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SENSITIVITY OF SPRAY AND CALPUFF MODELS TO SOURCE CHARACTERISTICS WHEN SIMULATING DISPERSION FROM FIRES

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Abstract: This paper discusses a case study regarding the application of dispersion modelling for the evaluation of pollutant dispersion from an incidental fire in a refinery. This task is particularly challenging, due to the high uncertainties associated with the characterization of the source term. The aim of the work is to compare how ground concentrations simulated with two dispersion models, i.e. CALPUFF and SPRAY, are affected by changing the source term parameters within the estimated uncertainty ranges. Thus, first it is necessary to make an initial estimation of the source height, diameter, temperature, and rise velocity (base-case). Finally, the effect of changing the different parameters on the model outputs is evaluated. The source parameter that most significantly affects the model output in terms of ground concentration on selected receptors is the source area. By considering the extreme values of the defined uncertainty range (10 m^2 - 100 m^2), the pollutant ground concentrations on selected receptors vary up to +/- 60%. On the other hand, if the SPRAY model is applied with the specific fire source option, then the modelled concentrations result almost independent from this parameter. These different trends are quantified and discussed, thereby considering the model equations for the buoyancy flux calculation.

Key words: *Atmospheric dispersion modelling; environmental impact; models comparison; sensitivity analysis; source characterization*

INTRODUCTION

In the case of complex sources, the retrieval of representative emission data for dispersion modelling studies may be extremely problematic. This is particularly true for accidental sources like fires. Indeed, for incidental fires, the source geometrical features are not directly measurable but they have to be estimated considering some correlations available in literature. For this reason, this paper focuses on the evaluation of two dispersion models sensitivity to the source parameters when simulating pollutant dispersion from fires. Due to the high uncertainty associated to the source term parameters estimation in case of fires, sensitivity analysis is strongly recommended to determine how an input parameter variation can affect the results in order to identify the most influential variables. Therefore, the proposed procedure explores and quantifies the impact of possible errors in input data on predicted model outputs. More in detail, this paper discusses a case study where the dispersion models are applied to the simulation of a hypothetical incidental fire of an oil refinery. Two Lagrangian models have been selected: the particle model SPRAY and the Gaussian puff model CALPUFF. To perform the simulations, different sources types are set in the models: with CALPUFF the fire is simulated as a buoyant area source according to the indications of the User's Guide (Scire et al., 2000) whereas with SPRAY the fire is simulated as a point source and as a fire characterized by 10% of the emitted particles with no buoyancy flux.

MATERIALS AND METHODS

Case-study description

The hypothesized case study regards an incidental fire in an oil refinery. The event is supposed to involve a portion of the gas oil treatment unit. In our hypothesis, the fire lasts three hours. In real cases, the duration is a fundamental point for the definition of the case study and must be evaluated on the depositions of the people who were on the spot. To optimize the choice of the geographic area to be considered, weather data showing the plume direction should be taken into account. For the selected case-study a rectangular domain that follows the trend of the plume is identified. According to this, the source is located at the north-eastern limit of the domain. Also, for a more precise analysis, some discrete receptors should be positioned in places (e.g. hospital, school, city hall) that are considered of particular interest to estimate the pollutant concentration resulting from the incidental fire.

Model choice

The model choice is based on the analysis of the scientific literature and the technical legislation. Moreover, the specificities of the hypothesized case-study have to be taken into account, such as the particular type of source (fire) and the large simulation domain. The use of simple Gaussian models is not advisable in case of large simulation domains because they consider steady state conditions: they can't adequately describe the dispersive phenomenon, since only one meteorological condition is not representative of the wind field variations on the entire domain. In the literature, there are several examples of studies carried out using puff models, and specifically CALPUFF, for the simulation of pollutant dispersions from fires (e.g., Ainslie & Jackson, 2009; Henderson et al., 2008). The authors justify the model choice because it can treat buoyant sources. There are not many articles regarding the application of SPRAY for fires, presumably because it is a more recently developed model. On the other hand, there are some papers in which both CALPUFF and Lagrangian particle models are used (e.g., Grimaldelli et al., 2005, Degrazia et al., 2016). As an example, in the first paper, the choice of using non-steady state 3D models to evaluate the impact from a fire from a waste storage plant is justified by the need to provide a 3D description of the meteorological field in order to account for some essential characteristics such as wind shear, variable emissions over time and buoyant area source. In the end, for this study, it was decided to use a puff model (i.e. CALPUFF) and a Lagrangian particle model (i.e. SPRAY), since both comprise specific tools for modelling fires.

Definition of the emission scenarios

For this study, first a "base-case" is defined by assuming a set of reasonable source term parameters, which is then used as a reference for the comparison with the other emission scenarios that are defined in order to evaluate the models sensitivity to the source input parameters. Thus, starting from the "base-case", it has been decided to investigate alternative emission scenarios by changing the most critical source parameters, i.e. those that are most difficult to be defined and that mostly affect the model results. After a preliminary investigation, it has been decided to focus the study on the uncertainties associated with the definition of the source area and height. Thus, reasonable ranges within which these parameters may vary are identified. To evaluate the alternative emission scenarios, the upper and lower boundaries of these ranges are considered for simulations. Another parameter that is investigated is the modelled source types. For both CALPUFF and SPRAY, the fire is modelled by applying the specific source type (*buoyant area source* for CALPUFF, and *fire* for SPRAY) and then compared with the model results obtained by assimilating the fire to a point source. Particulate matter (PM) is chosen as target species for the investigations, since it is the pollutant whose emission is considered to be most critical in the case of incidental fires. The quantity of PM emitted is estimated based on the quantity of fuel burnt by applying a suitable emission factor. For the choice of the emission factor the "SFPE Handbook of Fire Protection Engineering" (DiNenno et al., 2002) is used as a reference, thus an emission factor of 0.05 t_{PM}/t_{fuel} is applied. Table 1 reports the input parameters for the base-case and the alternative scenarios.

Table 1. Input parameters of the investigated emission scenarios

Scenario	A (m^2)	T (K)	H (m)	Quantity (ton)	v ($m\ s^{-1}$)	PM ($mg\ m^{-3}$)
BASE	20	1373	15	11.2	8.16	51.852
A1	100	1373	15	11.2	6.21	51.852
A2	10	1373	15	11.2	9.17	51.852
H1	20	1373	20	11.2	8.16	51.852

RESULTS AND DISCUSSION

Base case

As an example of the results of the simulations, Figure 1 shows the maximum 1-hour PM concentration maps resulting from the base-case simulation in function of the different source types considered.

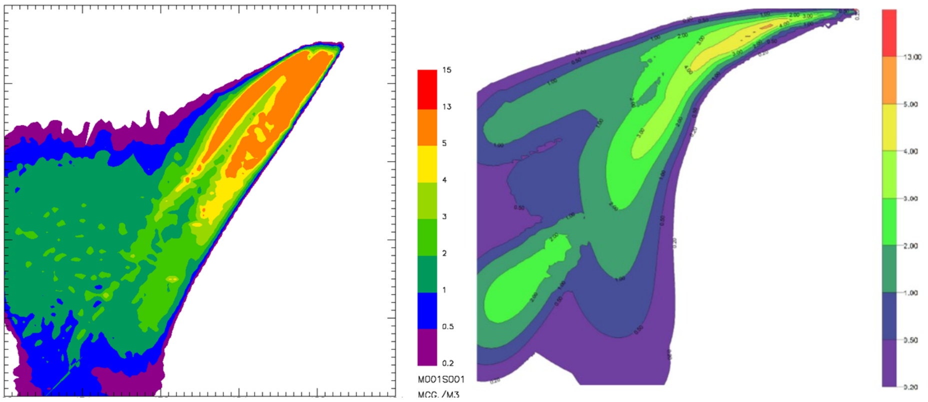

Figure 1. Maximum ground level concentration maps of PM resulting from Spray point source (left) and Calpuff point source (right)

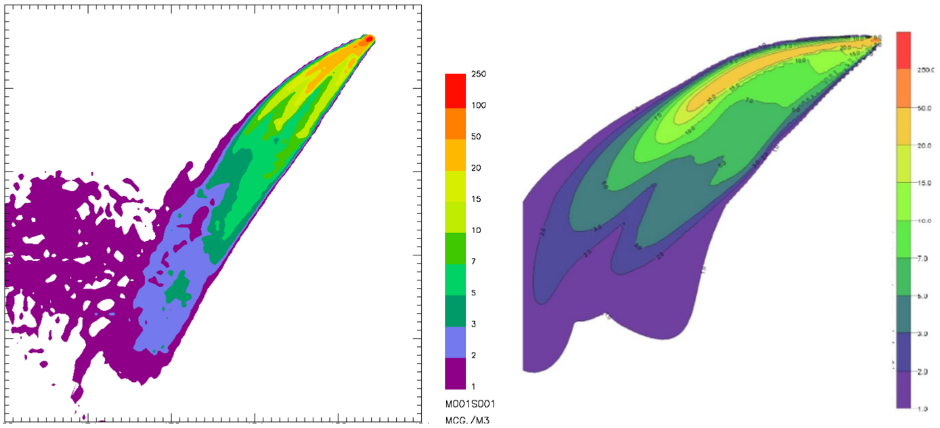

Figure 2. Maximum ground level concentration maps of PM resulting from Spray fire (left) and Calpuff buoyant area source (right)

Table 2. Maximum PM concentration values at selected receptors calculated by CALPUFF (left) and SPRAY (right)

CALPUFF			**SPRAY**		
Rec.	**Conc. (point source) (µg/m³)**	**Conc. (buoyant area) (µg/m³)**	**Rec.**	**Conc. (point source) (µg/m³)**	**Conc. (fire) (µg/m³)**
1	5.12	114.48	7	12.97	213.2
2	0.77	1.05	8	4.19	4.99
3	0.23	14.69	9	4.28	23.6
4	2.44	11.46	10	5.67	19.45
5	3.78	18.83	11	5.6	22.87
6	0.31	19.29	12	6.64	23.31

The maximum PM concentrations calculated by the models on a set of selected discrete receptors is reported in Table 2. It is important to highlight that the selected receptors are not necessarily the same for CALPUFF and SPRAY, even though they have been chosen by the same logic. For instance, receptors 1 and 7 correspond to the receptors where the maximum concentration has been calculated by the 2 models.
Figure 3 shows the trend of the of maximum 1-hour concentration of PM as a function of the distance from the source. For this purpose, 40 receptors placed along the plume axis starting from the source and spaced 250 m from each other are considered.

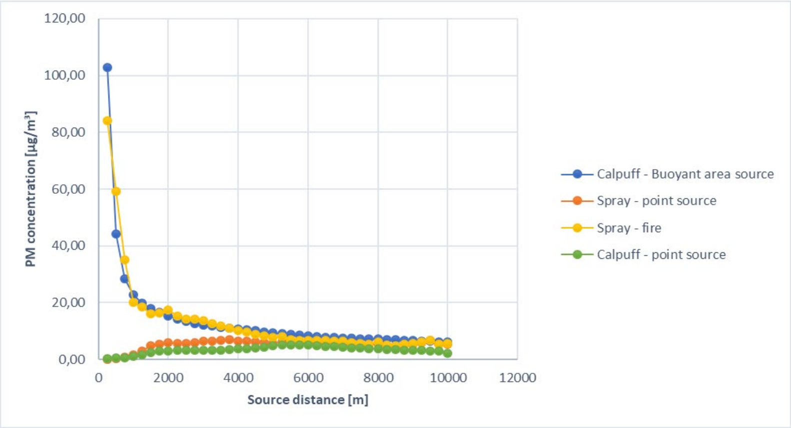

Figure 3. Maximum PM concentration trend in function of the source distance for the different combinations of dispersion models and source types considered

The different trends shown in Figure 3 can be explained by considering the different plume rise computations for point sources and for fires. According to the SPRAY model for fires, which considers the fact that combustion in fires is not complete, there is a cold fraction of particles that remains unburnt immediately falls to the ground, without being dragged into the plume rise. This gives the higher PM concentrations close to the source. As far as Calpuff is concerned, the buoyant area source model considers radiative heat losses due to the high plume temperature near the burning source. Consequently, the heat flux carried out by the plume along its trajectory will be reduced, leading to a lower buoyancy flux. On the contrary, for point sources, the maximized plume rise leads to very low concentration values close to the emission point. At high distance from the source (>5000m) the maximum PM concentrations computed by the different models tend to become very similar, giving concentrations ranging from 5 to 9 µg m^{-3} at 5000 m from the source and from 3 to 6 µg m^{-3} at 10000 m from the source.

Alternative emission scenarios

Table 3 shows the variability (%) of the maximum PM concentration values resulting at the selected receptors from the simulations relevant to the alternative scenarios compared to the base-case (Table 1). The area of the source is the parameter that most significantly affects the model outputs when using the CALPUFF + buoyant area source model or the SPRAY + point source model: the simulations conducted at the boundaries of the uncertainty range for the source area result in significant variations in the maximum PM concentrations at selected receptors. A decrease of the area from 20 m^2 to 10 m^2 generally results in an increase of the simulated maximum PM concentrations of over 50%, whereas an opposite effect is obtained by increasing the area from 20 m^2 to 100 m^2, generally giving decreased concentrations of over 60%.

Table 3. % variation of the maximum PM concentration values at the selected receptors resulting from the simulations of the alternative emission scenarios compared to the reference base-case for the different combinations of models and source types considered

CALPUFF - Buoyant Area				**SPRAY - Point**				**SPRAY - Fire**		
Rec.	**A1**	**A2**	**H1**	**Rec.**	**A1**	**A2**	**H1**	**A1**	**A2**	**H1**
1	-48.10%	42.10%	-17.30%	7	-52.40%	47.60%	1.50%	10.20%	-0.80%	-21.90%
2	-61.90%	7.60%	-0.90%	8	-24.80%	8.10%	0.00%	2.00%	-2.40%	3.40%
3	-40.50%	35.70%	-5.20%	9	-64.50%	50.90%	13.60%	2.50%	0.20%	-0.30%
4	32.90%	-53.30%	3.70%	10	-39.00%	24.70%	10.80%	2.10%	1.00%	1.90%
5	-67.10%	74.40%	-6.80%	11	-38.60%	23.20%	3.00%	1.10%	0.30%	-0.20%
6	-45.70%	21.00%	3.40%	12	-59.90%	49.90%	17.30%	1.30%	0.30%	-1.40%

When using SPRAY + point source model, this can be explained by considering that the buoyancy flux computation is performed according to the Briggs equation (Tinarelli, 2018), which is proportional to the square of the source radius:

$$F_b = g r_0^2 w_0 \frac{T_f - T_a}{T_a} \tag{1}$$

When using CALPUFF + buoyant area source model, the radiative heat loss from the plume to the ambient air, can be estimated through the following equation (Scire et al., 2000):

$$\frac{Q}{c_p} r^2 = -2\varepsilon\sigma r(T^4 - T_a^4)/c_p \tag{2}$$

Here, an increase of the radius implies a reduction of the heat losses. Consequently, the plume rise increases and the pollutant concentration decreases. On the other hand, if the SPRAY model is used in combination with the specific fire option, the effects of the source dimensions are in the parameterization of the entrainment in the formula that defines the final height H_F of the plume (Tinarelli, 2018):

$$H_F = \left[H_B^3 + \left(\frac{r}{\beta}\right)^3\right]^{\frac{1}{3}} - \frac{r}{\beta} \qquad \beta = 0.6 \tag{3}$$

Where H_B is computed by classical Briggs plume rise formula driven by a buoyancy flux F_b computed as:

$$F_b = \frac{gP}{\pi c_p \rho_{air} T_{air}}(1 - \varepsilon) \tag{4}$$

being P the heat release rate in the fire. Within the uncertainty range (10 m^2 to 100 m^2), H_F varies inside a range of 2% for fires having a heat release of the ones simulated.

CONCLUSION

This work aims to compare the application of the SPRAY and CALPUFF models for the simulation of pollutant dispersion from a fire in a refinery. More in detail, the two models are compared in terms of their sensitivity to some key source parameters, which are particularly difficult to be estimated in the case of incidental fires. For this purpose, different emission scenarios have been investigated and three different source types are taken into account: with CALPUFF the fire is simulated as a buoyant area source, whereas with SPRAY the source is simulated as a point source and then as a fire characterized by 10% of the emitted particles with no buoyancy flux. The source parameter that most significantly affects the model output in terms of ground concentration on selected receptors is the source area. By considering the extreme values of the defined uncertainty range (10 m^2 - 100 m^2), the pollutant ground concentrations on some receptors vary up to +/- 60%. On the other hand, if the SPRAY model is applied with the specific fire source option, then the modelled concentrations result almost independent from this parameter. Although this can be explained from a mathematical point of view, the problem remains open of choosing case by case the option that best approximates the real behaviour of the incidental source under investigation.

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