CHEMICAL ENGINEERING TRANSACTIONS
VOL. 26, 2012
Guest Editors: Valerio Cozzani, Eddy De Rademaeker

ISBN 978-88-95608-17-4; ISSN 1974-9791

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet

DOI: 10.3303/CET1226090

Consequences Assessment of an Accidental Toxic Gas Release Through a CFD Tool: Effect of the Terrain and Major Obstacles

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The main aim of this study is the establishment of a new methodology for the assessment of terrain and structures geometry effects on gas dispersion. Significant obstacles (such as the plant structures, buildings, or the terrain elevation) play a major role in gas dispersion, due to the eddies, wakes, stagnation and recirculation points they can introduce. A comparison between CFD simulations and integral model predictions have been worked out for a realistic case-study in order to point geometry role in gas dispersion.
Moreover, obstacles and terrain geometries are often not available in a suitable format. The proposed methodology uses easy-accessible data (such as SRTM data and geo-referenced aerial photography) to work out the required inputs, to reduce the time and cost associated to CFD modelling and make it practically applicable in industrial cases (design of new installations or assessment of existing ones).

1. Introduction

In safety studies concerning consequences analysis of gas releases, integral methods are widely used in order to obtain previsions of the dimensions of the area involved by the dispersion (Bernatik and Libisova, 2004). They are easy and low time-consuming tools, but they are liable to some deficiencies (one-dimensional modelling) and obey to certain assumptions. On the other hand, powerful computational tools based on fluid dynamics methods have recently been developed (Computational Fluid Dynamics, CFD) allowing for an integrated approach on complex scenarios and/or physicochemical phenomena. CFD codes perform three-dimensional computations of fluid properties variation, turbulence modelling, chemical reactions, in addition to accurately represent the geometry of the flow field. However, this level of details could be time-consuming.
The prediction of an accidental gas release, in term of both people and area involved by a toxic or flammable cloud dispersion, is of paramount importance for the definition of safety plans and actions to be undertaken to avoid and/or mitigate the consequences of such an accident; recent works (Pontiggia et al., 2011; Vianello et al., 2011; Cozzani et al., 2011) have pointed out that CFD approach cannot be given up when geometrically complex scenarios are considered. Nevertheless, geometry data are generally not available in a suitable format: incompatible 3D geometry encoding, too small level of

Please cite this article as: Pontiggia M., Busini V., Gattuso M., Uguccioni G. and Rota R., 2012, Consequences assessment of an accidental toxic gas release through a cfd tool: effect of the terrain and major obstacles, Chemical Engineering Transactions, 26, 537-542 DOI: 10.3303/CET1226090

details or lack of information, usually require time-consuming procedures for geometry conversion, clean-up or building from scratch.
In this work a new methodology for geometry creation and importation in a CFD simulation has been worked out based on easy-accessible data (SRTM data and geo-referenced aerial photographs). A realistic gas dispersion case study has been assessed in order to highlight the effect of imported geometries (obstacle and terrain elevation) on the dispersive phenomena. Results have been compared to integral model predictions for the same release, in order to highlight the limitation of this kind of models dealing with complex geometries. Two commercial suites, a general purpose commercial CFD code and a widely used integral model were used for the comparison.

2. Theoretical background and methodology

CFD codes solve the Navier-Stokes equations, together with specific model equations, such as energy balance, species diffusion, turbulence, etc. Accordingly to literature (Luketa-Hanlin et al., 2007), standard k-ε model for turbulence has been used; this model is well-known for the good arrangement among results accuracy, simulation stability and computational time required. In order to account for atmospheric stability, the ASsM approach has been adopted: as discussed elsewhere (Pontiggia et al., 2009), the ASsM approach requires an additional source term in ε balance equation, S_ε, to assure consistency between k-ε model predictions and Monin-Obhukov similarity theory profiles across the whole integration domain for neutral and stable stratification. Fully developed vertical profiles of velocity, temperature, turbulence intensity and dissipation rate have been used as boundary conditions at the inlet boundary, accordingly to the Monin-Obhukov similiraty profiles (Alinot and Masson, 2005).

3. 3D geometry building

Geometry data required for the set-up of a gas dispersion simulation are constituted by terrain elevation data and obstacle features.
Terrain information are obtained from the Shuttle Radar Topography Mission (SRTM) database, which is the most complete high-resolution digital topographic database publicly available. SRTM is available at the US Geological Survey's EROS Data Centre for download, and cover over 80 % of the Earth's land surface between 60° north and 56° south latitude, with a resolution of approximately 30 m for the US and 90 m for global coverage. Information are stored in the Digital Terrain Elevation Data (DTED®) mapping format. A specific routine has been developed in order to automatically convert the DTED® format in a set of point coordinates suitable for data importation in the CFD graphic pre-processor. In Figure 1 the domain selected for the case study is reported.
Obstacles can consist in plant structures, buildings, architectonical barriers (like confinement walls or earthworks), and natural barriers (like densely packed wood). 3D geometries of plant structures, when available, are generally provided with a too small level of detail: small features, while requiring a finely refined computational grid, and therefore very high computational loads, do not represent a significant contribution for gas dispersion calculation.

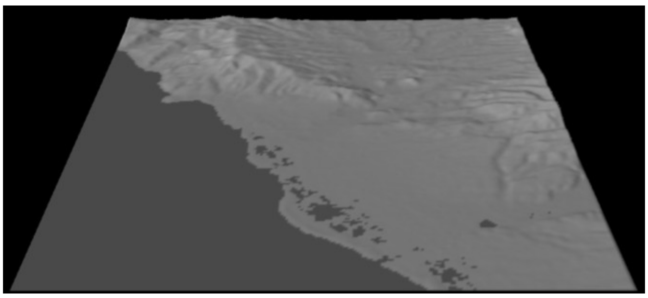

Figure 1: Domain selected from SRTM data for case-study simulation

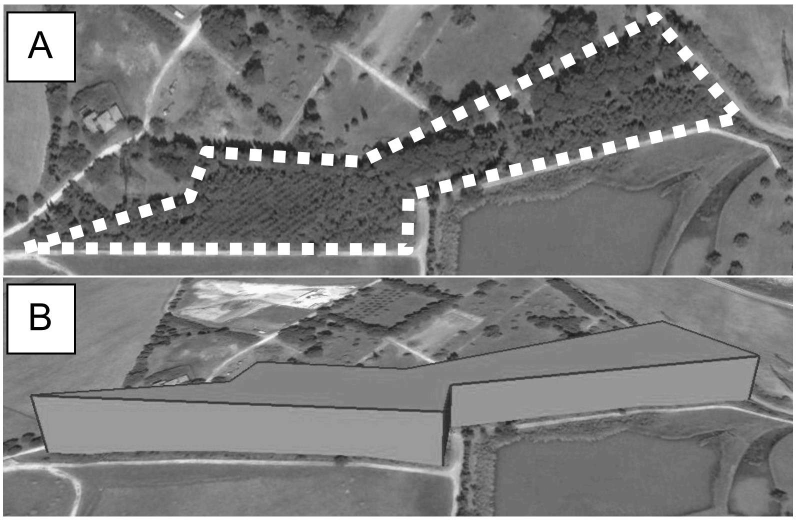

Figure 2: Obstacles importation procedure of a densely packed wood: (A) outline is selected on the aerial photography and (B) height is set to obtain a solid 3D geometry

As a result, a time-consuming procedure is usually required to clean-up the available geometry and speed-up the calculation. On the other hand, geometry of urban buildings and natural barriers is usually not available. In order to produce a suitable input for obstacle representation, geo-referenced aerial photographs have been used. The shape of the selected obstacle can be highlighted directly on the photograph (Figure 2A) and a specific routine has been developed in order to translate vertex points in a set of coordinates; these coordinates are subsequently imported in the CFD graphic pre-processor. An average obstacle height is then used to construct the solid geometry (Figure 2B).
Based on the analyst experience and detail requirement, obstacles can be reproduced with increasing level of detail (splitting obstacle on the base of different heights, clustering/un-clustering buildings and structures and so on).
In Figure 3 the obstacles used for the case study have been reported.

4. Case study

The proposed procedure has been assessed through analysis of a realistic case study, similar to the ones that can be found in the practical experience of risk analysis.

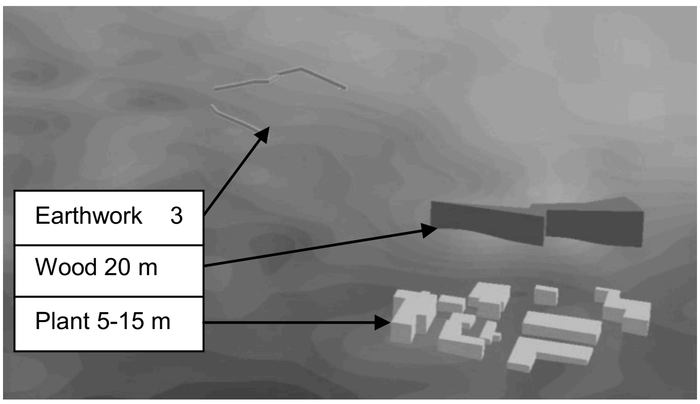

Figure 3: Obstacles used for the realistic gas-dispersion simulation, involving the Plant structures, a densely packed wood and an earthwork; average obstacles height is also reported.

Table 1: Discharge parameters calculated with DNV PHAST

Step	t start [s]	t end [s]	Liquid fraction [-]	Temperature [°C]	Velocità [m/s]	Mass flowrate [kg/s]
Step 1	0	180	0.01	-34	286	3.3
Step 2	180	210	0	-34	276	2.8
Step 3	210	255	0	-15	244	1.9
Step 4	255	300	0	32	129	0.7
Step 5	300	310	0	41	95	0.5

The case selected is as an accidental release of Chlorine from a 60 mm hole in a plant piping (operative conditions: 3 barg, 50 °C) releasing within the plant, with an external environment characterised by presence of obstacles (tree lines and some orographical feature) but not to a level of congestion to make the use of a 3D modelling clearly mandatory to obtain a realistic result.The pressurized chlorine source term has been simulated using DNV PHAST and discharge conditions have been applied at the chlorine inlet boundary in the CFD simulation, in order to ensure a consistent discharge mechanism for both the integral model and CFD dispersion analysis. Discharge data are resumed in Table 1. Liquid fraction at Step 1 has been neglected in CFD simulation.
Chlorine release is placed at 6 m above ground and directed downward (towards the ground). A wind speed of 2 m/s and a stability class F have been selected, in order to maximize the cloud dimension. Three different wind directions have been considered (summarized in Figure 4, both on the terrain map and on the simulation geometry):

- North-West, directed towards the open field and the minimum terrain slope;
- North, directed towards the Wood and the increasing terrain slope;
- South, directed towards a valley.

Results have been provided in terms of iso-curves at IDLH concentration (Figure 5) and iso-Probit curves (Figure 6). It is reminded that the "Probit" is a variable relating the dose to the vulnerability: a specific routine has been implemented in the CFD core solver in order to integrate the concentration over the time for each cell in the simulation domain in order to calculate the toxic dose; the Probit value is calculated as a logarithmic function of the toxic dose.
In Figure 5 ideal cloud centre-lines are also highlighted: centre-lines have been worked out accounting for wind direction and release point. It should be noted that the plant buildings wake effect, depending on wind direction, create a strong recirculation thus substantially shifting the effective release point: chlorine dispersion takes place from all the building wake rather than from a punctual source. This effect is particularly evident in NW and S wind directions (Figure 5A and 5B).
Terrain elevation is, on the other hand, responsible of the shifting of the cloud direction: referring to Figure 1, elevation raises form the plant position towards north and decreases towards south.

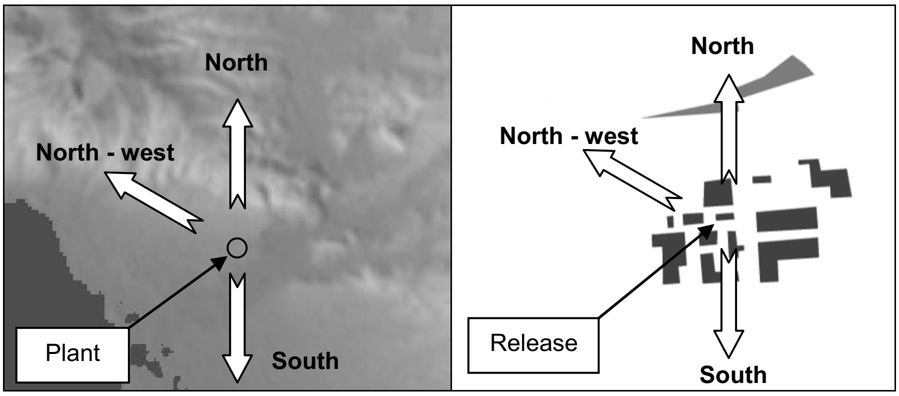

Figure 4: Wind directions (white arrows) analyzed in the CFD simulations

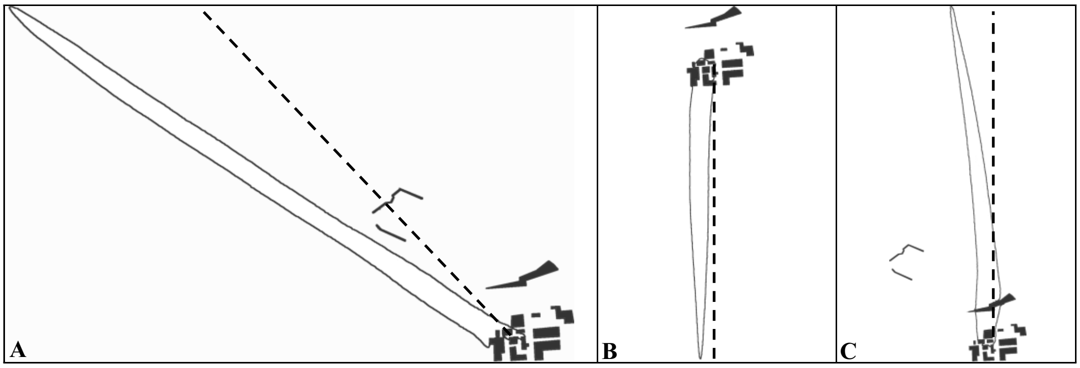

Figure 5: Iso-concentration curves at IDLH concentration for each wind direction, (A) North – West, (B) South, (C) North; dotted lines represent ideal cloud centre-line based on wind direction

Cloud centre-line is consequently shifted towards West in Figure 5A (wind blowing to NW) and it is bend in Figure 5C (wind blowing to N). No significant direction shift is observed in Figure 5B (wind blowing to S), since dispersion direction is aligned with decreasing terrain elevation.

The wood does not play a major role for the IDLH concentration cloud shape: the cloud is partially stopped and it slightly expands in the lateral direction before flowing over the wood, but, dealing with 10 ppm concentration threshold, gas buoyancy is almost neutral and the cloud is roughly twice as high as the obstacle, thus producing limited consequences. The effects of the wood on cloud dispersion is mainly highlighted by iso-Probit curves (Figure 6B): Probit values associated with higher concentrations (Probit greater than 1), and, consequently, smaller cloud heights: the concentred clouds is therefore blocked by the obstacle and cannot step over it.

Distances at IDLH and Probit values are listed in Table 2 along with results calculated with integral models. Dealing with wind blowing to NW, only the plant buildings wake effects influences damage distances, and CFD results are roughly 50 % of the integral model predictions, both for IDLH and Probit. More severe distances reduction are observed for wind blowing to N and S: in the former direction the wood heavily influences Probit, with a distance reduction up to 80 %. IDLH distance is less influenced by the wood, but the terrain slope bends the cloud with an overall reduction of about 60 %. In the south direction, due to the buildings and the wood acting as upstream obstacles and due to the the valley, IDLH is reduced up to 70 % and Probit up to 80 % of the integral model results.

As expected, the use of CFD modelling gives substantial differences with respect to the results obtained by the integral models (as widely used in Risk Analyses) where important obstacles are present, as it can be seen in the case of wind blowing to South direction in Table 2.

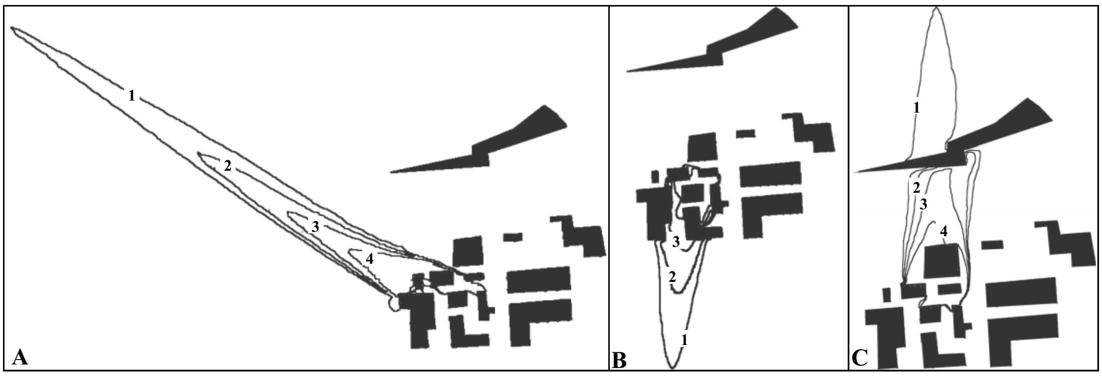

Figure 6: Isoprobit curves for each wind direction, (A) North – West, (B) South, (C) North; Probit values are reported with labels relevant to each Isoprobit curve.

Table 2: Distances comparison (Distances are expressed in [m])

Direction	**IDLH**	**Vulnerability 0 % Probit = 0**	**Vulnerability 0.0035 % Probit = 1**	**Vulnerability 0.15 % Probit = 2**	**Vulnerability 2.5 % Probit = 3**
North – West	3480	1241	721	472	309
North	2840	602	303	267	158
South	211	474	289	186	103
Integral model	6615	2450	1588	1023	646

However, a significant reduction with respect to the results obtained with analytical models is obtained also when the dispersion is directed towards an open terrain field (N and NW directions) where no major obstacles are present. In these cases the effect of the terrain slope and of the tree line is such to reduce by a factor 2 to 3 the results obtained with analytical models.

5. Conclusion

In this work a new methodology for terrain and geometry importation in CFD simulation has been worked out, relying on accessible data and presenting a case study of a realistic toxic gas release.
Geometry and terrain elevation have proved to be responsible of heavy variation to effective release point, cloud centre line direction and damage distances. Strong distance reductions have been observed (up to 80%) with respect to integral model predictions where the dispersion is affected by plant buildings. However, significant distance reductions are observed also where the dispersion is directed to open field, where no apparently important obstacles are present.
In cases where, as in the example shown here, the damage distances predicted by analytical models are very high, the use of CFD modelling even when no apparently significant obstacles are present can therefore provide the analyst and the plant owner with realistic damage distances, much more manageable from the point of view of the emergency planning and the local authorities and population concerns.
One of the main obstacles against the use of CFD modelling, that is the time consuming activity necessary for creating the 3D model of the surrounding environment, can be overcome by the methodology presented here based on publicly available terrain data,

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