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NUMERICAL ASSESSMENT OF THE APPLICABILITY OF GAUSSIAN MODELS FOR THE PREDICTION OF NEAR-FIELD DISPERSION NEAR URBAN ENVIRONMENTS

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Abstract: Monitoring pollutant emissions into the atmosphere is a key issue for industry and authorities. In urban environments, the presence of buildings disturbs the flow in their wake and poses specific problems of interaction between the emitted plume and the disturbed flow. Dispersion models based on a CFD approach can explicitly account for the presence of buildings and accurately represent the three-dimensional nature of the mean flow but suffer from high calculation times, often incompatible with operational time constraints. As a result, simplified, Gaussian models are still widely used to quickly provide an order of magnitude of expected consequences, especially for emergency response, despite their lack of obstacle modelling. The aim of this work is to study the applicability and scope of Gaussian models for the prediction of near-field dispersion of pollutants around industrial sites in peri-urban environments, in comparison to more complex models. To this end, the IRSN's operational Gaussian model pX and the SLAM (Safety Lagrangian Atmospheric Model) model were used to predict ^{85}Kr air concentration around the ORANO La Hague (France) reprocessing plant. The performance of each model was analysed through their ability to predict concentration peaks at various locations, and their sensitivity to meteorological conditions. Additionally, the sensitivity of pX to its parameterization was explored. The results show that for distances greater than one or two kilometres, the Gaussian approach can provide an acceptable prediction of field concentrations with an appropriate parameterization, while a CFD-based dispersion model tends to provide a real added value in the close vicinity of the site, where the flow and pollutant dispersion is still perturbed by the presence of buildings.

Key words: *Near-field dispersion, Gaussian models, Lagrangian***.**

INTRODUCTION

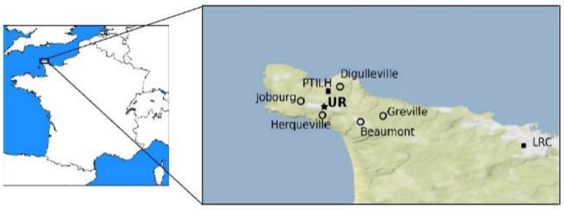
In case of chronic or accidental release of pollutants by nuclear facilities, atmospheric dispersion models are used to assess plume dispersion, to infer the potential environmental and health impact and support decision-makers in deploying protection measures. In the near-field region, the presence of buildings and obstacles may impact the dispersion of pollutants, through complex interaction mechanisms with turbulent structures (Li et al., 2021). CFD approaches allow to explicitly represent the flow field and pollutant dispersion in peri-urban environments around idealized obstacles and even realistic buildings and cities (Pantusheva, 2022). As distance to the discharge source increases, impacts of buildings and obstacles on the flow field tend to decrease, and the interest of CFD approaches over simplified dispersion models is unclear. Additionally, CFD approaches are time- and resources- consuming, and generally not compatible with operational time constraints associated to emergency response, so that simplified dispersion models are still widely used. The objective of this work was to explore the applicability of simplified approaches compared to more complex approaches to predict pollutant dispersion up to a few kilometres from an industrial site, their sensitivity to meteorological forcing and parameterization, and infer knowledge on the transition distance from which the Gaussian approach becomes acceptable. IRSN's operational Gaussian puff model pX was compared to the stochastic particle SLAM model coupled to a wind and turbulence field database. The models were applied to realistic meteorological and release conditions to predict pollutant dispersion around the ORANO La Hague reprocessing plant, and their results were compared to concentration measurements at various distances.

METHODS

Case study and simulation set-up

Gaussian puff models such as pX assume a Gaussian repartition of the plume concentration in the three directions of space, and its evolution under turbulent diffusion effect is parameterized by empirical laws, depending on the atmospheric stability. These parameterizations were generally fitted on flat-terrain, ground-sources experiments. They do not account for obstacles or complex orography. To counterbalance these limitations, adapted empirical diffusion laws may be used, such as the Briggs urban formulas that represent the increased vertical turbulence in a dense urban environment. A virtual source may also be used as input of Gaussian models to account for modifications of the plume centreline height due to building downwash effects. SLAM is based on a Lagrangian stochastic particle dispersion method, coupled with a wind field and turbulence field flow database generated with RANS $k - \varepsilon$ simulations with the ANSYS Fluent solver. The dispersion of particles is then simulated by interpolating between the pre-calculated flow fields, which ensures a reasonable computational time (Vendel, 2011; Charvolin-Volta, 2021).

The present study focuses on the ORANO La Hague Reprocessing Plant, which releases ^{85}Kr as a part of the reprocessing process from two production units, equipped with two 100m-high stacks. The site is in North-Cotentin in Normandy, France, with a rather complex orographic situation (Connan et al, 2014). The DISKRYNOC project conducted by IRSN consisted in gathering continuous measurements of ^{85}Kr concentration between November 2020 and December 2022 within 20 kilometres of the site. For the present study, measurements from six stations around the plant, ranging from 800m of distance to the discharge source to up to 5.2km will be considered (see Figure 1). This study focuses on a reduced period of interest, from December 2020 to January 2021, during which there are both significant releases as well as a significant density of concentration measurements (El-Ouartassy et al., 2022).



a)

Station	Distance to the source (m)	Nb. Of obs. Peaks
Jobourg	2200	9
Herqueville	800	50
Digulleville	2600	81
PTILH	2000	118
Beaumont	2600	90
Gréville	5200	74

b)

Figure 1. (a) Position of the ORANO La Hague Reprocessing plan (UR) and surrounding measure stations. (b) Observations per station for the combined periods of December 8 to 15, 2020 and January 7 to 26, 2021.

Source heights ranging from 0 to 100m (stack height) by increments of 20m were considered with the pX model, as well as laws of Doury, Pasquill, Briggs Rural and Briggs urban to describe turbulent diffusion. The stack height was used as input to the SLAM model. A time step of 150s and 20000 particles per source were chosen to meet computational time constraints while maintaining an acceptable precision.

Definition of successes and failures

A concentration peak is defined as a temporary rise in ^{85}Kr concentration levels above the detection threshold of measurement devices (1545Bq/m3). We are interested in characterizing the ability of dispersion models to identify the presence and intensity of these peaks, using three categories: successes (TP, for True positive), prediction failures (FN, False Negative) and false alarms (FP, False Positive). Classically, a success refers to a peak that is both observed and predicted by the simulation. A failure is a peak that is observed but not simulated, and a false alarm is a peak that is simulated but not observed. A dispersion model cannot exactly reproduce all concentration peaks. A direct comparison of peak concentrations at the frequency of measurement (10 minutes) would lead to disappointing results, and above all, would not be significant in terms of the overall quality of the model. Three types of tolerance need to be considered: temporal, spatial and in intensity. In the context of emergency response, dispersion results are used to predict the dose received over a relatively short period of time. Without deposition processes, there is a direct linear relationship between integrated activity and total dose received. We therefore consider the integrated activity over a one-hour period. Intensity tolerance refers to the ability to correctly predict peak values. In this study, we are interested in the response of models in emergency situations, where underestimation is to be avoided, thus we apply asymmetric intensity tolerance constraints: to be considered a success (TP), a simulated peak must have an intensity within a factor of 2 lower and a factor of 10 higher than an observed peak. Finally, no spatial tolerance was explicitly considered in this study.

Statistical indicators

Model performance over the periods of interest is measured by aggregating the proportion of TP, FN and FP using statistical indicators. These indicators are the Hit Rate (HR), which measures a model's overall ability to capture observed events, and precision, which assesses the relevance of simulated events. The F1 score combines these two indicators in a measure of overall model efficiency:

$$HR = \frac{TP}{n_{obs}}$$

$$precision = \frac{TP}{n_{sim}}$$

$$F1 = 2 \times \left(\frac{HR \times precision}{HR + precision}\right)$$

Perfect scores correspond to a value of 1. Furthermore, a criterion is defined to check the nature of non-compliance with the intensity tolerance:

$$R_{ov} = \frac{n_{opv}}{n_{opv} + n_{upv}},$$

where n_{opv} is the number of predictions overestimated by more than a factor of 10 and n_{upv} the number of predictions underestimated by more than a factor of 2.

RESULTS AND DISCUSSION

Global statistics

The total number of observations over the considered period is 672 (28 days x 24 hours), with a total of 422 observed peaks. The distribution of observed peaks is consistent with the meteorological situation over the study period in terms of wind direction and can be found in Figure 1b. For the Jobourg station, only 9 peaks were detected over the study periods, which is not enough for the application of statistical tools to provide significant results. Jobourg was therefore considered an *outlier*. Statistics were determined by compiling the integrated time series for each station (except Jobourg) and are illustrated in Table 1. First, statistics without the intensity tolerance criteria provide an indication of the overall peak detection capability of a model. The various pX parameterizations lead to very good peak detection rates, with a HR up to 87.7% with Briggs Urban law. In comparison, SLAM detects 58.1% of peaks. In terms of accuracy, both models predict around a third of false alarms. Without constraints on peak intensity, the best HR values with pX are systematically obtained with a ground-level source while the best precisions appear with a source at stack height. Imposing constraints on peak intensity leads to a reduction in the number of TPs, with important impact on statistics. A significant proportion of predicted peaks fail to meet the intensity tolerance constraints for both pX and SLAM.

Table 1. Global statistics and their evolution after application of peak intensity tolerances.

Intensity tolerance	Statistic	SLAM	Pasquill	Briggs Rural	Briggs Urban	Doury
OFF	HR	58.1	64.9 – 76.3	69.2 – 81.6	87.2 – **87.7**	52.3 – 73.8
ON		31.7	30.3 – 39.0	32.2 – **41.9**	39.7 – 40.2	23.2 – 35.8
OFF	Precision	**68.6**	66.6 – 68.0	66.6 – 68.3	66.8 – 67.0	56.9 – 62.8
ON		**37.4**	31.5 – 35.8	31.7 – 35.8	30.4 – 30.9	20.0 – 31.0
OFF	F1	62.9	66.4 – 71.1	68.8 – 73.4	75.7 – **75.8**	57.1 – 65.6
ON		34.3	31.0 – 37.3	32.0 – **38.6**	34.5 – 35.0	22.6 – 32.8

In Figure 2, which gives the R_{ov} ratio between the number of overestimated peaks and the number of simulated peaks not complying with the intensity tolerance criteria, a value below 0.5 implies a tendency to under-predict peak intensity. The SLAM model and the Briggs Urban parameterization tend to underestimate predicted peaks for all release heights while for other laws, the source height is a more sensitive parameter. The Briggs Rural, Doury and Pasquill laws underestimate the peak values when a 100m source height is used. Decreasing the source height increases the probability of detecting a peak with pX as well as their intensities, and therefore lowers the probability of underestimating the consequences. However, for source heights close to ground level, R_{ov} exceeds 0.5, indicating a tendency to overestimate peak concentrations. This highlights the need to compromise on source height to avoid under- or over-estimating consequences.

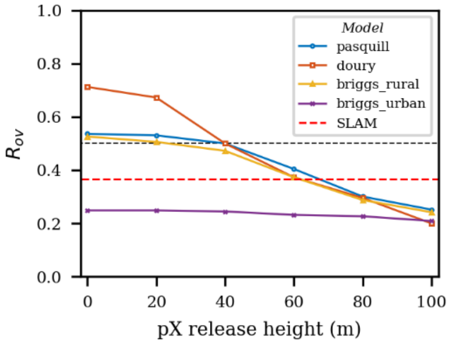


Figure 2. Proportion of overestimated peaks out of all peaks not complying with intensity tolerances.

While pX leads to the best HR with intensity constraints, its performances are highly dependent on the parameterization, which, if inadequate, can result in statistical performance inferior to that obtained with the SLAM model. In particular, the Doury law is very sensitive to the source height and leads to the worst statistical performances. The best statistical performances, in terms of F1 score, which represents the trade-off between detection rate and model accuracy, are obtained with Briggs Rural's law and a source height around 60 meters.

Statistics per station

The statistical performance per station of the dispersion models is illustrated in Figure 3, for pX simulations with a source height of 60m. The best F1 score is obtained at Herqueville with the SLAM model, and the Briggs Urban law achieves a similar HR, although the overall F1 score is lower. This station is the closest, located around 800 meters from the sources of discharge. For the PTILH, Digulleville and Beaumont stations, located about 2 kilometres away from the sources, the best performances are obtained with the Briggs Rural and Pasquill laws.

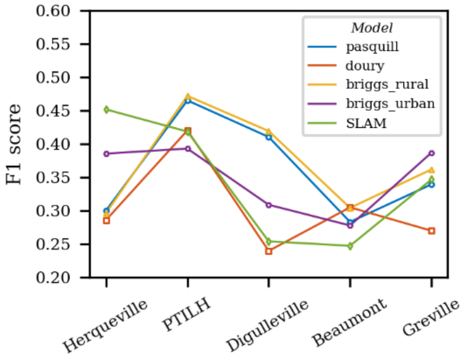


Figure 3. F1 score statistics (with intensity constraints) per station for SLAM and each pX parameterization.

Herqueville is located at a distance where buildings still have a strong impact on concentration levels near the ground, and the present results tend to confirm the added value of the SLAM model and CFD approaches for dispersion in the vicinity of industrial sites, while the Gaussian puff approach is acceptable at 1 kilometre or larger distances from the site.

CONCLUSION

This study presented a comparison between the performance of the pX operational dispersion model and the SLAM model on the DISKRYNOC measurement campaign. The aim was to investigate the potential added value of a CFD-based approach such as SLAM, and the sensitivity of pX to some of its parameters. Results have shown that the Gaussian approach can lead to acceptable results for the present case study for distances to the discharge source further than 1km. While SLAM does not bring real added value at those distances, the case of Herqueville tends to confirm its interest for shorter distances, where interaction mechanisms between pollutants and obstacles may have a significant impact on the consequences at ground. It should be noted that SLAM configuration in terms of time step and particles number was based on a compromise between precision and computational time and memory constraints. This may contribute to the lesser performance of the model at long distances. Additionally, it was shown that Gaussian models need to be used with an appropriate parameterization to compensate building effects. Specifying a source height at approximately half of the real emission height gives the best balance between over and under estimation of consequences. Using a source height at ground level has however shown to maximize the HR and is still a fair approach in the framework of emergency response, to avoid underestimation at all costs. The present results need to be consolidated using other time periods of the DISKRYNOC campaign, and Gaussian parameterizations based on similarity theory. Further studies planned by IRSN and ORANO will allow to complete the present comparison with on-site measurements within the ORANO La Hague site.

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REFERENCES

Charvolin-Volta, P., C.V. Nguyen, L. Soulhac, G. Lamaison, P. Laguionie, O. Connan, J. Chardeur, O. Cazimajou, L. Solier, I. Korsakissok, S. Vecchiola, A. Mathieu, M. Le Guellec, A. Tripathi, 2021; Evaluation of a Lagrangian dispersion model coupled with a CFD wind field database against a new full scale atmospheric tracer experiment. In *20th Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*. Tartu, Estonia

Connan, O., L. Solier, D. Hébert, D. Maro, M. Lamotte, C. Voiseux, P. Laguionie, O. Cazimajou, S. Le Cavalier, C. Godinot, M. Morillon, L. Thomas, S. Percot, 2014: Near-field krypton-85 measurments in stable meteorological conditions around the AREVA NC La Hague reprocessing plant: estimation of atmospheric transfer coefficients. *Journal of Environmental Radioactivity*, **137**, 142-149. https://doi.org/10.1016/j.jenvrad.2014.07.012

El-Ouartassy, Y., I. Korsakissok, M. Plu, O. Connan, L. Descamps and L. Raynaud, 2022: Combining short-range dispersion simulations with fine-scale meteorological ensembles: probabilistic indicators and evaluation during a ^{85}Kr field campaign. *Atmospheric Chemistry and Physics*, **22**, 15793–15816. https://doi.org/10.5194/acp-22-15793-2022

Korsakissok, I., Mathieu, A., Didier, D., 2013. Atmospheric dispersion and ground deposition induced by the Fukushima Nuclear power plant accident: a local-scale simulation and sensitivity study. Atmospheric Environment 70, 267–279. https://doi.org/10.1016/j.atmosenv.2013.01.002

Li, Z., T. Ming, S. Liu, C. Peng, R. de Richter, W. Li, H. Zhang and C.Y. Wen, 2021: Review on pollutant dispersion in urban areas – part A: Effects of mechanical factors and urban morphology. *Building and Environment*, **190**, 107534. https://doi.org/10.1016/j.buildenv.2020.107534

Pantusheva, M., R. Mitkov, P.O. Hristov and D. Petrova-Antonova, 2022: Air Pollution Dispersion Modelling in Urban Environment Using CFD: A Systematic Review. *Atmosphere*, **13**, 1640. https://doi.org/10.3390/atmos13101640

Vendel, F., 2011 : Modélisation de La Dispersion Atmosphérique En Présence d'obstacles Complexes : Application à l'étude de Sites Industriels.

Vendel, F., G. Lamaison, L. Soulhac, L. Donnat, O. Duclaux, and C. Puel, 2010: A New Operational Modelling Approach for Atmospheric Dispersion in Industrial Complex Areas, In *13th Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*. Paris, France.