steps gives less error with the wind rose of Brest and 9 wind directions (10.0%) compared to the second approach (14.0%). Inversely, the first approach gives higher error with the wind rose of Nîmes and 3 wind directions (48.7%) compared to the second one (42.8%). The results are, however, better for three quarter of cases using the first methodology, which can be seen in Figure 9 (A) and (B). Additionally, when taking all cases into account a mean relative difference of 18% on the error is obtained in favor of this methodology. Nevertheless, when considering more than a half of the wind directions available in the wind rose, the first approach was not evaluated, only the second one.

3.4. Estimation of the error with respect to the complete wind rose

As a last point of analysis, a study has been performed to assess the possibility of estimating the error induced by considering a partial wind rose with the first approach (regular steps) compared to a simulation of the full wind rose with 18 wind directions. Indeed, it has been shown previously that using this methodology, an overall error of 13.8% is obtained when considering 9 wind directions instead of 18. However, this error ranges from 10.0% to 17.5% as a function of the wind rose and from 5.6% and 21.3% as a function of the building layout considered in this work. Thus, even if an overall prior estimation of the error before doing the simulations is available, the specific case result can still be far from the expected ones given the large possible ranges of error. A way to assess the error more accurately once the simulations are done is therefore necessary.

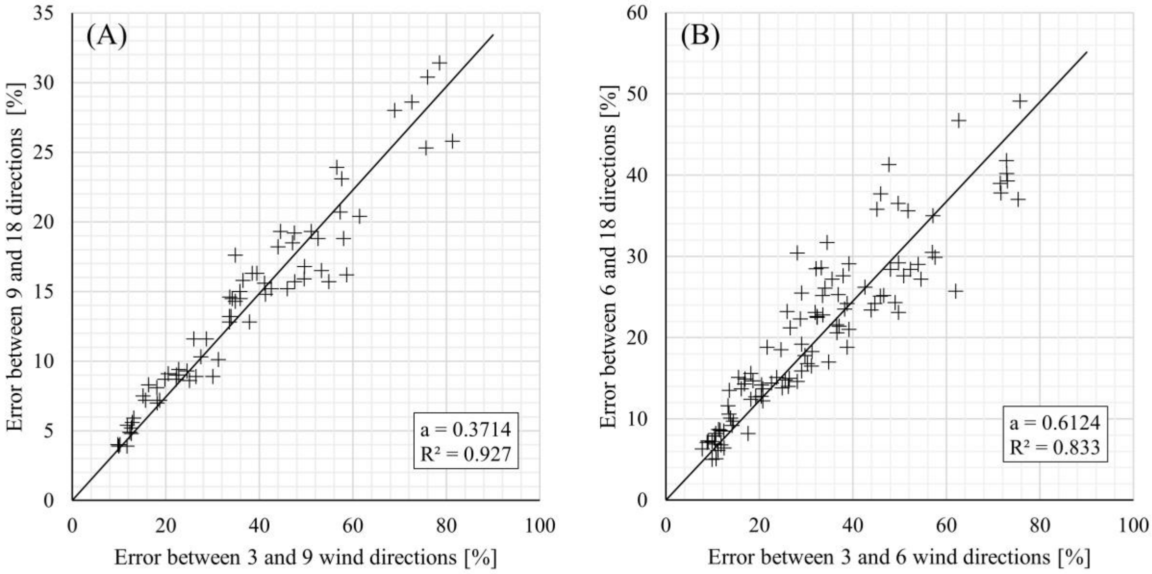

Figure 11. Estimation of the error using the first approach with regular steps when considering (A) 9 and (B) 6 wind directions.

In order to have a better evaluation on the error when using the approach with regular steps, the error between the results obtained with 9 and 18 wind direction has been plotted as a function of the error between the results obtained with 3 and 9 wind directions. The scatterplot is given in Figure 11 (A). Each point of this scatter plot corresponds to a given couple of wind rose and building layout as well as a given starting point. According to this figure, it can be seen that the scatter plot seems to be linearly correlated using a linear function with a slope of 0.3714, leading to a coefficient of determination R^2 of 0.927. The corresponding equation is given in (5).

$$E_{9/18} = E_{3/9} \times 0.3714 \qquad (5)$$

Thus, using Figure 11 (A) and results from 3 wind directions evenly spaced in a total of 9 wind directions simulated with a regular step, it is possible to assess the error compared to considering a whole wind rose. The same work has been carried out considering 6 wind directions and the results are given in Figure 11 (B).

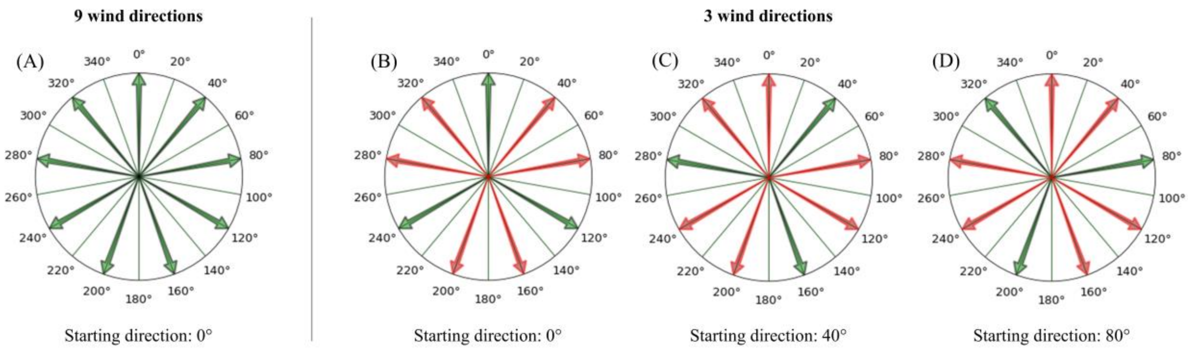

Figure 12. Illustration of the example to calculate the error made compared with considering the whole wind rose (green arrow: wind direction modelled / red arrow: wind direction not considered for annual concentration calculation).

As a practical example, if mean annual concentrations are calculated considering 9 wind directions starting at 0° as shown in Figure 12 (A), mean annual concentrations considering 3 wind directions already simulated can also be calculated with three distinct starting directions: 0°, 40° and 80° (Figure 12 (B), (C) and (D) respectively). If these last three annual concentrations give on average 25% of difference with the one calculated with 9 wind directions, then, according to Figure 11 (A), an error of around 25% × 0.3714 = 11% is made using 9 wind directions evenly spaced instead of considering the whole wind rose. The same methodology can be used when using only 6 wind directions but using Figure 11 (B) instead of (A). The methodology to determine the error is presented as a step-by-step flowchart on Figure 13.

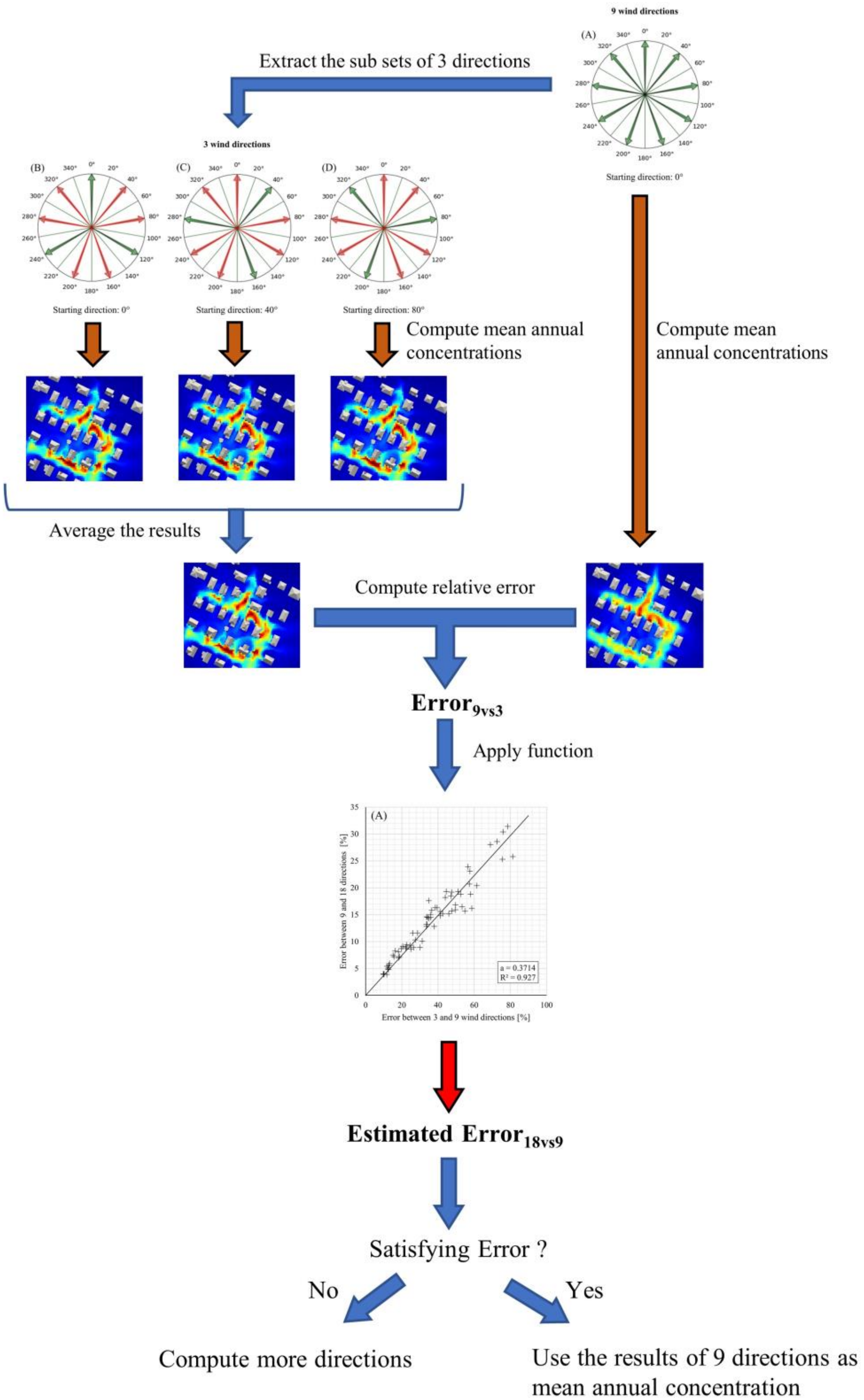

Figure 13. Flowchart of the methodology to determine the error for the method 1.

4. Discussion

This study provides information on how to decrease the number of wind directions needed for mean annual concentrations calculation based on CFD results in order to decrease the calculation costs without leading to high errors. It enables environmental engineers and scientists to assess the air pollution of a region more quickly and cost-effectively, while managing the resulting error and ensuring that it is within an acceptable range. Two approaches were considered with (1) ignoring some wind directions uniformly spaced and (2) considering the predominant wind directions. Additional work can be done to extend the use of these approaches and the major issues are discussed hereafter.

Several configurations of building layout were considered in this study which mainly included urban and peri-urban neighborhoods, with buildings overall ranging from 10 m to 25 m high with punctual structures of 2–3 m high, and both homogeneous and heterogeneous layouts. It has been shown that no specific trends are observed between the error and the building layout considered and that an overall maximal variation of 3.9 for the first approach (respectively 4.2 for the second one) is obtained. However, more densely built-up neighborhoods with higher buildings such as in city centers were not considered in the scope of this work. Since such urban configurations may lead to different results, further work can be done in this direction to extend the applicability of the methodologies studied in this paper.

Some wind roses were also considered in this study covering the four cardinal points of France (and Paris) and having different patterns: homogeneous in wind direction and velocity, homogeneous in wind direction with mostly intermediate velocities, heterogeneous with a preferential axis of wind direction and heterogeneous with a preferential direction of wind. It has been shown that homogeneous wind roses in wind direction and velocity led to the minimal errors while heterogeneous wind roses with preferential wind axis and direction led to the maximal errors when using the first approach (an overall maximal variation of 1.7 was obtained with the first approach and 1.9 with the second one). The wind roses used in this work were only located in France, nonetheless. Additional work can therefore be performed to extend the applicability of these approaches using wind roses from different countries, under different climates or with extreme wind roses highly homogeneous or heterogeneous or with mostly high and low wind velocities.

Additionally, according to the high variation in the errors as a function of the building layout, it is not possible to be sure in advance of the error made using one of the two approaches presented. Only an overall information is available prior to the choice of number of directions but given the spread of values it can be too vague. However, a methodology to assess the error afterward for the first approach has been presented, allowing the operator to estimate the error made compared with considering the whole wind rose finely. Based on the result, the operator might choose to keep the results as they are or simulate the missing wind directions if the error is not acceptable.

The reader must nonetheless be aware that these results were achieved under the following hypothesis.

- For the CFD simulation: RANS model, RNG k-ε turbulence model, surface emissions, passive scalar, neutral atmospheric conditions, unsensitive meshing, distances between boundaries respecting COST Action 732 guidelines.
- For the mean annual concentration: the calculation was done following the statistical approach provided in Reiminger et al. (2020b) and using annually averaged daily traffic emissions.

To use the raw results of our study for real-life settings, one should be aware that this work was done under this set of hypotheses, and that depending on how much the reader deviates from it (using LES models, chemical reaction, etc.) he should be careful with taking the result as they are.

The methodology developed here consists of reducing the number of directions to improve computation time while controlling subsequent error when calculating mean annual concentration. However, it can be applied to other set of hypotheses given some examples to produce adapted equations. The flowchart remains the same.

Finally, the whole work has been conducted considering wind roses with 20° steps in wind directions, thus 18 wind directions. Different discretization can also be found such as 22.5°, 30° or 40° corresponding respectively to 15, 12 or 9 wind directions. The interest of this work was also to give an idea of the mistake that can be made by using weakly discretized wind roses. As an example, in the case of a 40° discretized wind rose, an overall error of 13.8% is thus made compared with a more discretized wind rose of 20° (18 wind directions).

5. Conclusion

The objectives of this study were to find out the possibilities to limit the number of wind directions needed to be simulated in order to calculate mean annual concentration based on CFD results at a lower calculation cost. Two approaches were studied and compared throughout this paper and the main conclusions are as follows:

(a) Ignoring some wind directions evenly spaced (first approach) can highly decrease the calculation costs without leading to high errors: when simulating one wind direction out of two, an overall error of 13.8% can be expected for a calculation gain of 50%.

(b) The error made when ignoring some wind directions evenly spaced is depending on both wind rose and building layout. No specific trend can be identified as a function of the building layout. As a function of the wind rose, the trend is that the error is smaller when the wind rose is homogeneous than where there is a preferential wind axis or direction.

(c) Considering the predominant wind directions (second approach) can also decrease the calculation costs: when simulating the first twelve wind directions, an overall error of 10% can be expected for a calculation gain of 35%.

(d) The error made when considering the predominant wind directions is depending on both wind rose and building layout but no specific trend can be identified neither as a function of the building layout nor the wind rose.

(e) The first approach considering uniformly spaced wind directions is generally better than the second, leading to lower errors for the same number of wind directions considered. The first approach should therefore be preferred, it has not been studied when more than half of the wind directions are considered with the first approach, but it could be used as well.

(f) A way to evaluate the error made considering 6 or 9 wind directions evenly spaced with respect to the full the wind rose is provided for the first approach which can be used to have a better idea of the error made or to check if additional wind directions are necessary.

Eventually, the results of this study will allow environmental engineers and scientists to assess annual outdoor air quality optimally with a wider use of numerical methods to compare with regulatory values provided by the WHO, the EU or any other organization. Indeed, the cost of modeling is the main obstacle and, with the presented methods, can be significatively reduced while managing the resulting error and ensuring that it is within an acceptable range. Further work could be done to evaluate the error and optimal strategies with others numerical models such as plume models or LES CFD models.

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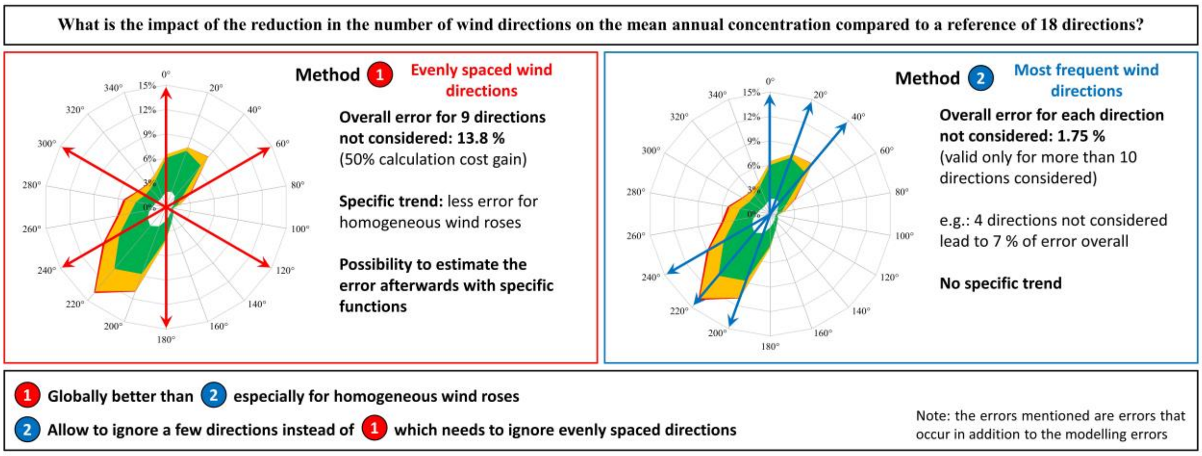
Graphical Abstract



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