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Hazardous gas releases in urban areas: Assessment of consequences through CFD modelling

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ABSTRACT

Release of hazardous materials in urban areas is a major concern in industrial risk assessment. The presence of high population density in such areas multiplies the magnitude of the consequences. In urban areas, many buildings with complex geometries are involved leading to 3D flow fields that strongly influence gas dispersion. Representing such complex geometries simply but realistically in detailed simulation models can be cumbersome and often limit their utility. In this work, a methodology for the construction of 3D urban models and their importation into CFD models was developed through the access to spatial geodatabases, leading to a relatively fast and simple domain design technique. Moreover, since the magnitude of consequences depends on the absorbed dose which in turn depends on both concentration and exposure time, a simple methodology for dose evaluation was developed and implemented in a CFD code that enables the estimation of regions with a given death probability. The approach was developed and applied to a case study with different atmospheric stratification conditions. The results were then compared with those obtained using integral models. It was found that integral models can both overestimate and underestimate the magnitude of consequences related to hazardous material releases in urban areas.

1. Introduction

Accidents involving hazardous material releases constitute an important concern in industrial- and transport-related risk assessment. They can lead to consequences of large magnitude since the hazardous cloud can spread widely across distances of kilometres and pose a hazard to both human health and the environment.

Urban areas are easily involved in hazardous gas releases not only because many industries form part of urban agglomerations as a consequence of the growth of cities, but also because of the transport of hazardous materials by road and rail. The latter, while usually involving quantitatively smaller amounts of substances, still are a serious hazard both in terms of safety and security since their mitigation and prevention systems are less effective; moreover, transport vehicles transit through areas with highly vulnerable populations such as schools and hospitals. Besides, such incidents in urban areas present an extremely hazardous scenario in terms of the magnitude of consequences, exacerbated by the high population densities present in these areas.

Furthermore, urban areas are characterized by complex geometries resulting from the large number of buildings of varied shapes and dimensions. These obstacles strongly influence wind velocity since wakes, stagnating zones, recirculation, and preferential paths that may be present or arise can significantly complicate the scenario in simulations. Representing such complex geometries simply but realistically can prove cumbersome and often limit the utility of detailed simulation models.

Accidental releases of hazardous gases have been the subject of studies since the early 1980s and were investigated by the executing trials of large spills and development of numerical models; these models continue to be currently utilized for loss prevention purposes in chemical- and process industries [1,2], and some of them, like DEGADIS, SLAB, ALOHA, and UDM, are among the most popular and widely used models in safety engineering applications [3,4]. These are lumped-parameter models, usually pseudo one-dimensional, and account for some physical phenomena using semi-empirical relationships whose parameters have been tuned on field test data [5]. Since the experimental setup of these field trials usually does not involve any particular obstacle, these models can provide reliable results only in open field conditions, that is, when almost no obstacles are present in the cloud region.

To analyze the effects of multiple large obstacles on gas dispersion, computational tools based on computational fluid dynamics (CFD) can be utilized to simulate the complex urban geometries involved. This approach enables performing full three-dimensional analysis, and predicting velocity, temperature, and concentration

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Nomenclature

c_p	constant pressure specific heat coefficient (J/kg K)
c_v	constant volume specific heat coefficient (J/kg K)
$C_{1,\varepsilon}$	k–ε model specific constant
$C_{2,\varepsilon}$	k–ε model specific constant
$C_{3,\varepsilon}$	k–ε model specific constant
C_μ	k–ε model specific constant
$\bar{g}$	gravitational acceleration (m/s^2)
G_b	turbulent generation term due to buoyancy (kg/m s^3)
G_k	turbulent generation term due to shear stress (kg/m s^3)
k	turbulent kinetic energy (m^2/s^2)
k_T	heat exchange coefficient (W/m K)
K	Von Karman constant
p	pressure (Pa)
S_ε	user-defined ε-generation term (kg/m s^4)
t	time (s)
T	temperature (K)
T_*	friction temperature (K)
u_i	i-th component of the velocity vector (m/s)
u_*	friction velocity (m/s)
$\bar{v}$	velocity vector (m/s)
x_i	i-th component of the coordinate vector (m)
Y_M	turbulent generation term due to compressibility (kg/m s^3)
z	height above ground (m)

Greek letters

ε	turbulent dissipation rate (m^2/s^3)
μ	molecular viscosity (kg/m s)
μ_T	turbulent viscosity (kg/m s)
ρ	density (kg/m^3)
σ_k	Prandtl number for k
σ_ε	Prandtl number for ε
$\bar{\bar{\tau}}$	stress tensor (N/m^2)
ϕ_m	semi-empirical function for atmospheric stability
ϕ_ε	semi-empirical function for atmospheric stability

fields in the integration domain. While this procedure might ensure more detailed results, it requires a large amount of resources both in terms of CPU time and analysts' skills.

Particular attention has to be paid in CFD simulations to turbulence modelling. The effect of turbulent fluctuations can be modelled by the RANS (Reynolds averaged Navier–Stokes) approach, or fully simulated by direct numerical simulation (DNS). The DNS places very large demands on resources and, nowadays, is applied only to very simple cases. An intermediate solution is to use large eddy simulations (LES) that simulate only larger eddies and use models for simulating the effects of isotropic dissipating eddies. Although LES is less demanding than DNS, it is still quite demanding in complex scenarios. Consequently, RANS remains a good compromise between result accuracy and computational efforts. The most popular closure model for turbulence effects in the frame of the RANS approach is the k–ε two-equation model, since it ensures reasonable results and good stability [6].

CFD results have been successfully validated against experimental field data [7,8] and lab-scale trials [9]. Some works have also been carried out in geometrically complex scenarios, involving few obstacles [10,11], or idealized urban canopies [12]. Realistic urban areas have been studied, analyzing the flow field in Hong Kong [13] and Manhattan [14]; in both these studies, flow of motions around buildings have been simulated while [15] the dispersion of a tracer gas has been also analyzed and the results obtained have been compared using integral models and hybrid models to assess concentrations in fields. However, where atmospheric stability was concerned, only wind-, temperature-, and turbulence profiles were imposed at the inlet boundary, without verifying whether the turbulence closure model maintains the profiles imposed at the wind inlet boundary throughout the integration field thereby assuring the correct representation of the physical phenomena involved.

In this work, realistic gas dispersion in a geometrically complex environment (i.e. urban terrain) was studied utilizing CFD tools, enabling a full 3D analysis of the effects of the obstacles in the impact area of the hazardous cloud. In particular, as a case study, ammonia dispersion was studied in the Lecco municipality, which is a small city located in a highly industrialized region in the north of Italy. The influence of the atmospheric stability was accounted for using the ASsM approach [16] which ensures consistency of the turbulence closure model with the Monin-Obhukov similarity theory. Moreover, since consequences of toxic gas dispersion mainly depend on the absorbed dose, a dedicated methodology was implemented in the CFD code for absorbed dose evaluation.

To represent simply but realistically the geometry of the urban buildings, a dedicated procedure was developed for the reconstruction of the 3D city model from the available topographic database and its direct import into the CFD code, since the realistic representation of all the buildings present in the integration domain represents one of the key problems when urban environments are involved.

Finally, the results obtained were compared with those computed using an integral dispersion model, commonly used in industrial risk assessment [3,4]. This enabled verification of the performance of integral models when dealing with complex environments.

2. Theoretical background

CFD codes solve Navier–Stokes Eqs. (1) and (2) together with specific model equations, such as energy balance (3), species diffusion, turbulence, etc.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \nabla \cdot (\bar{\bar{\tau}}) + \rho \vec{g} \tag{2}$$

$$\frac{\partial (\rho c_v T)}{\partial t} + \nabla \cdot (\rho \vec{v} c_p T) = \nabla \cdot (k_T \nabla T) \tag{3}$$

In the equations above, ρ is the density, t the time, v the velocity, p the pressure, τ the shear stress, g the gravity acceleration, c_v and c_p the specific heats, T the temperature, and k_T the thermal conductivity.

In this work, the k–ε model was used to represent the effects of turbulence. This model introduces two additional transport equations for turbulent kinetic energy k (4) and turbulent kinetic energy dissipation rate ε (5), respectively [17]:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon - Y_M \tag{4}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{\varepsilon 1}\frac{\varepsilon}{k}(G_k + C_{\varepsilon 3} G_b) - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} + S_\varepsilon(z) \tag{5}$$

where u_i is the velocity component along x_i direction, μ the viscosity, μ_T the turbulent viscosity, G_k the shear stress-related turbulent