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Simulation of Accidental Release by Means of two Different Modeling Approaches

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For the Seveso Directive, the determination of damage areas related to accidental scenarios, is a key issue. In the present work, the results of two simulation models used (the Gaussian model, named EFFECTS, and Lagrangian, named ARRISK) to determine the effects of the local buildings on the simulated dispersion are presented and compared. The selected test site is a depot of hazardous materials. The results show that Gaussian model exhibits a maximum impact distance greater respect to the Lagrangian code. Significant differences between the two modeling approaches are observed for the IDLH index. As expected, the impact of buildings on the spatial extension of dangerous areas is also found to be noteworthy.

1. Introduction

Due to the evolution of the Seveso legislation and the new implementation of the REACH Directive for the classification of chemical materials, a number of small establishments have recently fallen within the scope of the control of major accident hazards. The new activity in the Seveso sector will take additional risk factors such as congested area, wider range of hazardous materials and exposure for the workers. An example of “atypical” Seveso sites are the depots of chemical goods. The application of assessment and management methods to these “new entries” for the control of major accident hazards is neither simple nor obvious. In particular, these can mislead the simulation of accidental events, which are essential for consequence assessment and emergency planning. Up to now, amongst the different approaches, Gaussian models are the most used to determine the impact of accidental releases in Seveso establishments, even though, these conventionally can simulate stationary sources emissions and are unable to deal with obstacles and non homogeneous turbulence conditions. As a first approximation, it makes sense to neglect these factors, but other important effects need to be considered, to obtain more accurate results. Competent Authorities accept consequence simulations, based on Gaussian plume models, as well as simplistic assumptions about obstacles. In the Seveso practice, the use of non-Gaussian models for consequence simulation is unusual. Computer Fluid Dynamic (CFD) models to account for the effects of obstacles are mainly used in scientific research/academic environments. In recent papers Pontiggia et al. (2011) and Fiorucci et al. (2008), simulated major accidents in a congested area, addressing the impact of obstacles on the dispersion, as well as the potentials of CFD models to foresee such an influence. These models have been used in a recent paper by Hanna (2009) to demonstrate that, in the event of a heavy gas release in a congested area, the obstacles reduce the cloud dispersion thereby increasing concentrations. Operators and consultants tend not to use CFD models for preparing a “Safety Report”, because of their complexity, cost and difficulty in using them. There is an emerging need for investigating the potential of alternative dispersion models, able to deal well with obstacles without making the study so

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difficult. As for computational costs and degree of complexity, the “Lagrangian particles models” can be considered intermediate between Gaussian and CFD models, as reported by Alhajraf (2005). A better understanding of their potential is challenging from both research and Seveso contexts.

2. Aim and methodology

The study is aimed to evaluate the potential of a particle Lagrangian dispersion model for modeling the consequences of a toxic release in proximity of buildings located on a depot site and to compare the results with a conventional Gaussian model. The latter may provide useful suggestions for a possible application of particle models to simulate the releases in a more reliable way for Seveso application.

2.1 Conventional consequence analysis approach

Consequences of an accident release are usually calculated by means of conventional models, such as the Gaussian ones, as these are easy to use, do not require many input data and give an estimate of the impact within a short calculation time frame. During the simulations F2 (extremely stable; wind speed of 2 m/s) and D5 (neutral; wind speed of 5 m/s) atmospheric conditions are assumed.
One widely used consequence analysis model for consequence assessment in Seveso safety reports is the TNO developed EFFECTS code. It performs calculations to predict the physical effects (concentrations, radiation levels, peak overpressures etc) of the escape of hazardous materials. All models in EFFECTS are based upon the Yellow Book (1997) assumptions. EFFECTS can also model complex releases by linking individual models in such a way that they describe all physical phenomena that may occur during that release. The impact due to release in the EFFECTS code is based on the homogeneous turbulence assumption. Hence EFFECTS has been selected for comparing its results with those obtained with the Lagrangian approach, where no homogeneous turbulence is considered.

2.2 Microscale Lagrangian approach

In order to carry out the present study the ARRISK (2010) consequence analysis system has been used. It is based on the Micro-Swift-Spray (MSS) modelling system reported by Moussafir et al. (2004) which includes the Micro-SWIFT and Micro-SPRAY models reported by Tinarelli et al. (2007).
Micro-SWIFT is an analytically modified mass consistent interpolator for complex terrain and urban areas. Given topography, meteorological data and building geometry, a mass consistent 3-D wind field is generated. Starting from predicted or observed meteorological measurements, Micro-SWIFT makes an initial 3D reconstruction by means of an interpolation phase. This first guess field is then modified to take into account obstacles by creating analytical zones (displacement, cavity and wake) where the flow is modified according to buildings. Finally, this flow is adjusted in order to satisfy the continuity equation. It is also able to derive diagnostic turbulence parameters (eg. Turbulent Kinetic Energy, and its dissipation rate) to be used by Micro-SPRAY especially inside the ones modified by obstacles.
The Micro-SPRAY model embedded in the ARRISK system was used in this study. It is a Lagrangian particle dispersion model capable to take into account the presence of obstacles. It is directly derived from the SPRAY code reported by Tinarelli et al. (2007) and recently upgraded by Anfossi et al. (2010) and Mortarini et al. (2011).

3. Case study

The case study addresses a typical commercial depot of drummed and packaged chemical goods. The site features a few warehouses, very close to each other, a small mixing plant, a five-storey building for commercial, administrative and executive offices and, a courtyard for transfer operations. The place is small and densely populated. The total area of factory is 25,000 m^2 with one hundred workers plus customers and drivers. The Safety Report considers several “top events” involving the possible forking of drums by the forklifts. A single event has been selected and the scenarios have been developed by means of the modelling system described above.

3.1 Accident analysis and emission estimation

Among the possible accidents considered by the Safety Report, we selected the event involved with the breaking of 180 L drum containing thionyl chloride by a freight elevator. A liquid pool is supposed to be formed, before evaporating and reacting with the atmospheric humidity to produce H_{Cl} and SO_2. To

estimate the amount of formed gases, an intervention time of 10 minutes was considered, taking into account the emergency procedures which should neutralize and dispose of the product.
A conservative approach has been applied which considers the complete and instantaneous conversion of the $SOCL_2$ vapours in H_{Cl} and SO_2 with the consequent dispersion of toxic vapours.
A temperature of 20 °C and wind speeds of 2 and 5 m/s with F and D Pasquill stability classes respectively were considered for estimating the emission. A 7 m of pool diameter is estimated to be formed. Flow rates of 0.018 and 0.0134 Kg/s were estimated for SO_2 in D5 and F2 atmospheric conditions respectively. As for H_{Cl} flow rates of 0.020 and 0.0153 kg/s were obtained. Although both emitted toxic compounds were simulated for dispersion, results are presented for SO_2 only.

3.2 Models setup

The conventional consequence analysis approach using EFFECTS was setup to produce 600 seconds averaged SO_2 concentration results at 1 m height for prefixed threshold levels. The meteorological conditions D5 and F2 were applied using inhabitated land roughness conditions. The above reported correspondent emission factors for SO_2 were used, considering no reacting gases and semi-continuous release conditions.
In order to compare the results among models, their working parameters were kept as close as possible. For this reason the meteorological conditions, the roughness parameter and the SO_2 emission factors used for the EFFECTS model were also applied in the ARRISK system. For the latter a simulation domain of 398x298 m^2 with 2 m of lateral resolution was chosen. Its vertical extension was divided in 15 levels from 1m to 200 m with increasing resolution with height. To take into account the effects of the main buildings located inside the studied industrial facility, their spatial extension and height were extracted from territorial and proprietary data and then provided to the ARRISK system to produce model obstacles and “zones” as required by Micro-SWIFT model. A simulation without obstacles was carried out to evaluate their effects on the calculated concentration fields. Both 3D and surface concentration fields at 1 m height were produced using the Lagrangian Particle Models based ARRISK system. The results are presented below.

4. Results

To obtain information on the spatial extension of dangerous toxic concentrations, the Immediate Dangerous to Life and Health (IDLH) and the Lethal Concentration which kills 50 % of test animals (LC50) indexes were extracted from the 10 min averaged concentration fields of SO_2. As the reference values of IDLH and LC50 for SO_2 are provided for 30 min of exposure time, and the modelled accident is supposed to last 10 min, the above indexes values were recalculated for the effective simulation time (IDLH = 420 mg/m^3; LC50 = 9283 mg/m^3). The results obtained with both conventional consequence analysis approaches, with and without obstacles, are presented below.

4.1 Conventional approach results

EFFECTS was used to obtain the 10 min averaged SO_2 concentrations vs. downwind distance and the possible existence and its spatial extension of both IDLH and LC50 indexes. As for the LC50 index, it is never reached in both meteorological conditions. Conversely for the IDLH, they are overcome in F2 and D5 conditions. According to results the spatial extension of the IDLH zone is as large as 1.5m and as long as 55 and 20 m for F2 and D5 respectively, located at 15 and 2.5 m from the poll source. The above results are in agreement with what is expected using a Gaussian approach in pollutants dispersion as applied in the EFFECTS system.

4.2 Microscale Lagrangian approach results

As an example the wind field at 1 m height in D5 meteorological conditions is shown in Figure 1. The effect of buildings on wind speed is clearly visible within the zones between obstacles. It is worth noting how Micro-SWIFT produce wake and cavity zones downwind to north-east buildings, as well as the displacement zones in the buildings facing the un-modified wind (western buildings). As shown in Figure 1, these zones create large re-circulation areas among buildings, calm wind at the interface between wake and cavity zones and complex structures of wind field between obstacles. All these effects are expected to produce significant impacts on the calculated concentration fields.

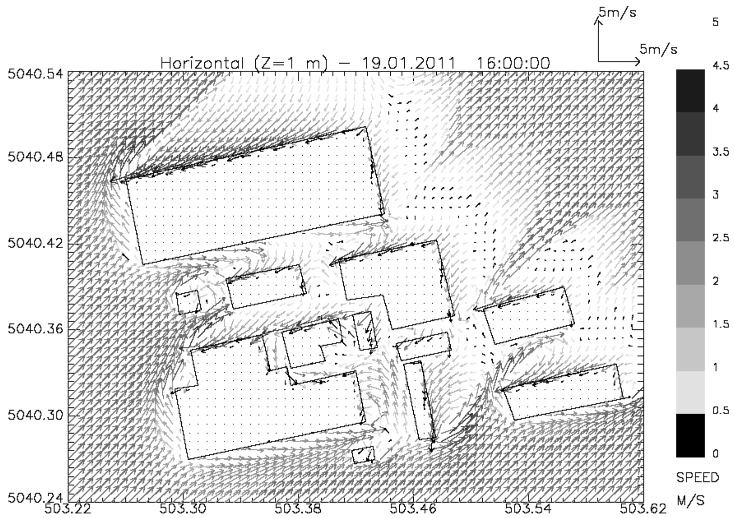
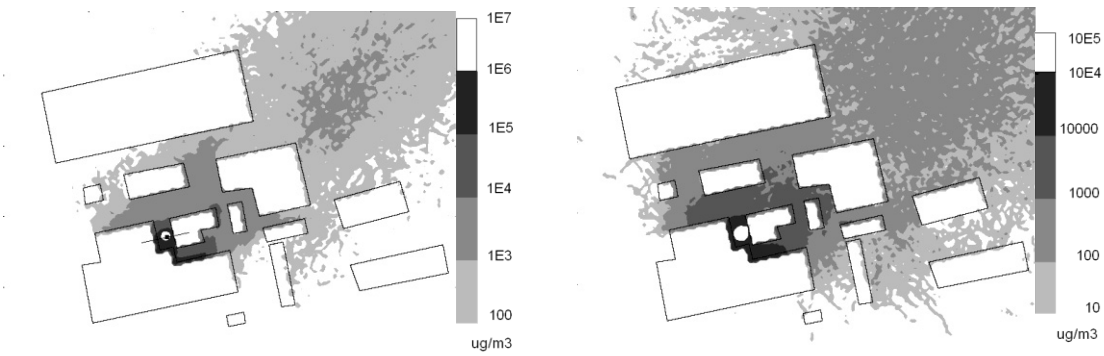


Figure 1. Wind field at 1 m height in D5 atmospheric conditions.

The SO_2 average concentrations after 600 s of the accident in atmospheric conditions F2 and D5 are shown in Figure 2. Compared to typical concentration field obtained without the influence of obstacles, it is clear how the latter play an important role in the pollutant dispersion phenomena. While the Gaussian approach of EFFECTS predicts maximum peak between 10 to 25 m depending on the atmospheric conditions, the correspondent values predicted by ARRISK are confined in the accident area limited by the buildings surrounding it. In addition, the buildings downwind the accident area seem to produce a shield to the dispersion of toxic pollutant. According to results shown in Figure 2, this effect is more effective in F2 conditions than in D5 one. In order to evaluate the amount of effects produced by buildings, a simulation without obstacles has been carried out.



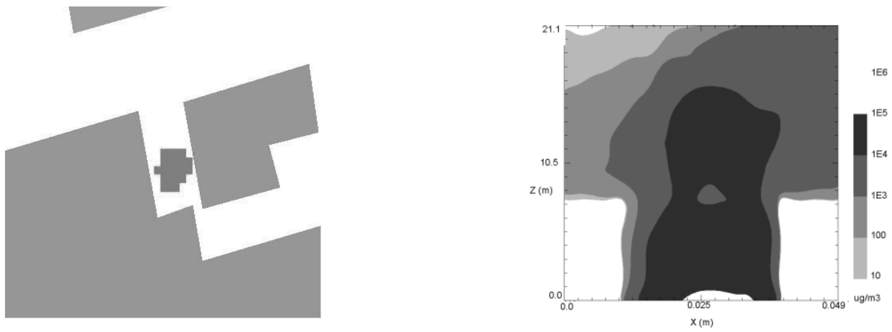
a) b)

Figure 2. SO_2 average concentration after 600 s of accident in stability conditions F2 (a) and D5 (b).

Table 1: Maximum SO_2 concentration (mg/m^3) after 600 s a different distances from the source.

Atmospheric conditions	15 m		60 m		150 m	
	Obst.	No Obst.	Obst.	No Obst.	Obst.	No Obst.
F2	316	103	64	13	1.7	4.9
D5	82	22	1.7	2.7	0.4	0.8

Table 1 shows the maximum SO_2 concentrations at three different distances with and without obstacles calculated over all possible directions. At closer distance from the source, the buildings increase the estimated concentration values for about a factor 3-4. Conversely at longer distances they reduce concentrations for about a factor 2-3. The above results have an impact on the spatial extension of the safety indexes. Figure 3a shows the zone with concentration values above the IDLH limit in F2 atmospheric condition. It is estimated to be as large as 11x9 m^2, which is much smaller than the value predicted by the Gaussian based EFFECTS system (3x35 m^2). In D5 conditions the IDLH zone extends up to 5x4 m^2, respect to its non existence when EFFECTS is used.

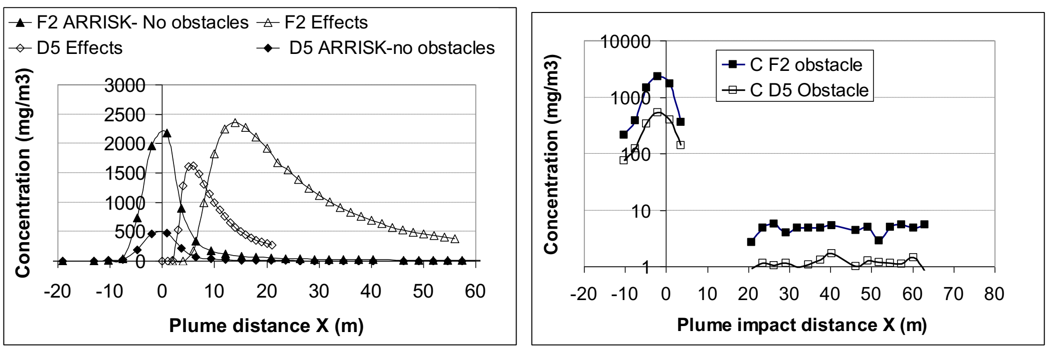


a) b)

Figure 3. IDLH zone in F2 atmospheric conditions (a), Vertical cross section over the pool source (b).

Figure 3b shows the vertical cross section of SO_2 concentrations over the IDLH zone. It can be observed that significant concentrations (10-100 mg/m^3) are estimated up to 15 m height, overcoming the buildings (white areas in Figure 3b) with likely impact on indoor concentrations by means of forced or natural ventilation systems. The LC50 limit is never overcame in both meteorological conditions, in agreement with what predicted by EFFECTS model.

In order to compare the results of the two models, the estimated ground impacts along the direction of plume dispersion have been extracted. In Figure 4 is shown both the results obtained with non obstacles present in the models (a) and including obstacles in the ARRISK model (b). While for F2 the maximum peak is quite similar for both models (about 2100 mg/m^3), it is interesting to observe the simulated impact distance that is quite different (about 1m for ARRISK and 15 m for EFFECTS). As for the D5 cases (Figure 4a), both peak values and their position are quite different in both models (maximum concentration of 500 mg/m^3 at 1m for ARRISK and 1600 mg/m^3 at 5m for Effects). Using the ARRISK model results, it is evident (Figure 4 b) how the influence of the obstacles on the ground pollutant impact with an increase of the maximum values respect to the simulation without obstacle (+4.6 % for F2 and +11.7 % for D5).



(a) (b)

Figure 4. Ground Plume impact along the direction of plume dispersion for different models and meteorological conditions: no obstacle (a) and obstacle (b) simulations.

5. Conclusions

In densely built environments, as occurs in a few atypical Seveso establishments, the common practice underestimates potential consequences for workers. Due to obstacles, like buildings and walls, the concentration close to the release point, can be higher than the Gaussian plume models foresee allowing the hazardous limits to be reached. On the other hand, the extension of the damaged areas can be overvalued. In order to evaluate the differences in the determination of risk area, we compared the results provided by two user friendly models (the EFFECTS and ARRISK code). Significant differences in the extension IDLH zones were found between the two models. The estimated ground plume impacts were also different even when obstacles were not considered. The latter was found to increase the concentration of a factor 3-4 at closer distance from the source. Conversely at longer distances concentrations are reduced about a factor 2-3 due to shielding effects. The cloud's vertical profile was found to be affected by the buildings. These form a sort of "chimney", which guide the hazardous material towards the roof. This roof dispersion requires attention as the presence of air-conditioners could transfer the pollutants inside the buildings and degrading the indoor air quality. The use a Lagrangian particle model seems a good trade-off between the need for simple and easy to use tools and the need for accounting obstacles.

References

Alhajraf S., Al-Awadhi L., Al-Fadala S., Al-Khubaizi A., Khan A.R., Baby S., 2005, Real-time response system for the prediction of the atmospheric transport of hazardous materials, Journal of Loss Prevention in the Process Industries, 18(4-6), 520-525.

Anfossi D., Tinarelli G., Trini Castelli S., Nibart M., Olry C., Commanay J., 2010, A new Lagrangian particle model for the simulation of dense gas dispersion, Atmospheric Environment, 44(6), 753-762.

ARRISK, 2010, Development of a conseguence analysis for accidental releases based on particles Lagrangian models and working in both local and micro scales (in Italian). Technical report ARIANET R2010.18. September 2010.

Fiorucci A., Pontiggia M., Derudi M., Alba M., Scaioni M., Pendino R., Uguccioni G., Rota R., 2008, Risk assessment of dangerous products release and dispersion: a comparison between CFD and integral models, Chemical Engineering Transactions, 13, 195-202.

Hanna S., Hansen O.R., Ichard M., Strimaitis M., 2009, CFD model simulation of dispersion from chlorine railcar releases in industrial and urban areas, Atmospheric Environment, 43, 262–270.

Mortarini L., Carlino G., Tinarelli G., Mauri L., Trini Castelli S., Anfossi D., 2011, Development of the microscale Lagrangian particle model MICROSPRAY for the simulation of the two-phase releases, 14th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes Kos, Greece 2-6 October 2011. H14-212, 704-707.

Moussafir J., Oldrini O., Tinarelli G, Sontowski J, Dougherty C., 2004, A new operational approach to deal with dispersion around obstacles : the MSS (Micro-Swift-Spray) software suite, 9th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes Garmisch, Germany, 1-4 June 2004, 5.26, 114-118.

Pontiggia M., Landucci G., Busini V., Derudi M., Alba M., Scaioni M., Bonvicini S., Cozzani V., Rota R., 2011, CFD model simulation of LPG dispersion in urban areas, Atmospheric Environment, 45, 913-923.

Tinarelli G., Brusasca G., Oldrini O., Anfossi D., Trini Castelli S., Moussafir J. , 2007, Micro-Swift-Spray (MSS) a new modelling system for the simulation of dispersion at microscale, general description and validation. In: Air Pollution Modelling and Its Application XVII, Borrego C., Norman A.L., (Eds.), Springer, 449-458.

YELLOW BOOK, 1997, Methods for the calculation of physical effects due to releases of hazardous materials (liquids and gases) – Editors: C.J.H. van den Bosch, R.A.P.M. Weterings - Committee for the Prevention of Disasters, The Hague, The Netherlands.