



# CFD analysis of dense gas dispersion in indoor environment for risk assessment and risk mitigation

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## ABSTRACT

Environmental risks are inherent in the operation of any complex chemical process industry. The indoor release of hazardous chemicals that are denser than air is a topic of special concern, since dense clouds tend to persist at ground level or human breath level which leads to a magnification of their harmful potential. In the present work, we propose a computational fluid dynamics (CFD) based model for indoor risk assessment considering accidental release of a sustained, small, undetected leak of a dense toxic gas (chlorine) in an industrial indoor environment. Results from simulations show that the denser chlorine gas spreads like a liquid and flows all along the floor. At the same time, its concentration at a point away from the ground level increases slowly, thus showing that both stratification and dilution effects are present as the dense gas spreads. The implications of this spreading pattern from a risk assessment and risk mitigation point of view are discussed.

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## 1. Introduction

Environmental risk assessment is usually associated with open installations and open areas primarily because of the major risk awareness initiatives that have been created after the occurrence of major accidents involving emission/discharge of hazardous substances from chemical and process installations [1–3]. However, there are particular cases wherein the risk posed due to indoor operations/handling of chemicals needs to be assessed [4]. These units typically operate in a large building, in the form of a hangar, wherein the quality of the indoor air is an important criterion for the safety of the workers.

The indoor risk assessment process consists of the following three stages:

- Transport and advection modelling of the hazardous gas due to an accidental release,
- Estimation of the concentration of the gas, and
- Evaluation of the potential damage to the facility and the impact on its occupants.

Modelling the dispersion of a hazardous gas is the most critical step in indoor risk assessment. An inadequate model may lead to a

wrong estimation of concentration prediction and may impact negatively on both human and financial resources. In this context, one may note that traditional gas dispersion models are based on Gaussian distribution and have been developed for an instantaneous (puff) or a continuous (plume) release of hazardous chemicals into the atmosphere [5]. They predict the transport and dispersion of gases under a set of atmospheric conditions (weather, stability class, etc.) and consequently model their fate in the atmosphere. Blackmore et al. [6] gave an extensive review of fifteen hazardous gas dispersion models that were evaluated using field experimental data. Many models and methods are currently available to predict the discharge and dispersion of toxic or flammable gases in the open environment [7]. A few of these models have been modified to allow for the representation of the complex environment within the manufacturing plant or urban area in determining the impact of continuous release from a plant [8]. Lately, powerful simulation tools such as those based on computational fluid dynamics (CFD) have been brought into play to investigate a number of accident scenarios [9–12]. The state-of-the-art in open environment scenarios has advanced to such an extent that fairly accurate predictions of release patterns and their consequences can be made even in complex scenarios [13].

In the present work, we focus on models/methodology specifically developed for indoor risk assessment and that too in the context of dense gas dispersion. A dense gas is defined as any gas the density of which is greater than that of the ambient air through which it is being dispersed. The release to the atmosphere of

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hazardous materials that may form mixtures that are denser than the surrounding air is a topic of special concern for two reasons. Firstly, in unfavourable atmospheric conditions, these dense clouds form a dense layer at ground level which spreads over long distances before becoming passive [14]. Secondly, the dispersion of a denser-than-air cloud (whether due to the molecular weight of the emitted substance, the temperature of emission or the presence of aerosols) is fairly complicated and follows several hydrodynamic stages: an initial acceleration and dilution which is dependent on the release mechanism, followed by a period in which negative buoyancy predominates, and finally, after further dilution and/or heat exchange, the transition to a behaviour dominated by ambient turbulence (neutral flotation). Recently, attempts have been made to model such scenarios using CFD and related techniques [15–22]. In the present study, we present an improved approach in modelling these scenarios where the predicted spatio-temporal variation in the concentrations obtained from the simulations is linked with the evaluation of exposure risk levels of the occupants and the effectiveness of mitigation plans for the minimization/curtailment of these hazards. The use of such a computational model would provide valuable information for the safe design of the ventilation system and investigation of evacuation/mitigation measures.

Thus, the main objective of the present study is to develop a computational fluid dynamics (CFD) based model for the assessment of risk arising from an accidental, indoor release of a dense gas. In CFD, the fundamental equations describing the conservation of mass, momentum and energy balance are solved numerically for a given flow domain, initial and boundary conditions. The temporal and spatial evolution of the concentration field for the different species is found by solving a species transport equation on a computational grid. This can then be used to determine more accurately the three-dimensional, turbulent dispersion effects present in an indoor environment on the spreading pattern of a dense toxic gas and the associated risks. In the present study, this computational analysis is applied to the spreading of chlorine in an indoor environment and the advantages of this approach are highlighted. (It is expected that the model would be equally applicable for the dispersion of lighter-than-air gases; however, caution must be exercised because the present model does not include stratification-induced suppression of turbulence in its calculations.)

The arrangement of the rest of the paper is as follows. The computational model used to monitor the concentration of a hazardous gas species at a particular location and at a particular time is described in Section 2. It is applied in Section 3 to the case of a chlorine room to demonstrate its applicability for risk assessment following an accidental release. The computed concentrations of chlorine at select locations within the indoor environment are linked to the threshold risk levels to examine the consequences. The effectiveness of specific risk mitigation measures is investigated through further simulations in Section 4. Conclusions from the study are given in Section 5. The point is made that use of such simulations can provide valuable information for the efficient design of the ventilation system, for developing new designs for optimal operations, and for planning emergency evacuation measures.

## 2. Computational model

### 2.1. Modelling of the carrier gas

The flow of a Newtonian fluid (such as air and water) is governed by the continuity and the momentum conservation equations for isothermal flow, described by Eqs. (1) and (2), respectively:

Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (1)$$

Momentum balance:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \frac{\partial u_k}{\partial x_k} \right] + \rho g_i \quad (2)$$

Here,  $\rho$  is the density,  $u_i$  is the velocity component in the  $i$ th direction,  $p$  is the pressure,  $\mu$  is the viscosity of the medium,  $\lambda$  is the second coefficient of viscosity (the term involving this variable is assumed to be negligible) and  $g_i$  is the component of gravitational acceleration in the  $i$ th direction. In practical applications, the flow is invariably turbulent and all flow variables exhibit fluctuations. Resolving these fluctuations requires huge computational resources; the often-used approach is to smooth out these fluctuations using, for example, Reynolds time-averaging procedures, leading to Reynolds-averaged Navier-Stokes (RANS) equations. The time-averaged form of the momentum equation (Eq. (2)) for a constant density fluid can be written as [22,23]:

Momentum:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \nu \frac{\partial \bar{u}_i}{\partial x_j} - \overline{u_i u_j} \right] \quad (3)$$

This equation is similar to the non-time-averaged momentum equation (2) except for the appearance of the “Reynolds stresses”, viz., the term  $(\overline{u_i u_j})$  in Eq. (3). Typically, these Reynolds stresses vary highly and in a non-trivial way even for simple flows and their spatial and temporal dependence cannot be expressed in simple algebraic expressions. Without knowing how these terms vary, it is not possible to solve the time-averaged momentum conservation equation. Thus, turbulent flows require “turbulence closure” modelling. The simplest generic turbulence modelling is that of the  $k$ - $\varepsilon$  turbulence model in which the Reynolds stresses are described in terms of turbulent or eddy viscosity ( $\mu_t$ ) which itself is calculated in terms of two additional variables characterizing the turbulence fluctuations, namely, the turbulent kinetic energy ( $k$ ) and its rate of dissipation ( $\varepsilon$ ) [22,23].

Exact transport for these can be derived but only an approximate form of these, given below, is often solved

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k \bar{u}_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + \mu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j} - \rho \varepsilon \quad (4)$$

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(\rho \varepsilon \bar{u}_j) \\ &= \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} \left[ \mu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j} \right] - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \end{aligned} \quad (5)$$

where  $C_{1\varepsilon}$  and  $C_{2\varepsilon}$  are constants and  $\sigma_k$  and  $\sigma_\varepsilon$  are the turbulent Prandtl numbers for  $k$  and  $\varepsilon$  respectively. The turbulent viscosity is linked to the turbulent kinetic energy and dissipation via the relation,

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (6)$$

The model constants are given by

$$C_{1\varepsilon} = 1.44, \quad C_{2\varepsilon} = 1.92, \quad C_\mu = 0.09, \quad \sigma_k = 1.0 \text{ and } \sigma_\varepsilon = 1.3 \quad (7)$$

For a large number of flows, the above model gives satisfactory results and it has been used successfully for analysis of accident scenarios [13]; hence this model is used in the present study.

## 2.2. Modelling of dense gas dispersion

For risk assessment, it is necessary to determine the concentration of the hazardous species (which is a dense gas in the present case) within the indoor domain of interest. This can be done by treating the dense gas as a non-reacting scalar and solving the scalar transport equation. In this species transport method, the concentration of any particular species within the fluid mixture is obtained by solving a species conservation equation written in terms of the mass fraction of the species,  $Y_i$

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho u Y_i) = -\nabla \cdot J_i + S_{\phi_i} \quad (8)$$

where the last term is a source term, and  $J_i$  is the diffusion flux of the species  $i$ , which arises due to concentration gradient and is expressed in terms of the Fick's law. This approach can be used to determine the evolution of a tracer fluid, for example, to determine the mixing time in a tank [24]. The concentration of the tracer within the fluid domain is determined by solving Eq. (8) along with the mixture mass balance (Eq. (1)) and the mixture momentum equation (2). For turbulent flows, the time-averaged form of these equations are solved and the diffusion flux is computed as,

$$J_i = -\left(\rho D_i + \frac{\mu_t}{Sc_t}\right) \nabla Y_i \quad (9)$$

where  $Sc_t$  is the turbulent Schmidt number, taken to be close to unity, and  $D_i$  is the mass diffusivity. The first term on the right hand side of Eq. (9) accounts for molecular diffusion, while the second term accounts for turbulent diffusion.

In a mixture of gaseous species with similar molecular diffusivities, an equation of the form given by Eq. (8) is solved for  $N-1$  species where  $N$  is the total number of fluid phase chemical species present in the system. Since the mass fraction of the species must sum to unity, the  $N$ th mass fraction is determined by difference. These equations are solved together with appropriate boundary conditions (see below) in the context of computational fluid dynamics techniques.

## 2.3. Validation of the model

The validation of the computational model was done by comparing the results of the simulation for the spreading and dispersion of Freon 22 performed in a 3D test room with the results of experimental studies by Gilham et al. [16]. The results showed that there was a liquid-like stratification effect in the spreading and the results were in good qualitative agreement with the experimental data [25].

The computational model for dense gas dispersion thus consists of the following elements:

- RANS-based governing equations with the  $k-\epsilon$  turbulence model.
- Evaluation of the local, instantaneous concentration of the dense gas species of interest by solving the scalar transport equation for the species.
- Using an ideal gas law-based equation of state to evaluate the relevant thermophysical properties of the gaseous mixture.

Its application to a chlorine leak scenario is discussed below.

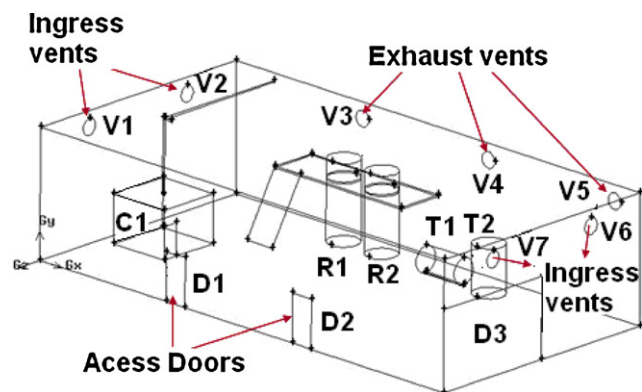


Fig. 1. Schematic diagram of the chlorine room.

## 3. Application to leak in a chlorine room

### 3.1. The physical problem

The simulated chlorine room is a typical indoor setting for a small scale industry with dimensions of 32 m × 16 m × 8 m (length × breadth × height) as shown in Fig. 1. It contains two large vertical reactors (R1 & R2), two intermediate storage tanks (T1 & T2) and an intermittent storage room for chlorine (C1). Compressed chlorine gas is stored in the storage room (C1) and is supplied through connecting pipelines. A chlorine vent, in the form of a long pipe of diameter of 100 mm, is provided at the top of the storage room to remove the vapours released accidentally during the normal operation. The room is normally closed, thus creating an indoor environment. A total of seven vents (V1–V7) are provided to maintain indoor air quality for the personnel working in the area. Of these, the front three (V3–V5) (see Fig. 1) are used for the egress of the contaminated air to the outside atmosphere, while the remaining four vents on the side opposite walls (V1, V2, V6 & V7) are used for bringing in fresh air. There are two access doors (D1 & D2) which are normally closed while a third door (D3) of larger dimensions is provided for transporting the raw materials and finished products from the plant. It is assumed that doors D1 and D2 can be opened at short notice for emergency evacuation while door D3 may not be readily accessible. Fresh air ingress at 3 m/s is specified at the four inlet vents to meet the air quality requirements for the personnel working in the indoor environment. Given the large volume of the environment compared to the number of personnel working in it, leakage of air from outside may be sufficient to cater to the fresh air requirements; however, an engineered venting system is thought to be necessary to meet with varying ambient climatic conditions. An equivalent amount of air is removed through the three exhaust fans, V3–V5.

Chlorine is a highly toxic dense gas. Its threshold critical concentration of chlorine being very small (IDLH of 10 ppm) [26], a small source rate is sufficient to exceed this level. Considering these factors, the scenario considered in the present study deals with an incident of slow leakage of chlorine from the vent pipe caused by a joint failure. It is assumed that the leakage is small enough not to have been detected by its depressurization effects or the violation of mass balance. Assuming a crack of length of 10% of the pipe diameter and a crack width of 0.01 mm, the mass flow rate of chlorine of the order of 0.01 kg/min was considered as the source release rate. It is assumed that because of depressurization, as the fluid comes out of the crack, a cloud of chlorine vapour is formed at the leakage location. This cloud will be much larger in size than the crack and is approximated in the present study in the form of one computational cell of equivalent chlorine concentration and flow rate. Thus, one grid cell is taken as a chlorine inlet and the

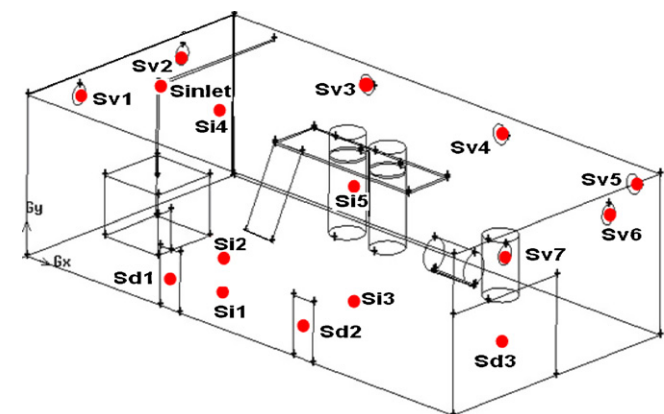
**Table 1**  
List of points at which chlorine concentration is monitored during simulations.

Sr. No	Abbreviation	Location of point	Group
1.	Sv1	Vent V1	Ingress air vents
2.	Sv2	Vent V2	
3.	Sv3	Vent V6	
4.	Sv6	Vent V7	
5.	Sv3	Vent V3	Exhaust vents
6.	Sv4	Vent V4	
7.	Sv5	Vent V5	
8.	Sd1	Door D1	Doors
9.	Sd2	Door D2	
10.	Sd3	Door D3	
11.	Sinlet	At the leak point	Leak location Interior points
12.	Si1	In front of Door D1 at ground level	
13.	Si2	In front of Door D1 at a height of 1.5 m	
14.	Si3	In front of Door D2 at a height of 1.5 m	
15.	Si4	In vertical alignment of Si2 at a height of 7.5 m	
16.	Si5	In vertical alignment of Si3 at a height of 7.5 m	

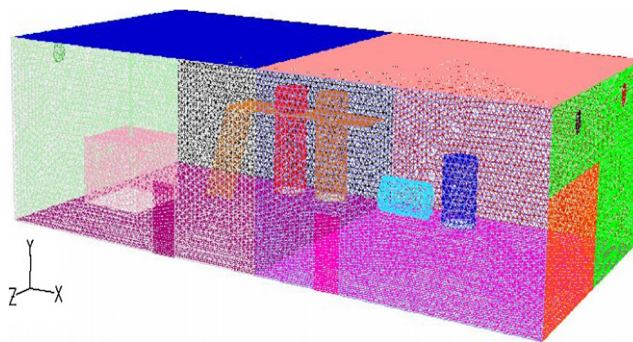
mass fraction and the velocity of chlorine in that cell are set such that the incoming flow rate is equal to that of the mass flow rate leaking from the crack. Its subsequent spreading is of interest. The chlorine gas is introduced after a steady flow pattern is established in the domain by the prevailing ingress and exit conditions of the air flow. To investigate the spreading and build-up pattern of chlorine, the concentrations at several locations within the domain are monitored. These are listed in Table 1 and Fig. 2. These consist of (i) the set of seven ingress and exhaust vents, (ii) the three doors, (iii) the leak source, and (iv) five interior locations of potential interest.

### 3.2. Details of the simulations

The computational model presented earlier is used for predicting the spatio-temporal variation in the concentration of dense chlorine gas following the accidental release. The commercially available CFD code FLUENT, which has been used in a number of accident scenarios reported in the literature, see [13] for example, has been used in the present study. Under normal conditions, all the doors are closed and fresh air enters at equal flow rates through the four vents, V1, V2, V6 and V7 at the specified rate of 3 m/s and leaves through the three exhaust vents V3, V4 and V5, which are specified as pressure outlet boundaries. No-slip conditions are enforced on all the walls. The flow is taken to be turbulent and the  $k-\epsilon$  turbulence



**Fig. 2.** Location of points at which flow variables are monitored to determine the spreading pattern.



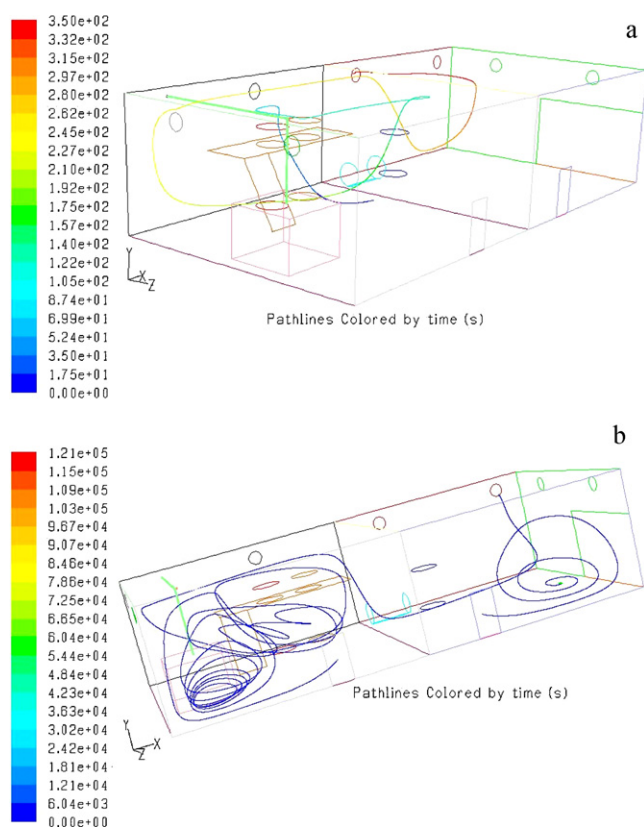
**Fig. 3.** Isometric view of the surface mesh of the flow domain.

model is used. Considering the domain size, wall functions are used at all the walls to keep the grid size at manageable levels. Since the velocities in the present study are fairly low and no heat transfer is considered, it is expected that no special, wall-induced effect (such as relaminarization under strongly accelerating conditions) will be encountered. Therefore a standard wall function approach should be adequate. All the simulations are nominally of second order accuracy in terms of discretization error. The mesh, generated using the software GAMBIT, consists of around 753,665 nodes as shown in Fig. 3. The simulations of the spreading gas were performed on an Intel® Core computer with a typical time step size of 5 s. Initial spreading calculations with a time step of 1 s have been performed, and comparison showed that a step size of 5 s would be adequate. A relative residual reduction factor of  $10^{-6}$  was used as the convergence criterion for the conservation equations. It is assumed that isothermal condition prevails throughout the period of simulation. Typically, each simulation took about a week of continuous computation. This precluded a systematic grid sensitivity analysis because decreasing grid size by a factor of two in each dimension would have taken months for each simulation. However, it may be noted that each of the obstacles in the flow domain has been represented accurately; care has been taken to ensure that that grid size in the interior is also fairly small. In terms of boundary conditions, wall functions have been used on all the walls. The outlet vents have been treated as constant zero gauge pressure boundaries while the inlet vents and the doors (when they are open) have been treated as Dirichlet boundaries. Here, the value of the normal velocity or the mass fraction in the case of scalar (corresponding to a chlorine concentration of 140 ppm) have been specified. The turbulence quantities have been specified based on turbulence intensity (5%) and the hydraulic diameter. The walls have been treated as zero-flux boundaries for the scalar. If there is a surface reaction occurring on the walls and if the reaction rate is known, then it can be readily incorporated as a boundary condition. Similarly, if the scalar participates in a homogeneous chemical reaction with some of the constituents of the gas, then that can be incorporated readily in the form of a source or sink term. Thus, the current approach can readily consider a reacting gas case. However, if there is a phase change, for example, condensation, then a two- (or multi-) phase formulation is required. The boundary conditions are consistent with the case of a dispersion of a non-reacting gaseous scalar.

### 3.3. Results and discussion

#### 3.3.1. Steady air flow pattern under normal conditions

The steady air flow pattern is governed by the location of the inlet and the exhaust vents, the flow rate through the vents and the location of the objects within the domain. For the case of 3 m/s of air coming in through the four inlet vents, namely, V1, V2, V6 and V7, and going out through the three exhaust vents, namely, V3, V4 and V5, the computations show that more or less equal flow distribution



**Fig. 4.** (a) Path line for a fluid particle initially located at point Si2. (b) Path lines for fluid particles located initially on doors D1 and D2.

occurs through the three outlet vents. However, the flow pattern is quite complicated. This is demonstrated in Fig. 4 where the path lines of air are drawn for fluid particles located initially at the interior point Si2 (Fig. 4a), and at doors D1 and D2 (Fig. 4b). Fig. 4a shows that a particle originating at the interior point Si2 goes through a convoluted path to go through the middle vent while the path lines in Fig. 4b suggest that there are stagnation zones on either side of doors D1 and D2. In all these figures, the path lines are coloured by the residence time of the particle in the domain. The time spent by a fluid particle varies considerably (from 1 min to 30 min for the cases shown) depending on its point of origin.

### 3.3.2. Spreading and dispersion of chlorine from sources

The spreading of the chlorine gas inside the domain is determined by injecting 0.01 kg/min of chlorine at a bend in the chlorine vent pipe. As seen in the previous section, the ingress of fresh air does not lead to very strong currents and fluid particles spend typically hundreds of seconds within the domain. In the absence of strong air currents, the spreading and dispersion of chlorine is characterized primarily by its (negative) buoyancy. Since the leak rate is small, the chlorine emanating from the leak flows down almost vertically until it hits the ground. This slumping motion is followed by spreading all over the floor (in the way a liquid spreads) before rising to higher levels. Simultaneously, there is a continuous entrainment of the less dense gas (air) into the bulk phase of chlorine gas leading to some amount of dilution.

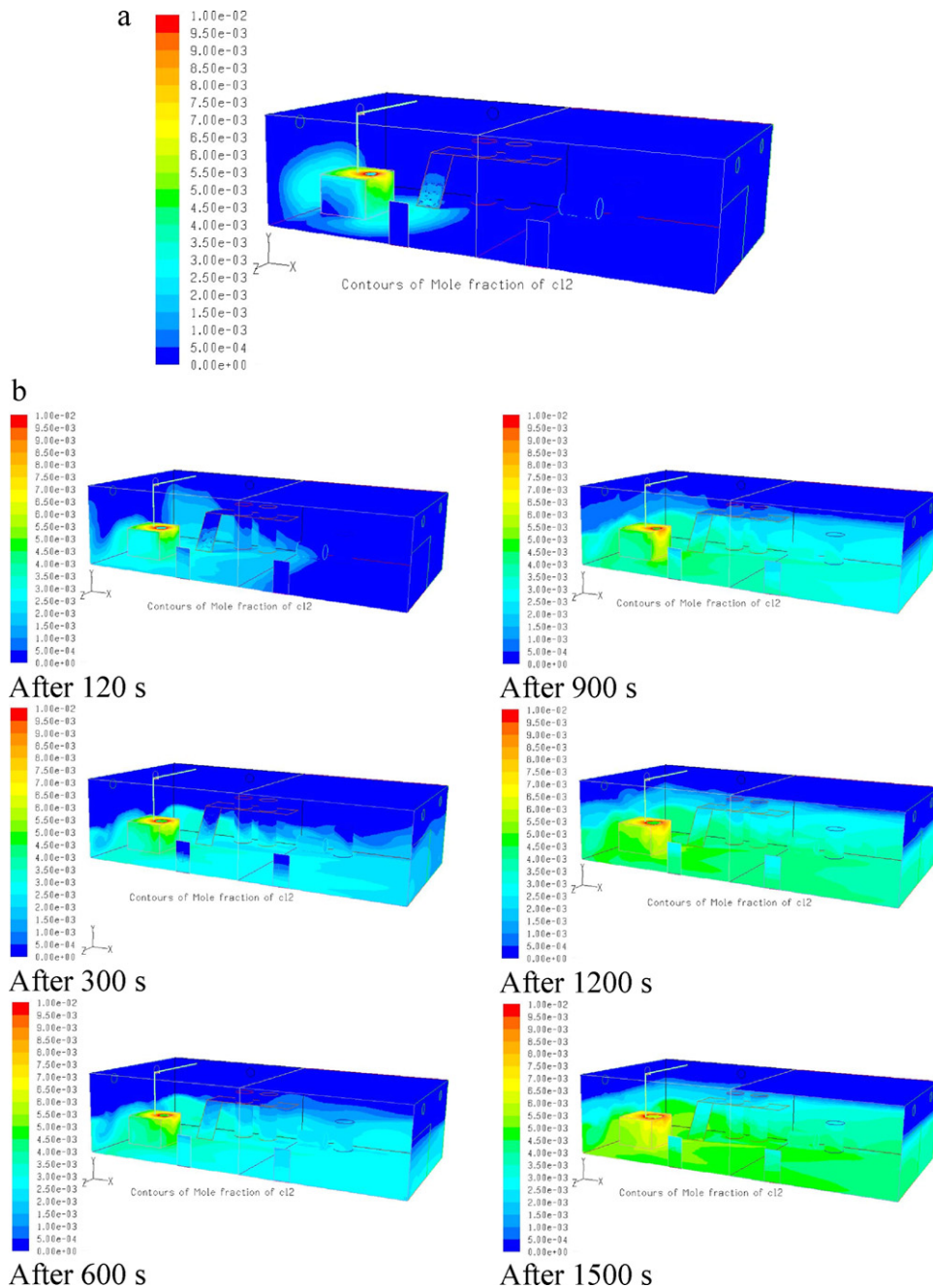
These aspects are evident in the contours of chlorine plotted in Fig. 5 at various time intervals. Here, the outline of the flow domain and the major internal components are shown to serve as a reference point along with the chlorine concentration field in terms of

mole fraction, at a particular time instant. Fig. 5a shows the contours at a time of 50 s after the start of the leak. (In the interest of bringing out clearly the spreading pattern of chlorine, the contour values in the range of 0–0.01 only have been plotted in all the figures. Any mass fraction higher than 0.01 is not shown.) It can be seen that the cloud of chlorine descends almost vertically down on to the chlorine equipment enclosure, flows over it and reaches the ground level. While this liquid-like motion is evident, it should also be noted that the concentration is not very high; the maximum mole fraction of chlorine is only of the order of 0.01. This slumping motion is followed by spreading all over the floor (in the way a liquid spreads) before rising to higher levels. Simultaneously, there is a continuous entrainment of the less dense gas (air) into the bulk phase of chlorine gas leading to some amount of dilution. As the source is a continuous one, the concentration builds up continuously within the domain during the entire tracking duration of 1800 s. The instantaneous chlorine mole fraction concentrations in the domain are shown in Fig. 5b at time instants of 120, 300, 600, 900, 1200 and 1500 s after the beginning of the continuous leak. It is observed that with the passage of time, the chlorine concentration at any specific location increases, and, that after the initial transient, the concentration at any specific time increases in the depth direction, indicating both stratification and dispersion. It may be noted that dispersion phenomena such as those shown in Fig. 5b, which are typical of a dense gas, may not be accurately modelled using models employing the Gaussian approach.

### 3.3.3. Chlorine build-up from the release

The risk arising from the accidental release may be assessed by tracking the chlorine concentration at different locations within the domain. Five interior points, denoted as Si1–Si5 in Fig. 3, have been selected for this. Of these, point Si1 is at the floor level; points Si2 and Si3 are at a height of 1.5 m from the floor while Si4 and Si5 are at a height of 7 m from the floor and are in line with the leak location. Fig. 6 shows the concentration profiles of chlorine at these locations inside the domain. It can be seen that the concentration reaches high values (>3 ppm) very quickly but not simultaneously. At point Si4, which is the closest to the source, it reaches a high value quickly and a constant high value is maintained there because the leak is continuous. Points Si1 and Si2 are at the same horizontal position but are vertically separated by a distance of 1.5 m. The fact that these two traces nearly coincide shows that the slumping down motion of the chlorine cloud is very fast. Point Si3 is horizontally displaced from point Si2 and therefore chlorine reaches there after some delay again indicating a vertical slumping motion first followed by in-plane spreading. Point Si5, which is at a higher location, receives chlorine after a further delay. This pattern is consistent with the hydrodynamics of a dense gas in terms of vertical slumping down, horizontal spreading and rising of the cloud.

After the cloud has spread to the lower parts of the domain, it rises gradually and is pumped out through the exhaust vents, V3, V4 and V5. Fig. 7 shows the concentration profiles of chlorine at these locations. As expected for a dense gas, the concentration at the exhaust is less than that at the ground level. Also, there is a time lag between the concentration levels at the bottom level and at the vents. If the chlorine detectors are located in the exhausts and are set to get activated at a chlorine concentration of 1 ppm, then Fig. 7 shows that the alarms are triggered at this level at about 360 s after the release. However, Fig. 6 shows that by this time nearly all the five interior points register a concentration level of 3 ppm or more. Thus, a chlorine detector located at the top may not work effectively as an alarm system in case of a dense gas release; a detector located ground level may allow a more rapid response.



**Fig. 5.** (a) Predicted concentration of chlorine after 50 s from release. (b) Predicted concentration build-up of chlorine at different time intervals from release.

## 4. Risk mitigation

### 4.1. Location of detectors

It can be seen from Fig. 6 that the variation of concentration of chlorine at Si1 and Si2 closely follow each other due to the dense gas nature of chlorine. Si3 then records the next higher level of chlorine concentration. This is followed by Si4 and Si5. Hence the predicted concentration at the five interior locations can be arranged in the following descending order, based on the concentration levels that they are exposed to: Si1 ~ Si2 > Si3 > Si4 > Si5. It has also been shown above that the concentration in exhaust vents increases much later and that, by the time it is detected, ground-based personnel can suffer a significant exposure to chlorine. Finally, it has

also been established earlier that, given the low threshold levels of toxicity for chlorine, it is not possible to have high ingress of fresh air continuously to flush out chlorine in case of accidental release.

Considering all these factors, the ideal location for the sensor of a toxic dense gas is at the ground level, say, in the wall a few inches above the ground for ease of access and for operational convenience. The precise location is not critical, as the spreading along the ground is quite fast. As shown earlier, a ground-level sensor will have the advantage, in addition to that of allowing for early detection, of not being sensitive to the source location of the dense gas. The analysis in the previous section shows that this is not so for a sensor location in the exhaust vent.

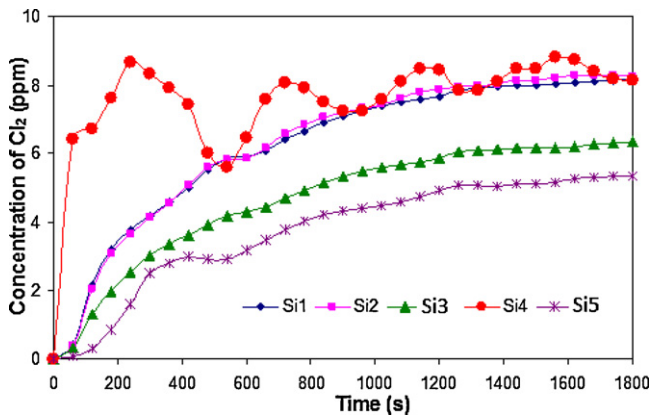


Fig. 6. The variation of concentration of chlorine at selected points within the domain for the case when the doors are closed.

4.2. Dispersion/dilution of the concentration

Given that a small leak from a pipeline is always possible, risk mitigation measures should include proper inspection and preventive maintenance procedures to monitor the health of the pipeline. Proper location of detectors will also help in buying crucial time for evacuation and engineered measures to mitigate the consequences of a release. As observed earlier, the concentration of chlorine reaches critical threshold levels in a short duration of time. This specific pattern of spreading of a dense gas, namely, that it collects at floor level and spreads quickly along the ground level, calls for special measures to evacuate/dilute its concentration to below the threshold levels.

One of the simplest methods for addressing the problem would be to open the doors D1 and D2 and let the incoming air provide for dilution of the gas cloud. However, simply opening of doors of the chlorine room may not be enough to dilute it because the outside air, which is lighter than chlorine, will do little to evacuate chlorine from ground level. There is also the danger of the chlorine cloud spreading out along the ground through the open door and endangering unsuspecting people outside. An effective measure therefore would be to induce air flow into the domain through the doors by switching on emergency evacuation fans located in the exhausts, which would be activated by the triggering of an alarm when the concentration reaches a level of 1 ppm. The predicted concentration rise in the exhaust vents is such that, if a detector is placed in the exhaust vent, the alarm would be triggered at about 360 s

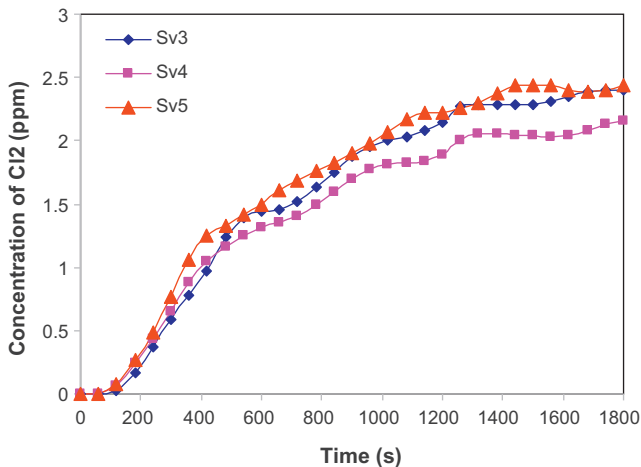


Fig. 7. The variation of concentration of chlorine at three exhaust vents for the case when the doors are closed.

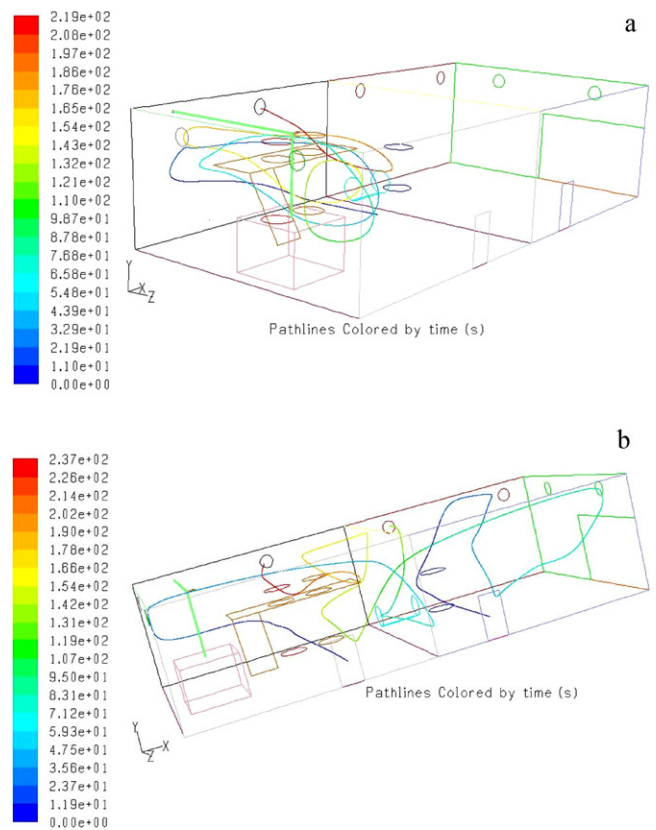


Fig. 8. (a) Path line for a fluid particle initially located at point Si2 for the case where air flow is induced through doors D1 and D2. (b) Path lines for fluid particles initially located at doors D1 and D2 for the case when flow is induced through these doors.

for the accidental release scenario considered (Fig. 7). For an alarm located at ground level, the detection can be as early as 80 s. Upon the detection of alarming levels of chlorine by the detectors, these fans would be turned on. The significantly higher evacuation rate of air from the room will then induce a draft of fresh air through doors D1 and D2 which are opened once the emergency fans are working at their full capacity. This contaminant-free air coming at high velocity will also aid in bringing down the concentration levels by mixing through turbulent dispersion and dilution.

This scenario of reducing chlorine concentration levels by dispersion, dilution and evacuation is simulated for the specific case of accidental release. It is assumed that early detection is possible through detectors located at ground level and the emergency fans become fully operational soon after the triggering of the alarm such that when the doors D1 and D2 are opened at a time of 360 s, a draft of fresh air enters the domain at a speed of 3 m/s. This has a significant effect on the air flow pattern within the enclosed domain. This is shown in Fig. 8a and b, which correspond to the case of steady flow field with induced draft of 3 m/s through doors D1 and D2, fluid particle locations discussed in Fig. 4a and b, respectively. Compared with the case when the doors are closed, one can see that the path lines have become simpler and that there is less residence time, indicating a faster evacuation rate on the whole.

The concentration profiles at the selected five interior locations corresponding to those in Fig. 6 and at the three exhaust vents corresponding to those in Fig. 7 are shown in Figs. 9 and 10, respectively, for the case when fresh air flow is induced through doors D1 and D2. Here, the simulation starts with the doors fully open and the flow field is fully established by the time the leakage starts. These show that there is a fairly significant and immediate reduction in the chlorine concentration at all locations. It can also be seen that, due to the change in the flow pattern, the chlorine concentration at

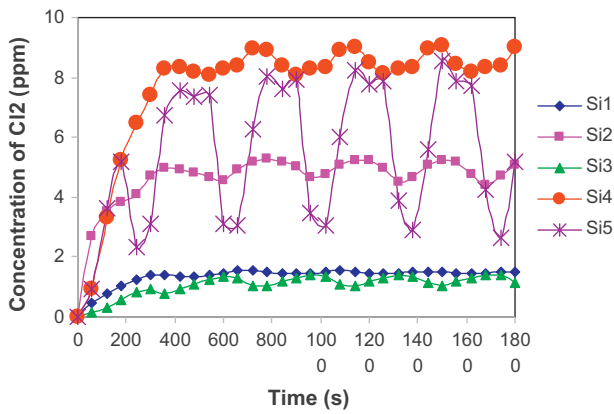


Fig. 9. Temporal variation of concentration of chlorine at five interior points from the instance of leakage; the steady state flow rate corresponds to that of Fig. 8.

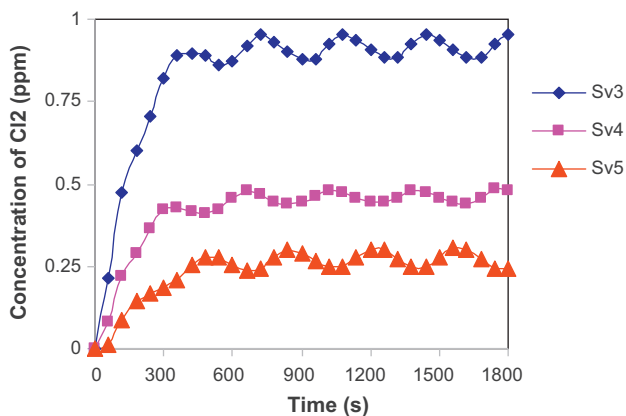


Fig. 10. Concentration of chlorine at three exhaust vents for the case shown in Fig. 9.

point Si2 is initially higher than that at point Si4, which is in contrast with Fig. 6. The chlorine concentration falls well below the 1 ppm level in the exhausts and below 3 ppm level at three interior points. However, significant concentration persists at two interior points. This situation persists for several minutes, and the evacuation rate is clearly not sufficient. The situation obtained with a higher evacuation rate, corresponding to an air inlet velocity of 6 m/s at the inlet, and is summarized in Fig. 11 where the concentrations are shown when the doors are opened 360 s after the beginning of the leakage of chlorine. Thus, for the first 360 s, the flow pattern corresponds to that of doors closed and only the inlet vents provide circulation within the domain. The chlorine concentration is essentially the same as in Fig. 6 for the first 360 s and it then responds to the

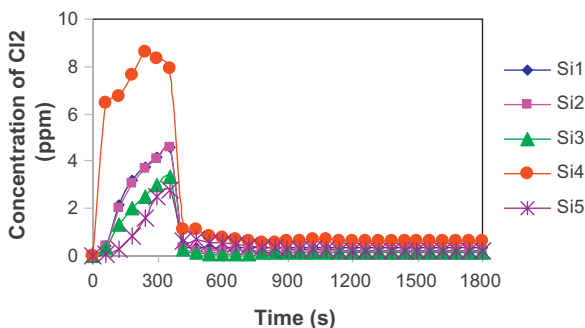


Fig. 11. Concentration of chlorine at five interior vents; doors D1 and D2 opened after 360 s with an induced air velocity 6 m/s.

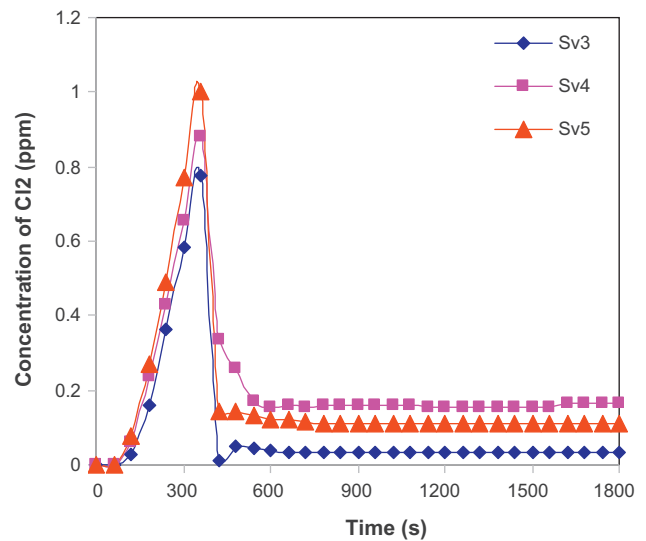


Fig. 12. Concentration of chlorine at the exhaust vents; doors D1 and D2 opened after 360 s with an induced air velocity 6 m/s.

change in the flow condition created by the sudden and sustained inrush of air at 6 m/s through doors D1 and D2. It can be seen that the chlorine level comes down to less than 1 ppm and is sustained at these level at all the monitoring points. The concentration at the exhausts also comes down to 0.2 ppm or lower, as shown in Fig. 12.

## 5. Conclusion

Dense gases that are toxic and flammable are increasingly being used in the chemical and process industries. A hazardous situation may develop if there is an accidental leak during their use, storage and transportation. In the present study, CFD simulations have been used to analyze the risk arising out of an undetected leak of toxic gas chlorine in a typical indoor industrial environment. CFD analysis of the accidental release scenarios provides useful insight in understanding the dynamics of the problem and is essential for a better understanding of the consequences of a dense gas release. This was done in the present study using the species transport method, wherein an additional scalar transport equation is solved to determine the concentration of the dense gas. The model was applied to the study the spreading and dispersion of dense toxic chlorine gas for accessing the risk posed due to it in an indoor environment and results showed that the gas spreads like a liquid in the lower parts of the domain. It was observed that when the doors of the industrial complex were closed, significant exposure to chlorine may take place to the occupants in the lower parts of the domain in between the period of accidental release and its detection by a sensor located in the vent. Risk assessment and mitigation measures should take account of the characteristic spreading pattern of dense toxic clouds to come up with effective engineered systems which prevent the build-up of concentration by early detection, dilution, dispersion and evacuation of the cloud. Mitigation action for this accidental release was done by opening the doors of the chlorine room, thus bringing fresh air in the control volume. Significant decrease in the chlorine concentration was achieved, helping in lowering the concentrations below the standard threshold levels and minimizing the risk posed to the occupants. The present study makes the case for a CFD-based assessment of risk and risk mitigation measures in the general context of consequence analysis of accidental release of hazardous gases in an indoor environment. Although the study has focused on a dense gas (chlorine), the computational model is generic enough to deal with cases of passive or positively buoyant



gases, either flammable or toxic releases of hazardous gases. While non-isothermal effects can be readily incorporated, further work needs to be done to enable it to treat phase change effects.

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