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Carbon Capture and Storage Hazard Investigation: Numerical Analysis of Hazards related to Dry Ice Bank Sublimation following Accidental Carbon Dioxide Releases

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Climate Change is caused by greenhouse gases such as CO_2. Worldwide increase in energy demand coupled with a continued reliance on fossil fuels have contributed to a significant increase in atmospheric levels of CO_2. Scenarios for stabilizing the emissions of CO_2 suggest mitigation actions including the deployment of Carbon Capture and Storage projects (CCS). One of the process steps consists in the transportation of the CO_2 to a storage location by buried pipelines. Any accidental release determined by failures is followed by a pressurized release of CO_2 with dry ice formation. Under specific conditions a dry ice bank will form contributing to atmospheric dispersion through superficial sublimation (Vianello et al., 2014). This study focuses on the importance of the bank sublimation emission to the near field dispersion of CO_2. The application of CFD techniques show that hazardous conditions exist over an area close to the source. Within 50 m from the pipeline the volumetric fraction of CO_2 still amounts to 7 – 10 % at 1.5 m above the ground, causing serious health effects on operators in a short time. In addition, a decrease in wind velocity coupled with an increase in both the ambient temperature and the intensity of solar radiation worsens the risk of health hazards. The danger persists for days after the accident given the slow dry ice bank sublimation process which becomes the dominant hazard source afterwards.

1. Introduction

The Intergovernmental Panel on Climate Change in 1992 stated the association between the increase of Earth average temperature and the growing in anthropogenic greenhouse gases (GHG) atmospheric concentration. Among these the carbon dioxide is by far the most important because of the link between worldwide economies based on fossil fuels and the emissions derived from combustion processes. CO_2 emissions from fossil fuel power generation represent not less than 25 % of the total emissions (IPCC, 2013). The stabilization of atmospheric CO_2 concentration can be achieved using a portfolio of various solutions including the Carbon Capture and Storage chain (CCS) which is the most indicated for the medium to long term (Kaggerud et al., 2006). It consists in the capture of CO_2 from related sources, the transportation to a storage location and long – term isolation from the atmosphere in underground geological locations (IPCC, 2005).

If CCS technology is to be widely introduced then extensive networks of CO_2 transportation facilities will be needed and the transportation by dedicated pipelines is the preferred solution to move large quantities of CO_2 over long distances (Leung et al., 2014). There is naturally the possibility of leakage from these infrastructure caused by component failure or third – party intrusions (adverse climatic events, terrorist attacks etc.). In most cases CO_2 is transported in pipelines with diameters in the range of 0.6 – 0.9 m, with operating pressures between 80 and 150 bar and temperature in the range -10 to 30 °C. If a pipeline leak occurs then the CO_2 undergoes an expansion that could give a bi-phase liquid – gaseous release. The unstable overheated liquid will then undergo a series of breakup mechanisms finally forming dry ice particles (Hulsbosch-Dam et al., 2012). Under specific conditions, particles in the jet will then snow out forming a sublimating dry ice bank (Vianello et al., 2014). For example, an important requirement is represented by the jet collision with the soil.

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This occurrence is surely found in the case of releases from a buried CCS pipeline and is very common given that a large part of the piping will be placed under the ground.

2. Modelling

2.1 Release characteristics, modelling

The present case concerns the pressurized release of CO_2 from a buried pipeline. The modelling aims at reproducing a full bore rupture that could be actually determined by wrong soil handling operations or earthquakes. The pipeline model example is that adopted by Vianello et al. (2012) describing a rupture of a 0.6 m – diameter pipeline with a total circulating flow rate of 251.67 kg.s^{-1}. The breach is located 4.2 km downstream of a shut – off valve. As modelled in the work mentioned, the velocity profile tends immediately to a stationary state mainly induced by the onset of sonic conditions. Considering this aspect, all simulations have been performed both in steady and transient method showing negligible differences. Steady results have been assumed as reference. The initial thermodynamic state for the released CO_2, consistent with the post – expansion state, is characterized by a pressure value of 1 atm and an equilibrium temperature of -78.4 °C. The computational inlet for CO_2 does not match the real one but it is located some lengths ahead in relation to characteristic length scale of breakup phenomena (Hulsbosch-Dam et al., 2012). The modelling of sublimating dry ice bank is more complex and follows a different approach. The inlet mass flow rate of Carbon Dioxide leaving the bank is estimated through an overall energy balance (Mazzoldi et al., 2008) as reported below.

$$E = SW_D - SW_U + LW_D - LW_U + H + LE + G \tag{1}$$

where E (Wm^{-2}) is the total energy available for sublimation, SW_D and SW_U respectively downward and reflected short - wave radiation, LW_D and SW_D long – wave radiation, H the sensible heat flux, LE the latent heat flux and G the flux derived by soil conduction. Further details are beyond the scope of this work and the reader should refer to other reference (Mazzoldi et al., 2008). Supposing the surface of the bank constantly at equilibrium temperature and applying the model under Italian average weather conditions (ISTAT, 2013), the simulation shows a trend similar to that found by the authors. In detail, a time weighted average based on 250 s, that is the stationary time of gaseous pressurized release, gives an emission value of 5.85 g.m^{-2}.s^{-1} of gaseous CO_2. This value is therefore adopted in the modelling of the emission from the dry ice bank source.

2.2 Geometry and computational approach

The geometry domain is three – dimensional and its length is equal to 250 m. It covers a height of 20 m and its depth is of 40 m. The crater geometry is here simplified as a truncated cone with sizes consistent with a real crater induced by the full bore rupture of the pipeline. The domain is discretized mainly with hexahedral elements that are computationally efficient and requires less unities than tetrahedral volumes. The grid is made up of approximately 1,400,000 elements, refined near critical areas like source points and boundaries.
The set of equations indicated below are solved simultaneously through an iterative GMRES solver (Generalized Minimum Residual) in conjunction with preconditioning settings to help convergence route.

2.3 Governing equations and boundary conditions

The simulation adopts RANS k – ε turbulence model to formulate conservation equations for mass, energy and momentum. Their general form is indicated below:

$$\frac{\partial}{\partial t}(\rho\boldsymbol{\Phi}) + \nabla\cdot(\rho\Phi\boldsymbol{U}) = \nabla\cdot(\Gamma_{\Phi}\nabla\boldsymbol{V}) + \left[-\frac{\partial(\rho\overline{u'\varphi'})}{\partial x} - \frac{\partial(\rho\overline{v'\varphi'})}{\partial y} - \frac{\partial(\rho\overline{w'\varphi'})}{\partial z}\right] + S_{\varphi} \tag{2}$$

In equation (2) Φ is the property described by the conservation law, ρ is the mean substance density while (u', v', w') velocity field instantaneous fluctuating components. The instantaneous continuity and Navier – Stokes averaged equations form a set of four equations with four unknowns (u, v, w, p). Since the averaging operation throw away all the details on the local state of the flow, to close the mathematical structure six additional unknowns need to be described and solved. This is achieved by using two more governing equations: one for mean flow kinetic energy k and the other for the rate of kinetic energy dissipation ε:

$$\frac{\partial}{\partial t}(\rho k) + \nabla\cdot(\rho k\boldsymbol{U}) = \nabla\cdot\left(\frac{\mu_t}{\sigma_k}\nabla k\right) + 2\mu_i E_{ij}\colon E_{ij} - \rho\varepsilon \tag{3}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\nabla\cdot(\rho\varepsilon\boldsymbol{U})=\nabla\cdot\left(\frac{\mu_t}{\sigma_{\text{å}}}\nabla\varepsilon\right)+C_{1\varepsilon}\frac{\varepsilon}{k}2\mu_t E_{ij}:E_{ij}-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} \tag{4}$$

All phenomena involved in the description are non – isothermal so the system of equations is supplemented also by the energy differential balance. In addition the Peng – Robinson equation of state has been used to link thermodynamic properties. Mass transfer phenomena due to convection and diffusion are described in terms of local mass fraction using a suitable convection conservation equation and Fick's law of diffusion.

The closure of the turbulence model requires six different boundary conditions. The description of bottom boundary condition is supported by wall functions defined at the nodes closest to the surface.

Inlet boundary condition concern the variation of the wind speed and the inflow of carbon dioxide from the sources. The latter has been modelled as previously described whereas wind entering profile is considered to be logarithmic and fully developed and so described by following equation (5):

$$u_{wind}=\frac{u_f}{K}\ln\left(\frac{\mathrm{z}+\mathrm{z}_0}{\mathrm{z}_0}\right) \tag{5}$$

In (5), u_f represents a friction velocity evaluated from terrain specific rugosity z_0 and wind mean speed at 10 m of elevation. K is the Von Karman's constant (assumed to be 0.42). At wind inlet also the turbulent kinetic energy k and its dissipation rate ε should be specified adding two following more equations:

$$k=0.33u_f^2 \tag{6}$$

$$\varepsilon=u_f^3[K(z+z_0)]^{-1} \tag{7}$$

These equations also contains variables related to atmospheric stability class.

At the outlet of the computational domain a zero normal gradient for all variables is specified. A specific study has been carried out to locate this boundary at a sufficient distance to prevent the propagation of computational errors in the domain, distorting results. A constant shear stress is imposed over the top boundary layer so that the flow is driven by both an energy dissipation at the top and on the ground of the computational domain. Side boundary conditions are usually modelled as symmetric non penetrating borders (Abuku et al., 2009) but in this work a more realistic approach is adopted by implementing a periodic flow flux. In these sense the fluid leaving the domain across one boundary is forced to enter the domain over the facing one reproducing the fact that the computational domain is a periodic part of a larger real geometry.

3. Results and discussion

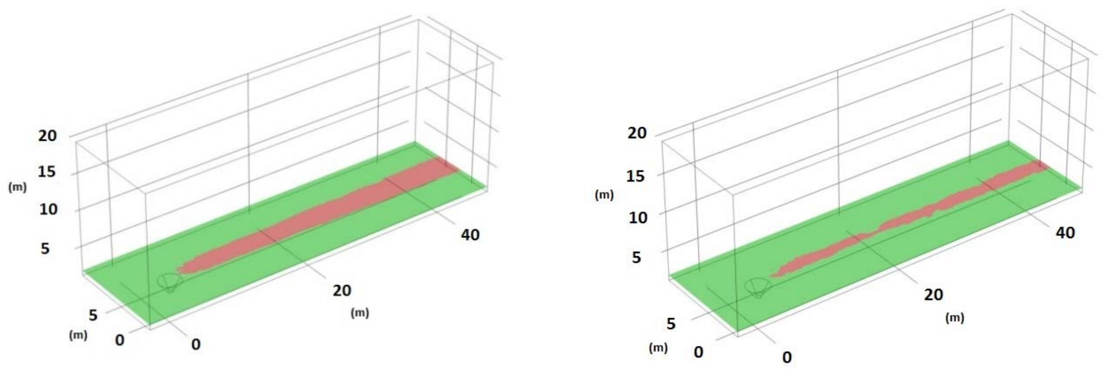
Extremely high concentrations of carbon dioxide could result in severe effects on the cardiovascular and central nervous system sometimes leading to death by asphyxiation. The lowest lethal inhalation concentration for humans is 100,000 ppm for 1 min. Concentrations of 20 – 30 % lead to convulsion and coma within the same time whereas unconsciousness may occur when inhaling a concentration of 12 % for 8 – 23 min. In light of these toxicological properties, gas concentration is therefore the most important parameter and most of the results represent the evolution of carbon dioxide concentration in space following the release from the dry ice bank and the ruptured pipeline. To give significance to the results, part of the data here reported refer to surfaces placed at 1.5 m above the ground matching the mean location of upper respiratory tract of a human being.

3.1 Dry ice bank downwind sublimation profiles

Simulations under Italian average weather conditions of dry ice bank sublimation returned the results presented in Figure 1 a - b. Local distribution of volume fraction of carbon dioxide are shown nearby the point of release at 1.5 m of height above the ground.

Figure 1-a shows the space distribution of areas covered by a concentration of 4 % by volume. The simulation assumes a completely downwind condition showing that the gas spreads out over an area at least 40 m downstream of the dry ice bank source.

At the same height from the ground, area covered by a concentration of 7.5 % by volume is more contracted and is located mainly in the centre of the plume. The domain is here limited to 40 m downstream of the source in order to focus the analysis near the release point and so on an area related to operators' intervention.



a b

Figure 1: CO_2 emission from the sublimating bank. Italian average weather conditions. a- CO_2 concentration distribution at 1.5 m, volume fraction 4 %. b- CO_2 concentration distribution at 1.5 m, volume fraction 7.5 %.

This analysis is very conservative since a situation of downwind condition increases local concentration of carbon dioxide. This occurrence has been validated with other simulations that showed an increase of the hazard near the release point against a situation under different directions. Results show that under Italian average weather conditions, the extension of the danger area induced by the dry ice bank sublimation is not negligible. In addition to that shown in Figure 1, calculations attest that dangers significantly increase approaching the release point. Here the gas concentration may culminate with volume fractions up to 18 – 20 % and so endangering operators lives very quickly. These conditions does not allow a stay longer than 15 – 20 min otherwise posing a serious risk that could culminate in a state of unconsciousness and even to death.
This problem is also complicated by the fact that the release of very cold carbon dioxide, denser than surrounding air, produces a stratification resulting in higher concentrations in layers closest to the ground as showed by Figure 2. A more detailed analysis of the local Richardson number confirms the domination of buoyancy linked to an insufficient kinetic energy to homogenize the fluid. Local Richardson number Ri is here defined as:

$$Ri = \frac{g\left(\rho_{CO_2} - \rho_{amb}\right)}{\rho_{amb}} \frac{\dot{V}_{CO_2}}{w u_f^3} \tag{8}$$

In (8), $\rho_{CO_2} - \rho_{amb}$ is the difference between the local density of carbon dioxide and that of surrounding air, $\dot{V}_{CO_2}$ the volumetric flow rate of carbon dioxide leaving the bank, w the local plume width and u_f the friction velocity already mentioned.

Figure 2 clearly shows a stratification of the carbon dioxide concentration profile. The carbon dioxide, in fact, as a dense gas reveals a vertical density profile stably stratified especially nearby the release point and the mixing between layers induced by turbulence is significantly reduced or inhibited.
The wind speed used is of 2 m.s^{-1} and given the weather conditions assumed, the environment is therefore considered to be unstable. An increase in local wind speed acts modifying the carbon dioxide distribution profiles despite the surface roughness of the terrain and mean features of the release. Figure 2-b shows that an increase in the local wind velocity acts increasing turbulence and consequently both mixing and carbon dioxide dilution mechanisms. As a result, its volume fraction decreases although the peak in concentration is always placed within a few meters downstream from the source. Stratification instead persists even for local increasing wind speed emphasizing the tendency of the carbon dioxide to stagnate in lower layers. However this tendency decreases away from the source where density differences reduce as a consequence of the progressive reduction of temperature gradients.
The modeling results also shows that other weather conditions like the environmental temperature and the degree of solar radiation have an effect primarily on the dry ice bank dynamics. Keeping the wind speed unchanged, an increase in the ambient temperature results in a greater sublimation process leading to local greater carbon dioxide concentrations even if the same temperature tendency acts at the same time increasing diffusive dilution mechanisms. Insolation has been modeled as a surface heat flux and represents an energy source supplied to the dry ice bank. Results collected show that insolation contribution is negligible when assessing carbon dioxide distribution in space near the dry ice bank. In fact several attempts with

different insolation degrees proved minimal influence on concentration profiles compared to that due to temperature and wind effects.

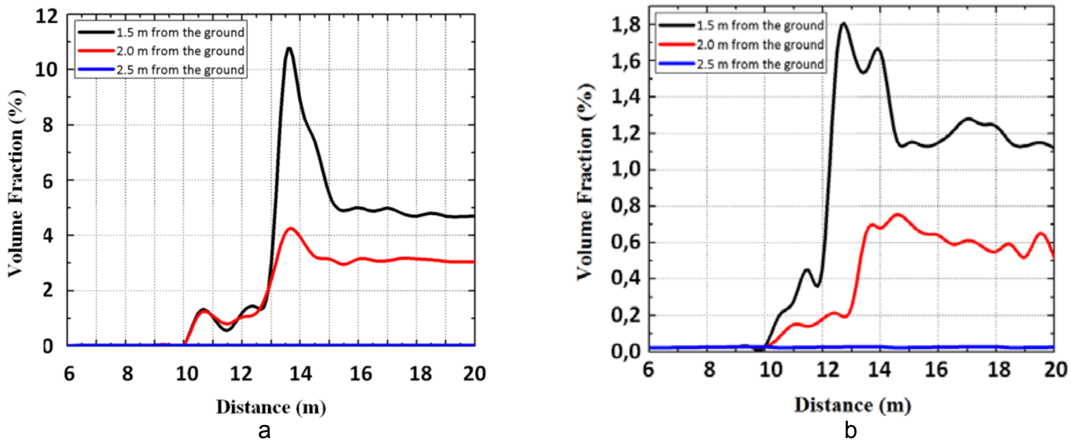


Figure 2: CO_2 volume fraction distribution in space at different heights from the ground. a- wind velocity 2 m.s^{-1}. *b- wind velocity 10* m.s^{-1}. *The source is located between 10 and 13 m (x – axis).*

3.2 Gaseous pressurized release and dry ice sublimation downwind concentration trend

Further investigations aim to establish the relative importance between the amount of carbon dioxide emitted from the sublimating bank and that due to the gaseous release resulting from the pipeline breach. This analysis may help to establish which scenarios are predominant in space and time during the accident.

Usually a pressurized release may result in a high – speed multi – phase jet of superheated liquid and gaseous carbon dioxide. The gaseous one is dispersed in the surrounding area while the instable liquid state undergoes a series of break – up mechanisms, evaporation and boiling. These steps lead to the final solidification and sublimation stages. This means that the resulting solid phase may fall on the ground forming a dry ice deposition (Vianello et al., 2014). Consequence analysis should therefore take into account both of these risk sources when assessing the carbon dioxide atmospheric dispersion following a pressurized release.

Despite different dynamic mechanisms some simulations were performed to investigate whether the presence of the emitting dry ice bank could influence the local distribution of carbon dioxide induced by the pressurized release from the rupture of the buried pipeline. To make comparable these different dynamics, the emission rate from the dry ice bank has been time averaged over a time period of 250 s that is the duration of the steady state of pipeline release sequence. The amount emitted from the dry ice surface is approximately equals to 18 gm^{2}s^{-1} and this value is used to compare the mutual influence of the release and of the dry ice bank. Weather conditions remain unchanged (wind speed of 2 m.s^{-1}, same insolation degree) and the survey inspected the carbon dioxide downwind space distribution.

Results show that the presence of the emitting dry ice bank does not change significantly the dispersion profiles due to the high – speed gaseous release. The location of maximum volume fraction and its value remain almost unchanged, the latter increasing slightly over 19 % (to be compared with Figure 2 – a). Main differences are observed especially in lower layers near the ground where the additional carbon dioxide source related to the sublimating bank increases the local concentration up to 40 % by volume. It should be stressed that the jet and the emission from the bank have very different time scales. The release from the guillotine rupture produces a mass release that lasts usually in a few minutes depending on the position of shut – off valves. On the contrary, the formation of a dry ice bank and its sublimation follow extremely slower dynamic mechanisms (Figure 3). So when assessing CCS failure risks, the determination of events' timeline is of crucial importance.

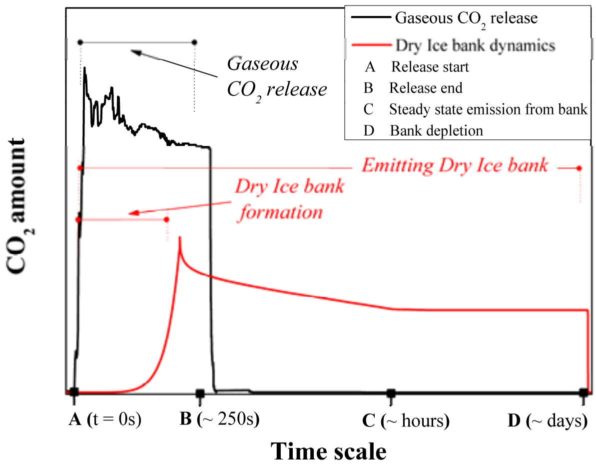


Figure 3: Relative time scales between the pressurized release and the dry ice bank sublimation dynamics.

4. Conclusions

This study investigates the accidental release of carbon dioxide from CCS pipelines and the consequences related to sublimating dry ice bank that may occur. Making use of a commercial CFD code, the atmospheric dispersion of carbon dioxide was modelled studying also the influence of atmospheric conditions and of the presence of a high – speed pressurized jet. Simulations show primarily that serious risks are associated to the sublimating dry ice bank near the release point. Under Italian average weather conditions, the dispersion of carbon dioxide generates volume fraction peaks of about 11 % that are incompatible with prolonged stays near the sublimating bank. Other simulations conducted by varying some meteorological parameters show that hazards increase with a decreasing mean wind speed and a raise in ambient temperature. A difference of 20 K in ambient temperature can double the local volume fraction peak near the release point.

A relative comparison between the incidence on carbon dioxide amounts of the pressurized jet and the carbon dioxide released from the dry ice bank leads to the conclusion that the incidence of the latter is minimal when the time horizon of the analysis is limited only to the time evolution of the release. However the sublimation from the bank becomes the predominant source of risk when the pressurized release goes down and its effects last for hours and days. Unless special measures are taken, even a brief expsosure may cause danger especially to operators locally involved in recovery operations and maintainance.

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