EXTENDED ABSTRACT

Comparison of micro-scale dispersion simulations with PMSS and GRAL applied to health risk assessment in an industrial site in central Italy

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Introduction

Microscale dispersion simulation is gaining more and more interest among industrial operators in order to facilitate a more realistic and faster health risk assessment in case of accidents. In the present study, a production site located in central Italy, characterized by complex geometry of the built elements, was considered. The aim of the study was to evaluate the application of two different Lagrangian dispersion models: the Parallel Micro-Swift Spray (PMSS) and the Graz Lagrangian Model (GRAL), to simulate an accident scenario consisting of the evaporative release of tetrahydrofuran. The simulations were conducted by reconstructing the site geometry, maintaining the same horizontal and vertical resolution and dispersion conditions for the two models.

Methodology

A chemical production industry located in Italy was selected as a case study. The industrial complex covers an area of approximately 145,000 m^2. It is primarily oriented in the northwest/southeast direction, with an approximate extension of 450 meters. The height of built elements is between 2.0 and 17.3 m.

The emission was generated by a damage occurring to a storage tank filled with tetrahydrofuran. The storage tank damaged had a cylindrical geometry (diameter 15 m, height 9 m), and it was placed within a containment basin of square footprint (height 2 m, side length 30 m). Tetrahydrofuran is a multipurpose toxic solvent; it is polar and highly volatile.

The emission rate was calculated with an evaporation model taking into account ambient conditions (temperature and wind speed). The approach proposed by van den Bosch, 2005 [1] was applied. MathWorks Matlab® was used as the modelling tool. The total duration of the event (complete evaporation of the pool) was 30 hours.

To simulate the dispersion of pollutants in the atmosphere, Parallel Micro-Swift Spray (PMSS; Oldrini et al., 2017 [2]), and the Graz Lagrangian Model (GRAL; Oettl, 2015 [3]) were used. Parallel Micro-Swift Spray is a micro-scale modelling system consisting of PSwift and PSpray. PSwift is a diagnostic meteorological pre-processor based on the principle of minimizing the divergence of the velocity field, which includes semi-empirical parameterizations to reproduce the effects of wakes and recirculation induced by the presence of buildings. PSpray is a parallelizable Lagrangian dispersion model. GRAL is also a Lagrangian dispersion model developed at the Graz University of Technology, since 1999. In GRAL, meteorological input information can be provided in several ways. In this case, it was based on 7 stability classes (PGT-classes), wind speed, and wind direction. Some of the turbulence parameterizations used in this model have been derived from own sonic anemometer observations in Austria. The perturbation of built elements is also implemented in this model.

The spatial domain of the studied case consisted of a grid of 560 x 450 m, with horizontal resolution of 2 m (281 x 226 points). Weather data provided by a meteorological monitoring station located 6 km west of the industrial site, with hourly resolution, were used. Meteorological data included the following parameters: wind speed and direction, solar radiation, temperature, atmospheric pressure, and precipitation.

To evaluate the impact of the resulting concentration fields on the modelled domain, concentrations were compared to the threshold limit values proposed by the American Conference of Governmental Industrial Hygienists (ACGIH). The TLV-STEL (Threshold Limit Value - Short Term Exposure Limit) was considered. The TLV-STEL is the limit for short exposures, representing the average concentration that can be tolerated for a maximum of 15 minutes, no more than four times a day, with at least one hour between exposure periods. The recommended TLV-STEL for tetrahydrofuran is 100 ppm (295 mg/m^3). In dispersion modelling, concentration averaging depends on the time resolution of meteorological input, which for this scale of analysis is usually hourly. For this, concentration values must be corrected to take into account the possibility that a shorter-period mean could be higher than a 1-hour mean. In the specific case, two different approaches were adopted depending on the applied model. 90th percentile was selected to represent concentration peak. For PMSS (which does not implement the calculation of concentration variance), a simple and relatively consolidated approach involves the use of a power law function, according to Bartzis (2007). This method yielded a fixed peak-to-mean ratio of 2.0.

The concentration-variance model implemented in GRAL (already existing) consists of two steps: (i) computation of the spatial distribution of the concentration variance, and (ii) calculation of R90 by applying a slightly modified two-parameter Weibull probability density function (PDF).

The area of concentration exceedance was defined as the ratio between the modelled peak concentration and the TLV-STEL, assuming, as a precaution, that the value of R90 is comparable to a short exposure of 15 minutes (in reality, it refers to a shorter period).

This gives an indication of short-term inhalation risk, assuming an exposure factor equal to unity (e.g. constant presence of workers who intervened to mitigate the incident).

Results and discussion

The comparison of the two models shows differences both in terms of distribution and absolute value of concentrations, which is reflected in the extent of the area around the source in which the TLV-STEL is exceeded.

The comparison of the calculated wind fields at 2 m height, and arbitrarily selected time frame is reported in Figure 1. Although the resulting wind fields are generally comparable, differences can be identified both in terms of calculated velocity and in the effect of the disturbance induced by buildings. The wind fields produced with GRAL provide a higher velocity and apparently less interference caused by elements (the vectors are less deflected than in the PSwift field).

The comparison between the average hourly concentration calculated during the entire event is shown in Figure 2. This concentration map shows that PMSS provides higher values than GRAL, particularly at the emission source. The difference can reach 2 orders of magnitude in the area adjacent to the source, while at a greater distance from the source the values are similar.
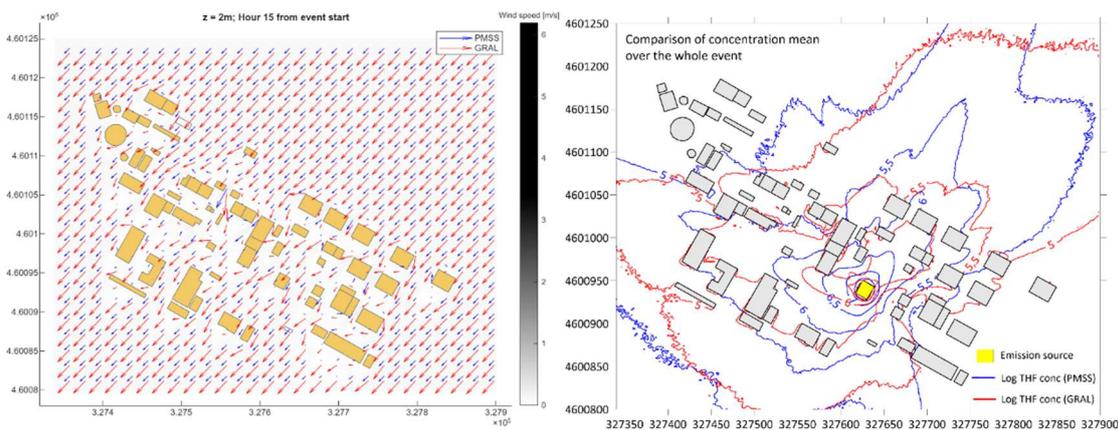

Figure 1 (left). Comparison of the calculated wind fields at 2 m height, and arbitrarily selected time frame (15 hours after the event start).
Figure 2 (right). Comparison of the average hourly concentration calculated during the entire event. Concentration unit is log (μg/m^3).

The comparison of the time trend of the instantaneous concentration (hourly average) at three receptors is shown in Figure 3. The figure shows how the concentration peaks, caused by the change in wind direction, are captured in a similar way by both models. This figure confirms that the values calculated with PMSS are higher. The wind direction at the time of the peaks is consistent with the position of the receptor relative to the source. The PBL height value is reduced, as is the wind speed, indicating neutral or stable atmospheric conditions. However, the peak occurring at receptor R10 at the 26th hour is an exception, where the wind speed is 3.08 m/s and the PBL height is 800 m. In this case,

the direction does not correspond to the position of the receptor relative to the source. This could be due to a disturbance caused by the presence of a building located near R10.
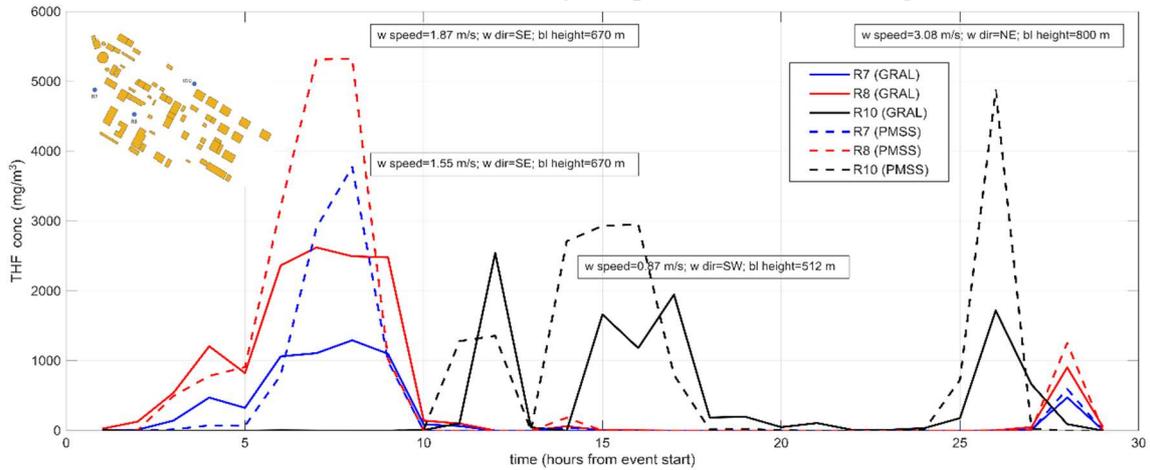

Figure 3. Comparison of concentration hourly average against time at receptors R7, R8, R10.

The comparison between the calculation of the area within which the concentration exceeds the TLV-STEL threshold is shown in Figure 5. The figure shows that, unlike the previous results, the impact area of peak concentrations is greater for the PMSS simulation. The same exceedance area covers zones that are not covered by the PMSS data processing. This indicates that the peak concentration calculation method applied to the PMSS data is less conservative than the one implemented in GRAL.
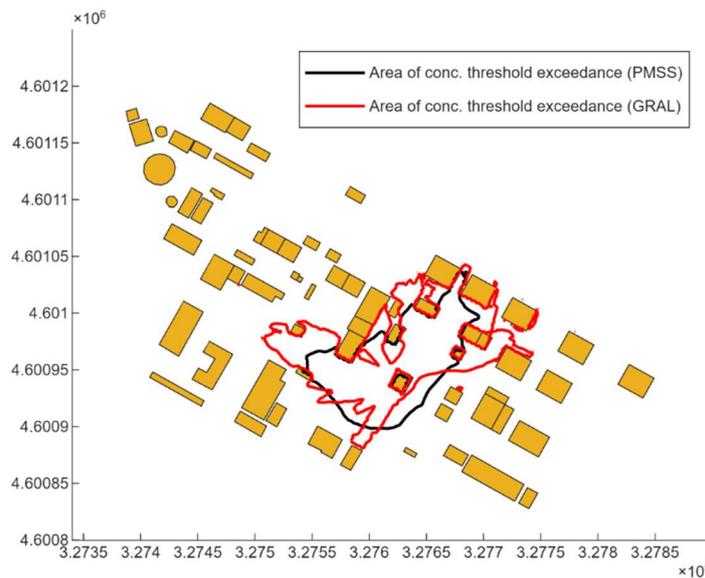

Figure 4. Comparison of the calculated area within which the concentration exceeds the TLV-STEL threshold of THF.

Discussion

The differences found in the simulations with the two models can be traced back to the structure of the models themselves. The main differences concern the following aspects: reconstruction of the wind field (both the undisturbed field and in presence of buildings),

calculation of vertical and horizontal dispersion (turbulence component), definition of the number of particles emitted, and finally calculation of peak concentrations.

In PSwift, interpolation procedures used for meteorological parameters are described in detail in Moussafir and Wendum (1985) [4]. To implement the presence of obstacles, the approach proposed by Kaplan et al. (1996) [5] was adopted. This method is based on a modification of the interpolated wind field according to prescribed zones surrounding obstacles; next, the wind is adjusted including the impermeability conditions on walls and roofs of buildings. In PSpray, dispersion calculation is based on the Thompson's scheme (1984 and 1987 [6]).

Meteorological input in GRAL is based on the most common input format for regulatory applications in Europe. When stability classes are used as input, the Obukhov length is computed based on the suggestions of the German standard boundary layer model (VDI 3783-8). GRAL simulates the flow around obstacles by solving the well-known Reynolds averaged Navier-Stokes equations (RANS), neglecting molecular viscosity, Coriolis and buoyancy forces, and utilizing an eddy viscosity turbulence model. The microscale wind-field model is only applied in regions around buildings up to 15 times the building heights (this value can be increased by the user). For the vertical wind component fluctuations, the model of Franzese et al. (1999) [7] is implemented in GRAL. A set of Langevin equations derived from Anfossi et al. (2010) [8], is taken to model the horizontal dispersion. Finally, the selected method for calculating R90 had a strong impact on the resulting concentration peaks.

References

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