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Application of a Gaussian Model to Simulate Contaminants Dispersion in Industrial Accidents

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The increase of the industrial production and the development of new processes led to the necessity of better regulations of activities concerning potential risks for human health and environment. Accomplishing such purposes requires studies on both the chemistry of the involved phenomenon and the dispersion mechanism in the surrounding environment. While the chemistry of reaction can be determined at small scale via laboratory experiments and models, the dispersion in the environment is an extremely complex phenomenon to model, because it is strongly affected by the atmospheric conditions. Several models with the purpose of simulating pollutants dispersion were developed (Gariazzo et al., 2012; Alemayehu et al., 2015; Fang et al., 2018); among those, Gaussian models found many applications in safety engineering, due to both their effectiveness and relatively low computational costs. The US-EPA recommends the use of the Gaussian model AERMOD for the simulation of dispersions within 50 km from the emission source. It is important to underline that most of these models were developed with the aim to simulate the dispersion of continuous emissions such as those from industrial chimneys. Such systems can be assumed to work under steady-state conditions, since they are supposed to work for a long time. Nonetheless, industrial accidents, which can have a severe impact on people and environment, generally occur at a relatively small time scale, thus their dispersion has not yet reached the steady state conditions.

In this work, we developed a modified non-steady-state Eulerian Gaussian model able to simulate the dispersion of contaminants produced by an industrial accident, which is hypothesized to be a point source. The model requires as input data time-dependent meteorological conditions and topographic information of the site, concerning: the source, physical properties of the pollutant, emission height and release temperature. The proposed model was applied to the 2,3,7,8-Tetrachlorodibenzodioxin (TCCD) dispersion after the Seveso accident (1976) near the source (radius of about 4 km). Results highlighted a good agreement with available literature experimental data.

1. Introduction

Chemicals release coming from industrial chimneys and accidents play an important role in atmospheric pollution. Hence, the simulation of dispersions became an important aspect in environmental assessments, helping understanding how the concentration of pollutants evolves in space and time around the release spot. CFD codes are among the most valuable methods to afford such a target. However, they are based upon specific codes for every different application requiring a lot of information about release properties and atmospheric conditions. Also 3-D domains and computational meshes have to be properly developed in order to describe the release zone. Such tasks require a lot of preparation and computational times (Derudi et al., 2014; Pontiggia et al., 2010, 2011). For this reason, simplified models can provide faster and still robust information about pollutants dispersions. Among these, the most commonly used approaches are based on Gaussian models. Most of these software products are developed for continuous emissions, such as plumes from industrial chimneys. However, a lot of events, such as industrial accidents, can be treated as instantaneous emissions.

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In this work, a Gaussian model has been developed for instantaneous emissions and validated by simulating the Seveso accident occurred in 1976, which lead to huge human and environment damages over a wide area.

2. Mathematical model

Modelling the dispersion of an instantaneous release requires an unsteady-state model, since the phenomenon itself is a transient, in which a fixed amount of pollutant is carried by source effects, wind and buoyancy forces.

$$\bar{C}(x,y,z,t) = \frac{S}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} exp\left(-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right) \tag{1}$$

Where S is the total mass released [kg],

$$\bar{C}(x,y,z,t) = \frac{S}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} exp\left(-\frac{(x-\bar{u}t)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right) \tag{2}$$

Total ground absorption (u_y,=u_z=0, source positioned at point (0,0,h))

$$\bar{C}(x,y,z,t) = \frac{S}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} exp\left(-\frac{(x-\bar{u}t)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}\right)\left[exp\left(-\frac{(z-h)^2}{2\sigma_z^2}\right) - exp\left(-\frac{(z+h)^2}{2\sigma_z^2}\right)\right] \tag{3}$$

The dispersion coefficients have been considered as follows:

$$\sigma_x = \sigma_y = ax^b \tag{4}$$

$$\sigma_z = cx^d \tag{5}$$

Where *a, b, c, d* are parameters that depend upon the Pasquill stability class of the atmosphere (Lees, 1996).
In order to run the simulations, some data about the release are needed, and they can be classified into 3 groups: meteorological, release and morphological data, detailed below.
Once that all the parameters are set, the code gives as output the ground concentration of the pollutant.

2.1 Meteorological data

Meteorological data can be freely downloaded by National and International Environmental associations, according to one's own country. The required elements needed for the computation of this model are:

- Wind speed and direction
- Air temperature
- Average radiation

Wind information are needed in order to evaluate the release direction and the phenomena evolution in the surroundings of the release. In combination with air temperature and average radiation, the atmosphere Pasquill stability class is crucial in order to define properly the dispersion parameters required by the Gaussian model.

2.2 Release data

The model hypothesizes an instantaneous point-source, then it requires a limited amount of information:

- Total mass released
- Release height
- Release temperature
- Release velocity

The point-source approach is consistent if the total emission time is much lower than the total release time.

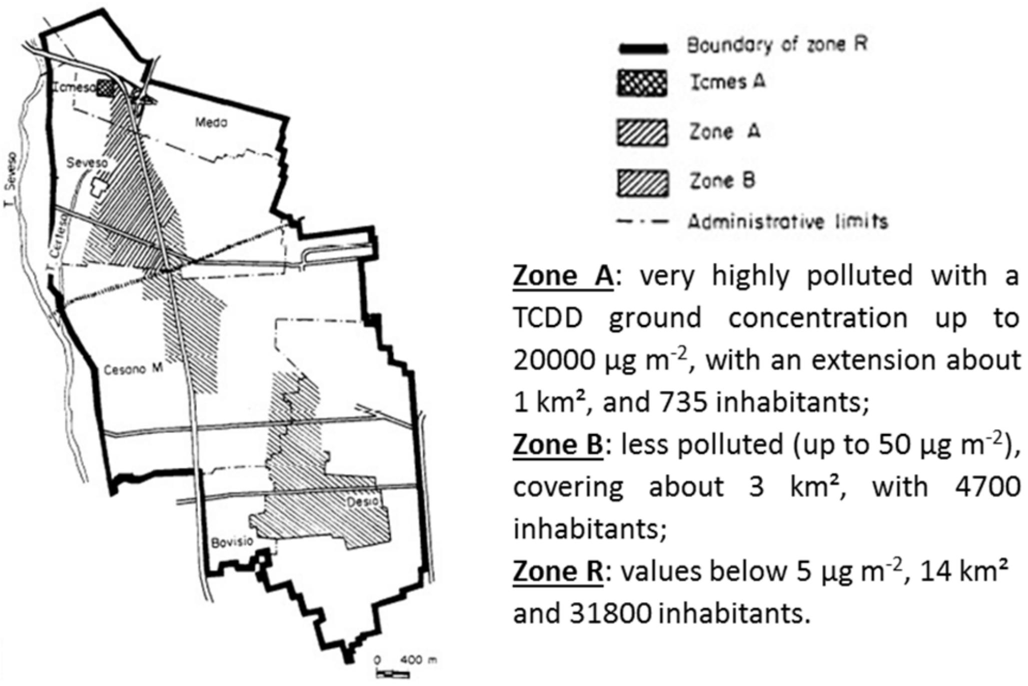
2.3 Morphological data

To convert the morphological area of interest in a matrix with elements containing the local height of the point, the software MATLAB® has been used through the function "*readhgt*". This function, developed by François Beauducel, imports .HGT "height" binary data files from NASA SRTM global digital elevation model of Earth land, corresponding to 1x1 degree tiles of 3-arc seconds resolution (SRTM3, around 90 m) and 1-arc second (SRTM1, around 30 m), and returns coordinates vectors latitude and longitude, and a matrix of elevation values.

3. The Seveso accident

The notorious Seveso accident took place on 10 July 1976 during the period of 10.40 GMT to 11.10 GMT, corresponding to the local noon. The accident occurred at a facility called ICMESA, located around the city of Seveso, in the north of Italy. The plant was provided with a batch reactor for the production of trichlorophenol, a component for several herbicides. At the day of the accident, the reaction went out of control reaching temperatures over 200°C, triggering a runaway reaction that lead to production of 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin (TCDD), known as one of the most toxic dioxins for human health and environment. The runaway reaction was never considered a possibility, so no emergency collecting system was installed. The dioxin was dispersed in a toxic cloud all around the plant, covering a total area of about 18 km^2~~,~~ with more than 30000 inhabitants.

After the accident, measurements of TCDD in the soil where performed, and the area affected by the dispersion was divided in 3 zones (Cavallaro et al., 1982), represented in Figure 1.



Zone A: very highly polluted with a TCDD ground concentration up to 20000 µg m^{-2}, with an extension about 1 km^2, and 735 inhabitants;
Zone B: less polluted (up to 50 µg m^{-2}), covering about 3 km^2, with 4700 inhabitants;
Zone R: values below 5 µg m^{-2}, 14 km^2 and 31800 inhabitants.

Figure 1: Map of Zones A, B and R drawn of the basis of environmental samples analyzed until 31 August 1976 (Cavallaro et al., 1982).

3.1 Release properties

Table 1 reports all the parameters of the TCDD release from ICMESA factory. The temperature of the release was hypothesized from the decomposition temperature of TCDD.

Table 1: Characteristic of the ICMESA TCDD release (Lees, 1996)

Release property	Value
Vent height	8 m
Vent diameter	12.7 cm
Temperature	250 °C
Total mass of TCDD	2-130 kg
Pressure	376 kPa
Velocity	274 m s^{-1}
Release time	20 min

The release pressure is the same of the emergency venting, which was installed for eventual faults in the compressed air cleaning system. For the total mass released, several estimates have been produced in the literature, ranging between 2 and 130 kg of TCDD released.

3.2 Orography

The topographic map around ICMESA has been recovered with the abovementioned “*readhgt”* MATLAB® function. The coordinates of the facility are 45° 38’ 54,73’’N – 9° 09’ 09,31’’E. Hence, the SRTM map to look for is between 9°-10° E, and 45°-46°N. Figure 2 shows the map centered at ICMESA spot, in a 16 km² area. It is noticeable that the zone is almost all plane. Hence, it is expected that the orography has low impact on the dispersion.

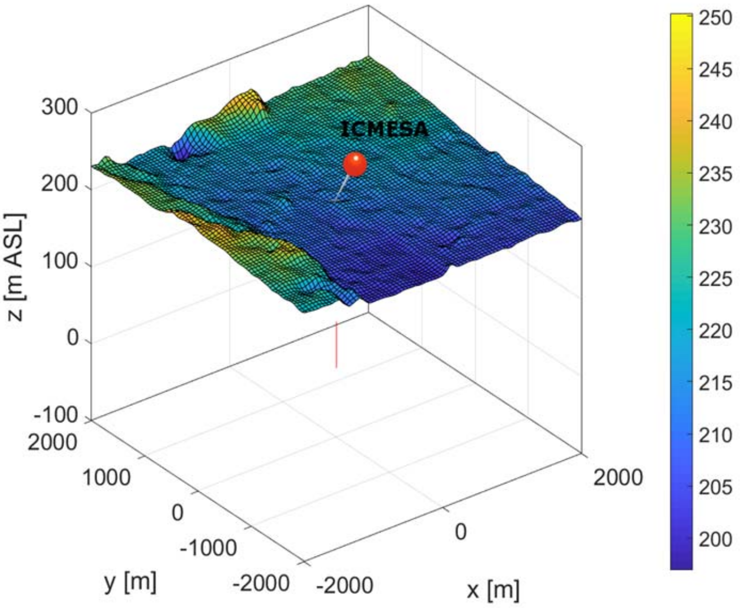


Figure 2: Map around ICMESA site, covering a square of 16 km²

3.3 Meteorological data

Atmospheric conditions at the time of the accident were recovered and presented in Table 2. In 1976, the closest atmospheric measurements site was at Linate Airport (Milan), which is 24 km distant from Seveso. We kept the same temperature and wind speed provided in Table 2, located on the ground. The atmosphere was quite unstable, due to wind variability. According to Table 1, the Pasquill Class for 10 July 1976 is estimated as an E class. For the direction, it was determined that, by means of graphic interpolations, based on weighted vector averages, the path of the toxic cloud could not be a straight line, and it was confirmed by deposition maps (Cavallaro et al., 1982).

Table 2: Weather conditions on 10 July 1976 at 12.00 GTM (station located at Milan airport, distant 24 km from Seveso and 100 m lower) (Cavallaro et al., 1982)

Height [m]	Temperature [°C]	Wind speed [m s^{-1}]	Height [m]	Temperature [°C]	Wind speed [m s^{-1}]
1400	14.9	6.7	600	22.9	3.6
1300	15.9	6.3	500	23.9	3.3
1200	16.9	5.9	400	24.9	3.1
1100	17.9	5.4	300	26.0	3.5
1000	18.9	5.0	200	27.0	3.9
900	19.9	4.6	100	28.1	4.3
800	20.9	4.3	Ground	29.1	4.6
700	21.9	4.0			

We also recovered more recent atmospheric data around the Seveso zone: the Italian association ARPA (Agenzia Regionale per la Prevenzione Ambientale), dedicated in collection of meteorological conditions in Lombardy since 1999, has two stations near Seveso, located at *Carate-Brianza* (distant 11 km from ICMESA) and *Vertemate con Minoprio* (14 km distant). It was interesting to notice that, in 2004, the average wind speed is much lower of the conditions presented in Table 2 (2-3 m s^{-1} vs 4.6 m s^{-1}). This could mean that at that time, the particularly high wind speed brought to an unpredictable spread of the toxic cloud.

4. Simulations and Results

The conditions reported in Section 3 have been applied to the Gaussian model described, estimating the ground concentration of TCDD in a zone of 16 km² around ICMESA site. In order to validate the model, we decided to consider the Zone A only: this zone was definitely the most investigated and analysed after the accident. Also, the dispersion of the toxic cloud in the proximity of the site is more strictly related to pure atmospheric dispersion phenomena, which are described in the presented model. Investigations around Zone A have been carried out by Istituto Superiore della Sanità (ISS). Between 11 and 13 August 1976, they collected in total 107 samples. The isopleths represent concentrations equal to 25, 50, 250, 500, 750, 1000, 1500, 2000, 3000, 4000, 5000, 10000, 15000 and 20000 μg m^{-2}.

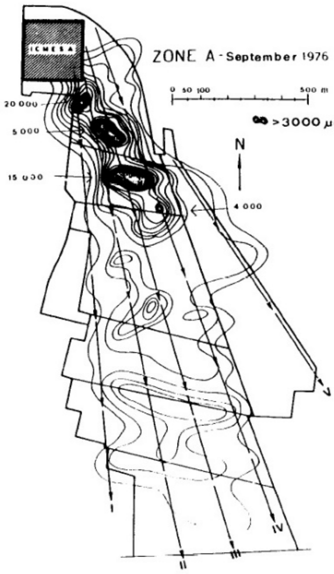


Figure 3: Chemical map of TCDD around ICMESA, September 1976 (Cavallaro et al., 1982)

Since from this reference we can only get the ground concentration, we need to estimate the amount of TCDD that is absorbed through the ground by using a gaussian model. In order to reconstruct this profile, we used the following trick: by subtraction the Gaussian term involving total ground reflection with the Gaussian term involving total ground absorption, we can get a virtual profile of pollutant: this amount of TCDD is actually the portion that is absorbed through the ground, and it is possible to recover it via integration with the vertical axis:

$$\bar{C}_{ground}(x,y,z,t) = \int_0^H \frac{S}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} exp\left(-\frac{(x-\bar{u}t)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}\right)\left[2exp\left(-\frac{(z+h)^2}{2\sigma_z^2}\right)\right]dz \qquad (6)$$

H should be the Planetary Boundary Layer, but due to the lack of information required to estimate it, it was assumed conservatively equal to 100m.

However, this definition is not conservative: since we want to estimate the amount of pollutant that deposits overtime, we need to take in account the amount of pollutant that is already absorbed. This is done by considering the mass of pollutant *S* that is absorbed:

$$S_{abs}(x,y,z,t) = \int_{\varphi} \bar{C}_{ground}(x,y,z,t)d\varphi \qquad (7)$$

Where φ is the ground. It Is possible then to evaluate the proper ground concentration:

$$\bar{C}_{ground}(x,y,z,t) = \int_0^H \frac{S - S_{abs}}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} exp\left(-\frac{(x-\bar{u}t)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}\right)\left[2exp\left(-\frac{(z+h)^2}{2\sigma_z^2}\right)\right]dz \qquad (8)$$

The results of the simulation are reported in Figure 4. As it is possible to see, the concentration of the areas around the release point are underestimated if compared to the experimental data. This could be explained by the fact that the model does not take into account some “dead zones”, where the impact with buildings, trees and so on could have caused an unexpected accumulation of TCDD. In addition, the present model does not take into account buoyancy effects that can have an influence considering the TCCD dispersion behavior. Despite this the cloud extension and the concentration at the outer edges show a good agreement with the experimental data. This aspect is very important during safety and environmental risk analysis because this model is able to underline what are the safe areas according to the different atmospheric conditions.

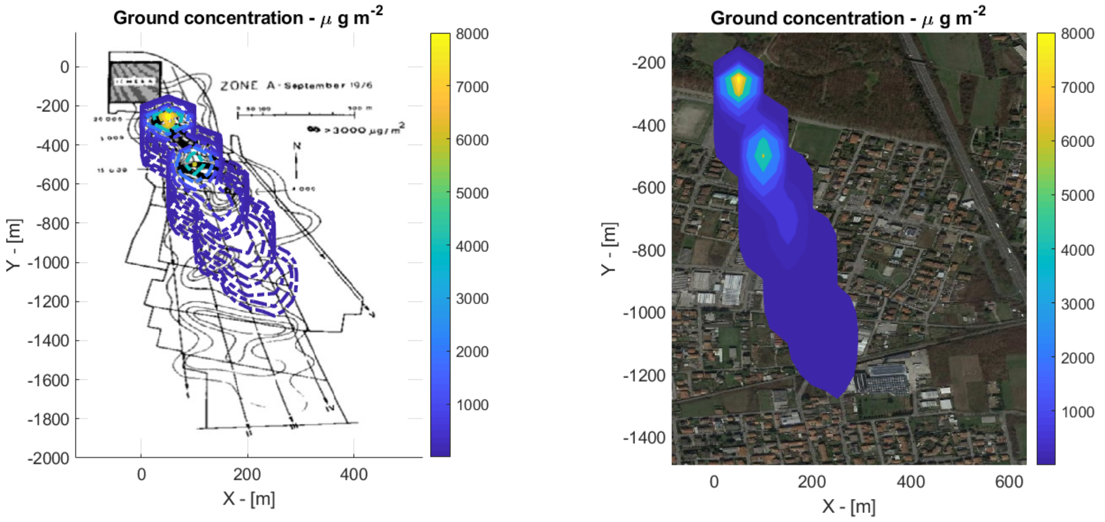


Figure 4: Ground concentration of TCDD (isopleths above 7.5 μg/m³)

5. Conclusions

This work proposes a simplified Gaussian model to estimate dispersions of instantaneous emissions. The model has been developed in a MATLAB® environment, which is supplemented with a function that allows to load topographic data from NASA SRTM database. The model was validated by simulating the Seveso accident, comparing the model results with measurements performed near the release area at the time of the catastrophe. Results showed good agreement between predictions and experimental data. The developed code can be potentially applied to provide fast and consistent estimations of dispersion of instant pollutant emissions with a limited amount of required data.

References

Alemayehu D., Hackett F., 2015. Gaussian dispersion model to estimate the dispersion of particulate matters ($PM_{2.5}$) and sulfur dioxide (SO_2) concentrations on Tribal Land, Oklahoma. American Journal of Environmental Sciences, 11, 440-449.

Cavallaro A., Tebaldi G., Gualdi R., 1982, Analysis of transport and ground deposition of the TCDD emitted on 10 July 1976 from the ICMESA factory (Seveso, Italy). Atmospheric Environment, 16, 734-740.

Derudi M., Bovolenta D., Busini V. Rota R., 2014, Heavy gas dispersion in presence of large obstacles: Selection of modeling tools, Industrial and Engineering Chemistry Research, 53, 9303-9310.

Fang D., Zhang X., Yu Q., Chen T., Tian L., 2018, A novel method for carbon dioxide emission forecasting based on improved Gaussian processes regression, J. Clean. Prod., 173, 143-150.

Gariazzo C., Pelliccioni A., Bragatto P., 2012, Simulation of accidental release by means of two different modeling approaches. Chemical Engineering Transactions, 26, 555-560.

Lees F. P., 1996 Loss Prevention in the Process Industry, 2nd Edition, Butterworth-Heinemann.

Pontiggia M., Derudi M, Alba M., Scaioni M., Rota R., 2010, Hazardous gas releases in urban areas: Assessment of consequences through CFD modelling, J. Hazardous Materials, 176, 589-596.

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, 3913-3923.