



## Emergencies planning and response: Coupling an exposure model with different atmospheric dispersion models



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### HIGHLIGHTS

- The D-F and D-M coupled systems are a very interesting tool for risk analysis.
- D-F is an excellent tool in the planning stage of emergencies and disasters.
- D-M is appropriate to provide efficient real time responses to emergencies.

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### ABSTRACT

Information on spatial and time dependent concentration patterns of hazardous substances, as well as on the potential effects on population, is necessary to assist in chemical emergency planning and response. To that end, some models predict transport and dispersion of hazardous substances, and others estimate potential effects upon exposed population. Taken together, both groups constitute a powerful tool to estimate vulnerable regions and to evaluate environmental impact upon affected populations.

The development of methodologies and models with direct application to the context in which we live allows us to draft a more clear representation of the risk scenario and, hence, to obtain the adequate tools for an optimal response. By means of the recently developed DDC (Damage Differential Coupling) exposure model, it was possible to optimize, from both the qualitative and the quantitative points of view, the estimation of the population affected by a toxic cloud, because the DDC model has a very good capacity to couple with different atmospheric dispersion models able to provide data over time. In this way, DDC analyzes the different concentration profiles (output from the transport model) associating them with some reference concentration to identify risk zones.

In this work we present a disaster scenario in Chicago (USA), by coupling DDC with two transport models of different complexity, showing the close relationship between a representative result and the run time of the models. In the same way, it becomes evident that knowing the time evolution of the toxic cloud and of the affected regions significantly improves the probability of taking the correct decisions on planning and response facing the emergency.

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### 1. Introduction

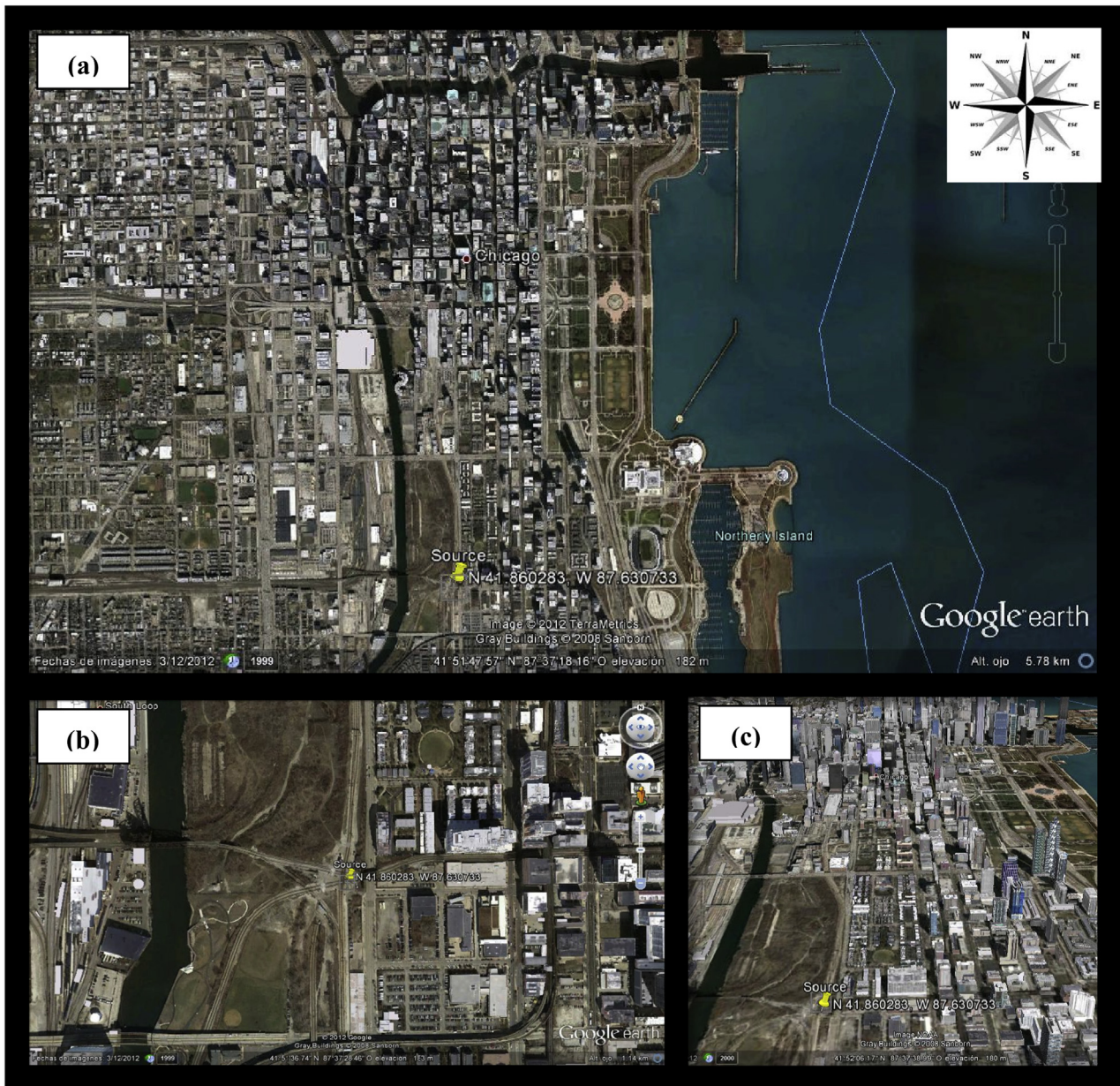
The adverse health effects of an accidental release of hazardous substances into the atmosphere are motive of concern in very populated urban areas, due to the size of the potentially affected

population and to the complexity of the scenario. Simulation models of chemical incidents constitute an important tool both for a real time emergency response and for planning it in several contexts. The appropriate model to be employed in an emergency will depend on the level of detail required and on the execution time available; both characteristics are closely related (Warner et al., 2008; Hanna et al., 2009).

Nevertheless, many exposure models for chemical incidents currently applied have serious constraints when authorities try to use them in actual situations. Firstly, they do not take into account

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**Fig. 1.** Aerial view of study area. In (a) a wide view of the emission source and its environment is observed. In the same picture the Chicago River can be seen to the left of the source, and also the tall buildings to the North. In (b) the railway junction and the plain open terrain around the source are visualized. (c) shows an angled view of the scenario, with a densely built (characterized by tall buildings) adjoining the open area around the source. Source: Google maps, 2011.

time as a variable: they only describe the expected final state, although time is a conditioning factor on emergencies responses. Moreover, the adverse health effects calculated by most current models are overestimated according to conservative decisions, and often their severity is not quantified (Reynolds, 1992; Ruiz Boada et al., 2003; Acquesta et al., 2011; Sanchez and Acquesta, 2011).

Taking into account the above-mentioned constraints, we have recently implemented the exposure DDC (Damage Differential Coupling) model, which computes the time evolution of the exposure to concentrations, permitting therefore a continuous monitoring. The method estimates maximum and minimum levels (hereinafter referred to as maximum damage and minimum damage, respectively) of adverse health effects caused by the exposure to a toxic cloud, using a recursive algorithm for that purpose (Sanchez, 2012; Sanchez et al., 2010, 2011; 2012a,b). DDC is applicable to acute exposures: therefore it employs the

toxicological indices of acute exposure (AEGLs, ERPGs and TEELs), incorporating the exposure characteristics described in the technical reports that justify these values (Craig et al., 2000; ERPG and WEEL, 2007; US EPA, 2012). As described in Sanchez et al.

**Table 1**

AEGLs for chlorine, corresponding to the 2012 update of the U.S. EPA July 2006 final statement.

Index	Exposure time (minutes)				
	10	30	60	240	480
AEGL-1 (mg m <sup>-3</sup> )	1.5	1.5	1.5	1.5	1.5
AEGL-2 (mg m <sup>-3</sup> )	8.3	8.3	5.9	3	2.1
AEGL-3 (mg m <sup>-3</sup> )	147.7	82.7	59.1	29.5	21
AEGL-1 (ppm)	0.5	0.5	0.5	0.5	0.5
AEGL-2 (ppm)	2.8	2.8	2	1	0.71
AEGL-3 (ppm)	50	28	20	10	7.1

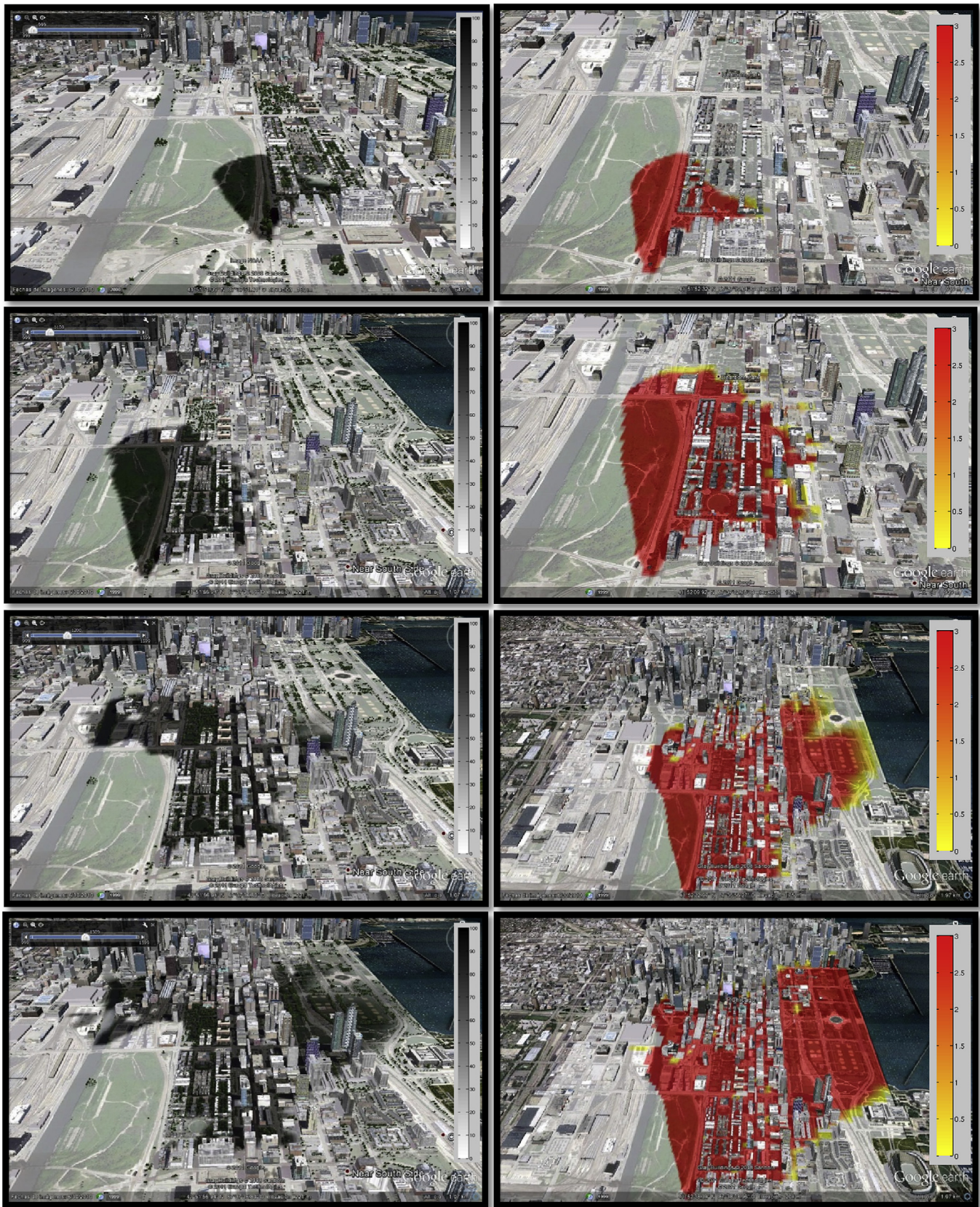
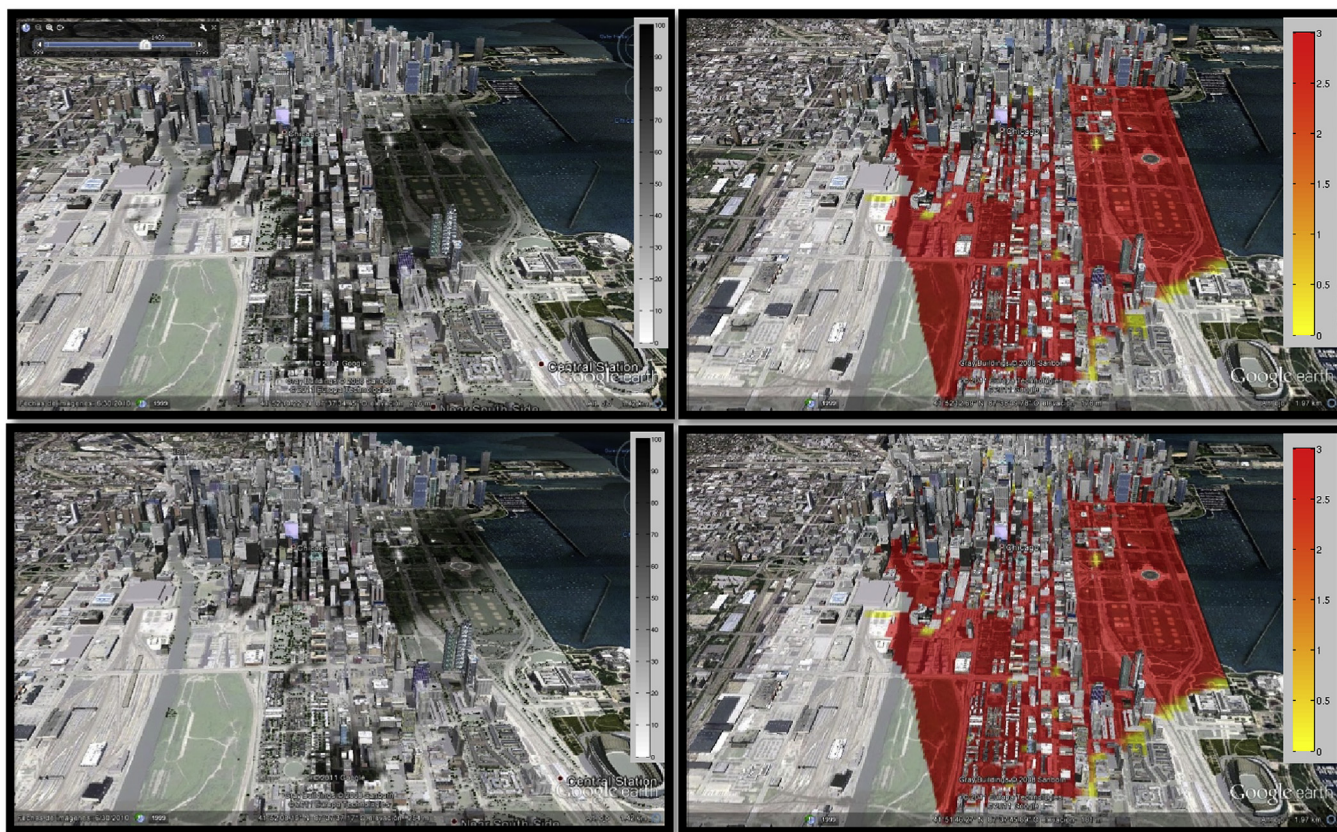


Fig. 2. D-F coupled system. Representation of the evolution of the toxic cloud (1st column) and maximum damage regions (2nd column) on a satellite image provided by Google Earth (2011), where 0.31 ppmv contours are shown, for  $t = 200, 400, 800$  and  $1200$  s;  $t$  is the time after the chlorine release starts.



**Fig. 3.** D-F coupled system. Representation of the evolution of the toxic cloud (1st column) and maximum damage regions (2nd column) on a satellite image provided by Google Earth (2011), where 0.31 ppmv contours are shown, for  $t = 1600$  and  $2000$  s;  $t$  is the time after the chlorine release starts.

(2013), the toxicological indices (AEGIs, ERPGs and TEELs) are comparable in terms of levels of adverse health effects; therefore we shall denote different levels of the indices of reference with the acronym HEL (Health Effects Level); for example, AEGL 1 corresponds to HEL 1.

DDC applies a methodology of differential analysis which ensures that the expected effect on health is among the maximum and minimum damage mentioned. To estimate the HEL as a function of exposure time, DDC assumes that there is a continuous field of the toxicological indices mentioned for time and concentration, and that the incremental estimation of the maximum and minimum damage by means of exposure differentials is not commutative. A more detailed description of the methodology developed for the DDC approach may be consulted in Acquesta et al. (2011).

DDC not only achieves more precise estimations of the expected health effects than those obtained by means of currently used methods, but also it is very useful in triage situations, where resources are limited and errors could be tragic (Sanchez, 2012; Sanchez et al., 2011, 2012a,b).

The purpose of this work is to study the coupling of DDC with two very different pollutant dispersion models, namely the computational fluid dynamics (CFD) FLACS (Flame Acceleration Simulator) model (GexCon US, 2012), and a simple numerical model (Sanchez, 2012), to use them in an integrated risk management. We refer to the couplings as D-F and D-M, respectively.

FLACS, whose outputs (see Hanna et al., 2004a,b) used in this work were kindly supplied by Dr. Steven R. Hanna, was originally developed to simulate explosions. At present it is also employed to simulate other phenomena, such as dispersion of pollutants in the atmosphere, and its application has been validated by means of several works (Hanna et al., 2004b, 2009; GexCon US, 2012). A

detailed description of FLACS may be consulted in Warner et al. (2008) and Hanna et al. (2004a,b). On the other hand, the simple numerical model above mentioned is composed of the implicit solution of the advection–diffusion–reaction equation by a finite differences method, plus an upwind schema for the advection term and a first order reaction term. A detailed description of this model may be found in Sanchez (2012).

## 2. Methodology

Why the above-mentioned coupling? Let us comment on the CFD and the simple finite-difference models. CFD models are more adequate for a deep analysis in densely populated areas, due to the fact that such models are capable of very accurately describing different scenarios (Delaunay, 1996; Hanna et al., 2007; Sanchez et al., 2013). But those models require large amount of data and too much computing time; such characteristics are adverse factors when using them in a real time analysis (Sklavounos and Rigas, 2005). Therefore, for real-time analysis simpler models (for instance, Gaussian models) are employed. Those models usually simplify the description of phenomena, in particular in a complex terrain, but their response is fast and they can then attain a first approximation to the problem with a short execution time (Hanna and Drivas, 1987; Hanna and Strimaitis, 1988; Reynolds, 1992; Delaunay, 1996; Gavelli et al., 2008; Long et al., 2009).

### 2.1. Scenario description

We have taken Chicago as scenario of the case study, because Dr. Hanna and his collaborators kindly allowed us to use their data and

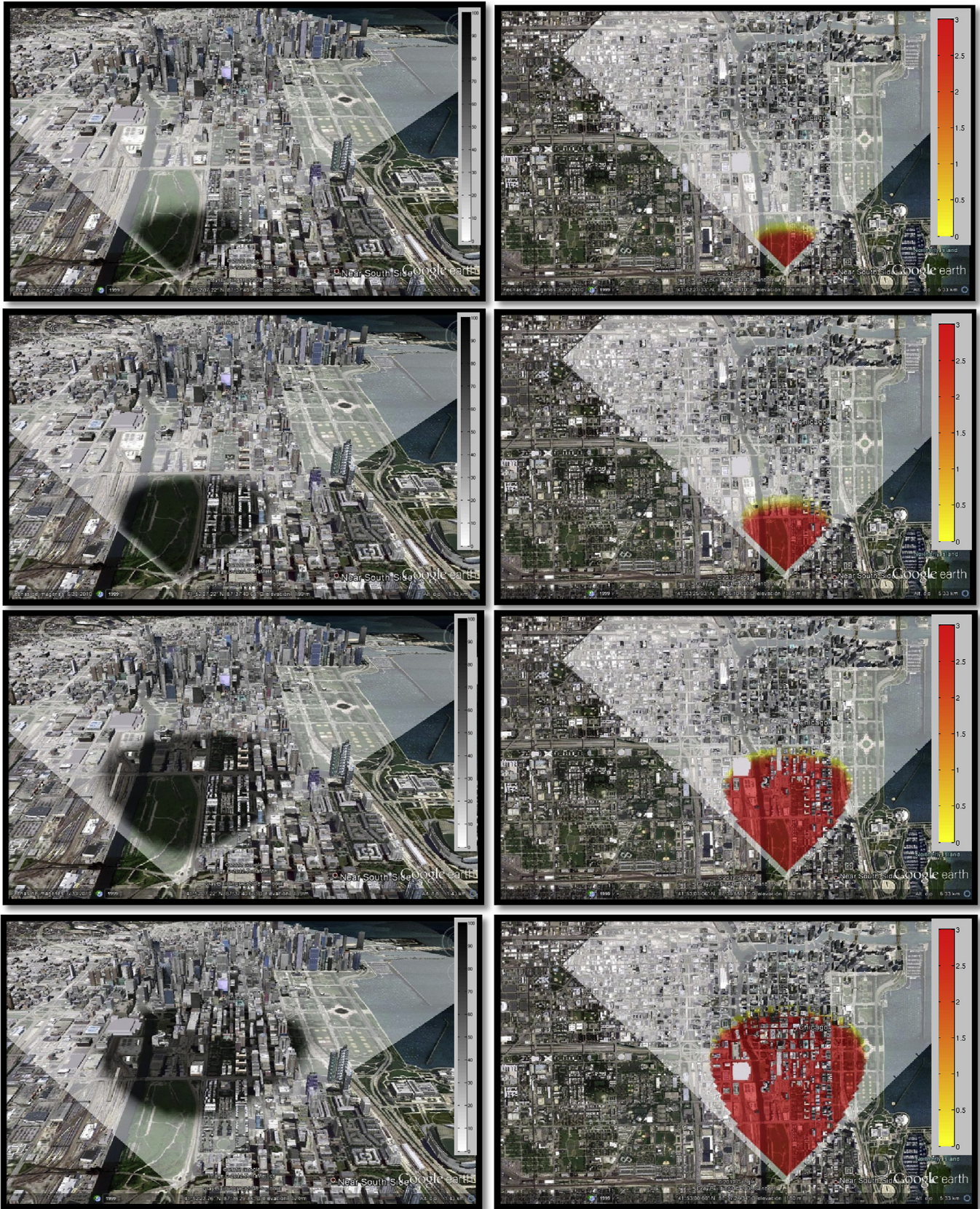


Fig. 4. D-M coupled system. Representation of the evolution of the toxic cloud (1st column) and maximum damage regions (2nd column) on a satellite image provided by Google Earth (2011), where 0.31 ppmv contours are shown, for  $t = 200, 400, 800$  and  $1200$  s;  $t$  is the time after the chlorine release starts.

runs with the CFD FLACS model (Hanna et al., 2009), as we already mentioned. They chose the source location (N 41.860283, O 87.630733) at an important railway junction, near downtown Chicago. The scenario is real, but the release of pollutants to atmosphere was purely hypothetical. As Fig. 1 shows, the emission context is a plain open terrain around the source, composed of grass, trees, bushes and sand/gravel areas. Hanna et al. simulated a leak of pressurized chorine from a tank on a freight train through a 10 cm diameter hole. A 689.48 KPa tank pressure is assumed at a 25 °C temperature. Chorine was released during 5 min at a 225 kg s<sup>-1</sup> rate. The atmospheric conditions were supposed stable with 3 m s<sup>-1</sup> light winds. As initial condition a vertical velocity gradient corresponding to a logarithmic law was selected. More details about the Chicago scenario can be found in Hanna et al. (2009). The plume is transported northwards to a region with many buildings, usually tall, with a 3949 inhabitants per km<sup>2</sup> population density (Wendell Cox Consultancy, 2012). The computational mesh cells have a 5 km N–S times 2.5 km E–W size at a 500 m height, totalizing  $9 \times 10^5$  cells for the D-F coupled system, and square cells with 5 km sides, at a 500 m height, totalizing  $5 \times 10^5$  cells for the D-M coupled system.

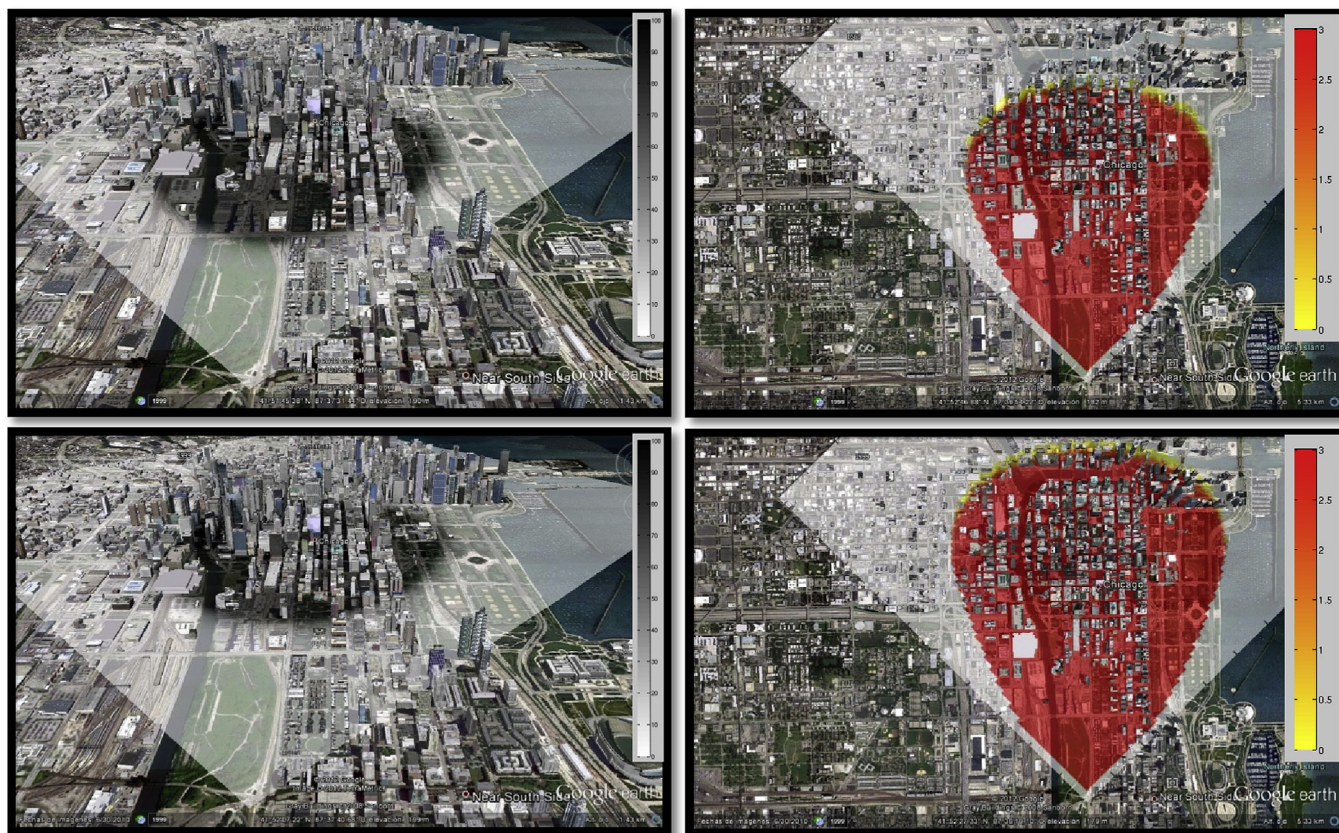
We focus on chlorine for several reasons. On the one hand, chlorine is one of the most widely used chemicals in industry; besides, as it is 2.5 times as heavy as air, it forms a dense cloud that remains close to the ground when moving. Due to the presence of buildings and other structures, sophisticated algorithms are required for computations to be useful for an accurate prediction. The body's response to chlorine inhalation depends on the concentration and on the total exposure time, and can range from sensory detection to sensory irritation and bronchial spasm

reflex to death by pulmonary edema or lack of oxygen during an asthma attack. Amore and Hautala (1983) concluded that the odor threshold (sensory detection) is 0.31 ppmv, and a range of 0.2–0.4 ppm has been reported in other studies (Fauske and Epstein, 1988; Ruiz Boada et al., 2003; National Research Council, 2004; MANHAZ, 2006; Hansen et al., 2007). DDC will use the AEGL index, due to its availability and priority in the hierarchy mentioned in the Introduction. AEGL values for chlorine can be found in Table 1, which shows the relationship between exposure time values and concentration values, associated with a health effect. The AEGLs have been developed primarily to provide guidance in situations where there can be a rare, typically accidental exposure to a particular chemical that can involve the general public.

## 2.2. Description of coupling

In order to coupling DDC with the other two models, DDC uses as input data the estimated concentration at each mesh cell on the plane  $Z = 1$  m, where  $Z$  is the height over the terrain level. Potential adverse health effects are estimated by means of the toxic load formula, which relates concentration and exposure time. Therefore, DDC estimates the adverse health effect on the population exposed to the toxic cloud. A 30 s time step was employed for both models.

By the way, an attractive feature of DDC, which will not be developed in this work but is worth mentioning, is the possibility of intersecting and superposing demographic layers with outputs of the couplings. This allows us to know the size of affected population and the characteristics of the information associated with demographic layers.



**Fig. 5.** D-F coupled system. Representation of the evolution of the toxic cloud (1st column) and maximum damage regions (2nd column) on a satellite image provided by Google Earth (2011), where 0.31 ppmv contours are shown, for  $t = 1600$  and  $2000$  s;  $t$  is the time after the chlorine release starts.

3. Results and discussion

Figs. 2–5 show data outputs of the coupled systems D-F and D-M for the Chicago scenario, according to the description in Section 2.1. These figures represent snapshots of the continuous simulation of the coupled systems, and show regions bounded by a 0.31 ppm concentration for the toxic cloud and no adverse health effects. Although both couplings show that the toxic cloud spreads over more than 1000 m windward from the emission source during the first 400 s, only the D-F coupling detects that the chlorine cloud travels faster and less diluted through plain and open terrain than through regions with buildings. Besides, the turbulent mixing near the densely built area that the cloud finds during its displacement, bounding its spread downwind, is detected only by the D-F coupling. As can be seen in Figs. 2 and 3, the spread of maximum and minimum regions is mostly restricted to a 2500–3000 m windward front (where tall buildings predominate). On the other hand, in the D-M coupling system the toxic cloud moves uniformly without interacting with obstacles and/or terrain and does not take into account the atmospheric turbulence, and only in the D-F coupling it is observed that eventually a gas volume becomes trapped in a southwest area, among tall buildings acting as trapping areas.

Remark that the representation of the toxic cloud shows time-averaged concentrations, using always the same time step.

As can be seen in Figs. 2–5, the DDC simulations shown in the second column represent regions according to a (dimensionless) scale of HEL. The range,  $0 \leq \text{HEL} < 1$  represents exposure levels that would produce a light odor, taste or other light sensorial irritation ( $\text{HEL} = 0$  corresponds to 0.31 ppmv odor threshold). The range  $1 \leq \text{HEL} < 2$  represents exposure levels that would affect the population at large (including susceptible people such as children, asthmatic and elderly people, and people with other illnesses). These effects are transient and reversible once the exposure ends. For  $2 \leq \text{HEL} < 3$  the above population could experience serious and/or irreversible lasting effects and their ability to escape could be inhibited. For  $\text{HEL} = 3$ , the population may experience life-threatening effects and might die. Finally, each integer HEL between 1 and 3 corresponds to the levels 1, 2 and 3 of the AEGL presented in Table 1.

In Table 2 the sizes of the maximum and minimum damage regions are presented under different ranges of HEL for the different times of simulation of the D-F and D-M coupled system. The time is counted from the start of the chlorine release.

A first view of Figs. 2–5, and of Table 2, shows us that for any simulation time from the start of the release of chlorine the greatest damage level predominates in more than 85% of maximum and minimum regions, that is,  $\text{HEL} = 3$ , closely related to severe effects on health or even to death. Such situation is directly connected with the magnitude of chlorine release. For such reason, we focus the discussion of our results on the total surface of the maximum and minimum regions, without discrimination of damage level, despite the fact that in Table 2 we have detailed information of that.

From the analysis of Fig. 6, we can see that, until a 400 s simulation time, the coupled system D-M covers a larger area than the coupled system D-F. However, this situation reverses from then on, due to the fact that the D-F coupled system has better descriptive properties: the toxic cloud simulated with such coupled system detects dispersion in places such as streets that the coupled system D-M is unable to represent.

On the other hand, Fig. 6 shows that the growth rate of the maximum region, for the D-F coupled system, diminishes after an 800 s simulation time. This time matches the time that the cloud spends passing through tall buildings which bound its spread downstream. Conversely, the D-M coupled system maintains an approximately constant growth rate of the maximum region area,

Table 2

D-F and D-M coupled systems. Area of the maximum and minimum damage regions according to ranges of HEL. Maximum Damage Region (MAX. D.R); Minimum Damage Region (MIN. D.R).

Time (s)	HEL	D-F		D-M	
		MAX. D.R.	MIN. D.R.	MAX. D.R.	MIN. D.R.
Area (km <sup>2</sup> )					
200	$1 \leq \text{HEL} < 2$	0.003	0.002	0.08	0.07
	$2 \leq \text{HEL} < 3$	0.005	0.005	0.03	0.04
	$\text{HEL} = 3$	0.082	0.082	0.29	0.29
	Total	0.090	0.090	0.4	0.4
400	$1 \leq \text{HEL} < 2$	0.034	0.033	0.13	0.03
	$2 \leq \text{HEL} < 3$	0.028	0.028	0.04	0.14
	$\text{HEL} = 3$	0.487	0.485	0.73	0.73
	Total	0.550	0.546	0.9	0.9
800	$1 \leq \text{HEL} < 2$	0.288	0.282	0	0
	$2 \leq \text{HEL} < 3$	0.106	0.087	0.22	0.21
	$\text{HEL} = 3$	2.040	1.900	1.87	1.88
	Total	2.434	2.269	2.09	2.09
1200	$1 \leq \text{HEL} < 2$	0.083	0.080	0	0
	$2 \leq \text{HEL} < 3$	0.168	0.159	0.26	0.25
	$\text{HEL} = 3$	4.000	3.720	3.23	3.14
	Total	4.251	3.958	3.49	3.39
1600	$1 \leq \text{HEL} < 2$	0.063	0.060	0	0
	$2 \leq \text{HEL} < 3$	0.319	0.405	0.26	0.25
	$\text{HEL} = 3$	5.370	4.890	4.77	4.4
	Total	5.752	5.355	5.03	4.65
2000	$1 \leq \text{HEL} < 2$	0.003	0.000	0	0
	$2 \leq \text{HEL} < 3$	0.364	0.414	0.26	0.24
	$\text{HEL} = 3$	6.250	5.720	6.43	5.66
	Total	6.617	6.134	6.69	5.9

due probably to the fact that, atmospheric conditions being constant, it has no interaction with obstacles.

Fig. 7 shows the difference between values of maximum and minimum regions. This concept is closely related to the velocity of the toxic cloud, because the estimated minimum damage becomes zero in those cells where the concentration is less than a certain threshold value given by the DDC boundary conditions (Acquesta et al., 2011).

As the emission of the source is continuous, there are always high concentrations around it and therefore up to 400 s simulation

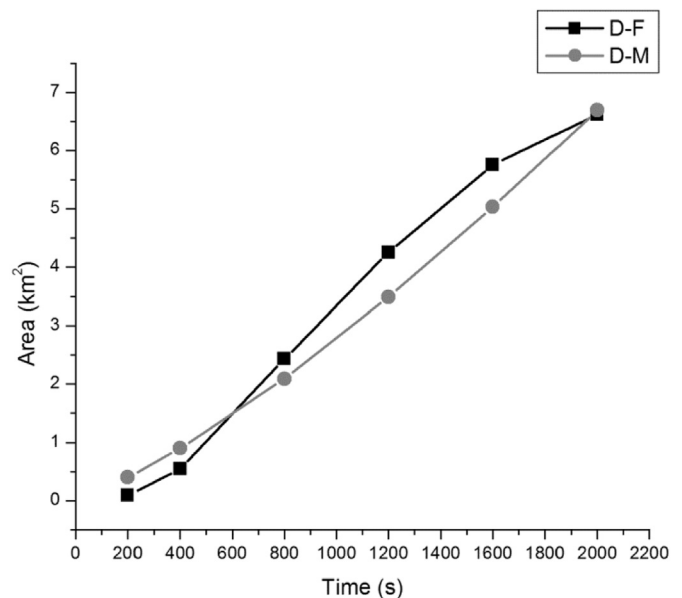
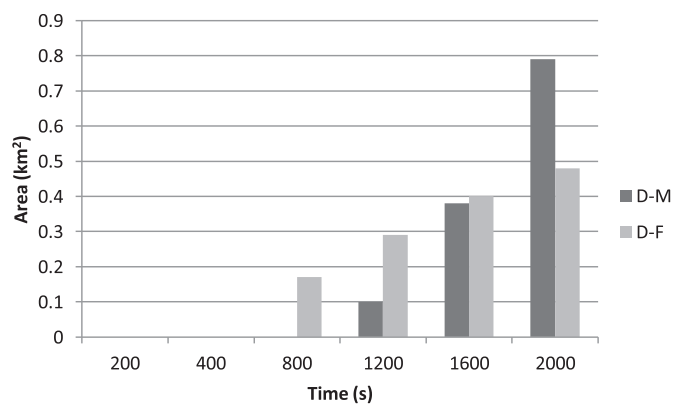


Fig. 6. Areas of maximum and minimum damage regions for the D-F and D-M coupled systems.



**Fig. 7.** Analysis of areas of maximum and minimum damage regions: difference between the size of maximum and minimum regions as time passes by for both coupled systems, where time is the exposure time after the chlorine release starts.

time the difference between the maximum and minimum covered areas is small. However, from an 800 s simulation time on, the coupled system D-F shows an important difference between maximum and minimum regions, provided in principle by the velocity of the cloud over the open area; the growth rate (with respect to the D-M coupled system) is small due to the constraint created by the densely built zone. Conversely, the D-M coupled system simulates the velocity of the cloud taking into account only the mean atmospheric velocity field, without considering the complexity of the terrain.

Finally, with the present example we pretend to analyze the importance of presented coupled systems for planning tools and emergency response in cities. The results presented show the descriptive character of D-F, however the simulation CPU clock times are large because many equations must be solved for each time step.

Hanna et al. (2009) explain in his work that the first 850 s of the simulation with FLACS was performed with the dense gas effects accounted for, and the simulation CPU clock time was 3 days on a PC with a single 3 GHz processor with 4 GB of RAM. However, after 850 s a neutral gas assumption was applied, and the next 2150 s of the simulation took less than 1 h of CPU clock time.

Moreover, D-M is an excellent tool to emergency response in real time, since the D-M simulation was performed in a few minutes by low numerical complexity.

#### 4. Conclusions

The D-F and D-M coupled systems constitute a very interesting tool for risk analysis, because knowing at each time step the affected regions and the health effects level supplies the decision makers the relevant information to be employed for getting an efficient response in a chemical emergency. These couplings allow us to extract conclusions about the time available for evacuating those people who would be reached by the toxic cloud in the near future, about how many inhabitants will need immediate medical assistance (according to the degree to which they are affected) and about how much logistics will be required to respond to an emergency, among other things.

With the present example we pretend to analyze the importance of presented coupled systems for planning tools and emergency response in cities, because we assume that an improvement in planning is closely related with early warning systems, contributing substantially to improvement in an emergency response.

The D-F coupled system, which includes a complex CFD model, can very accurately describe the scenarios; however, due to its

complexity, its high computational time cost and the huge amount of data that it requires, its application in real time for a fast emergency response is unfeasible. Nevertheless, D-F is an excellent tool in the planning stage of emergencies and disasters.

On the other hand, to provide efficient real time responses to emergencies, the D-M coupling is appropriate, due to its short execution time; it therefore supplies a fast and accurate estimation of the evolution of the toxic cloud and of the regions that could be affected.

Finally, in this work we showed how the description level of a model is based on its complexity and on its execution time and, therefore, on its correct application in emergencies and disasters management.

We think that, even when a dispersion model may offer very accurate details of the flow displacements, the output is not sufficient in emergency situations if an analysis is not included that takes into account the toxicological aspects of the exposed population. In that sense, it is essential to estimate where and when the toxicological levels, be they AEGL, ERPG and/or TEEL, are surpassed.

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