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Atmospheric dispersion of CO₂ released from pipeline leakages

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Abstract

During the onshore Carbon dioxide transportation potential risks such as leakages or even pipeline breaches can occur. In such cases CO₂ will be released and dispersed in the ambient having short-time impact on the environment and potentially on human health and long-time consequences on the climate. The hydrodynamical characterization of the released jet expansion and plume dispersion is decisive for understanding the pollutant impacts on the atmosphere and it is an essential part of risk assessment for the CCS-technology. Numerical simulations of gaseous CO₂ expansion and dispersion will be used to analyze the release conditions influence on harmful concentration distances.

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1. Introduction

Emissions from high pressurized pipelines can be determined on the basis of hydrodynamical and thermophysical calculations of the escaped fluid. If a leakage hole occurs when carbon dioxide is onshore transported in liquid form there will be initially a large pressure drop in the pipeline Gorenz et al. [1] and the pressure will fall until the liquid becomes a mixture of saturated vapour/liquid Molag and Dam [2]. In the vicinity of the leak orifice, liquid CO₂ will escape and immediately vaporize and expand, some of the

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liquid will desublimates into dry ice, which will precipitate onto the ground, Molag and Dam [2] and Mazzoldi et al. [3]. The period of time taken for a large amount of carbon dioxide to be discharged would be short. Initially CO₂ will escape by pushing the overlying soil upwards at an explosion-like speed. After the pressure in the pipe falls the flow profile of the escaping gas will almost be as described for gaseous material transport. The expansion of carbon dioxide will occur at sonic speed and will continue to do so until the pressure ratio between the CO₂ and the ambient air is lower than about 1.9, Kruse and Tekiela [4]. As a result of the expansion also the temperature of the escaping gas will fall and a plume of cold gas will form which is then dispersed and slowly mixed with ambient air. In this study a two-phase model is applied to characterize from hydrodynamical point of view the jetting expansion and the plume dispersion of the released CO₂ in the ambient medium by means of CFD simulations. The numerical method includes multiphase flow treatment, namely a turbulent two-component model. This model is used to analyze the influence of the jet release pressure and leakage dimension on the time and spatial development of different pollutant concentration levels.

2. Numerical formulation

For the mathematical modelling of gaseous carbon dioxide dispersion resulting from accidental pipeline releases fully three-dimensional fluid dynamical equations are considered. As already recognized in the literature, e.g. Mazzoldi et al. [5], CFD models are more suitable to simulate the jetting and dispersed flow compared to other simpler models which consider only a normal probability distribution of the pollutant. In this study a two phase separated flow of the released CO₂ jet and of the ambient medium is considered. The present model treats the two-component fields as a single continuum with an effective variable density ρ and an effective variable dynamical viscosity μ , which can be discontinuous across the phase interface. The governing equation system for the total fluid consists of the Navier-Stokes equations for pressure field p and velocity vector u , as already described in Herzog et al. [6]. For a point inside the jetting fluid the volume fraction α takes the value 1 and for a point inside the ambient medium it is 0, whereas for points in the transition interfacial region it takes interim values. From the definition of the phase volumetric rate, the effective local density and dynamic viscosity of the entire fluid are estimated as

$$\rho = \alpha\rho_j + (1 - \alpha)\rho_e, \quad \mu = \alpha\mu_j + (1 - \alpha)\mu_e \quad (1)$$

where, the subscripts j and e correspond to the jetting and external fluid. The phase volumetric rate α satisfies a transport equation like

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \vec{u}) = 0 \quad (2)$$

In this paper the individual flow components are considered to be incompressible, whereas the multi-component flow has variable density and viscosity as given by equation (1). The mass fraction (concentration) C of the jetting fluid is then given by the relation

$$C = \alpha \frac{\rho_j}{\rho_e} \left[\alpha \left(\frac{\rho_j}{\rho_e} - 1 \right) + 1 \right]^{-1} \quad (3)$$

For performing the simulations the interFoam module of the open source computational fluid dynamics package OpenFoam version 2.1.1 [7] was used. The transition zone between the two flow components is treated with the volume of fluid method (VOF), which is based on the interface-capturing technique by means of the volumetric rate. To overcome accuracy in the determination of the interface position, especially when dealing with highly nonlinear interfaces, the interface is captured by using 3-D Segment-Lagrangian improved VOF-method, described in Biauxser et al. [8]. The large turbulent structures in the flow are resolved by the governing equations, while the effect of the sub-grid scales are modeled by means of the one equation eddy viscosity Large Eddy Simulation (LES) model. For increasing the computational efficiency the simulations were performed on a standard Unix cluster and involved 16 cores running in parallel. The feasibility of this numerical methodology to simulate jetting CO₂ flows, their expansion and dispersion into the ambient medium, was already benchmarked and tested in our previous publication Herzog et al. [6].

3. Atmospheric dissipation of carbon dioxide plume

Purpose of this section is to present computer simulations of realistic carbon dioxide release scenarios by following the plume dispersion in the atmosphere over a long time interval. In Herzog et al. [6] a parametrical study of high pressurized gaseous CO₂ releases from leakage holes was presented only for the first release seconds. The initially large release pressure existing when the leakage occurs will decrease in time. Due to the lack of data regarding the gradual reduction of the release pressure, following assumption was taken as hole exit boundary condition. Namely, in the first few seconds the release is considered to be high pressurized with a constant pressure p_j , and afterwards the release pressure jumps to the ambient medium pressure p_e , while the plume expansion and dispersion is continued. Based on the findings of Gorenz et al. [1] the carbon dioxide release pressure is in the range of 20 - 40 bar at the leakage orifice. At such pressures CO₂ is already below the vaporization line of the phase diagram being gaseous. The value $p_j = 30$ bar will be considered as release pressure in this paper whereas the atmospheric pressure is of 1bar. For density and viscosity of the two flow components following values were considered: $\rho_j = 1.815$ kg/m³, $\mu_j = 1.47 \cdot 10^{-5}$ kg/ms for the pollutant gas and $\rho_e = 1.2$ kg/m³, $\mu_e = 1.8 \cdot 10^{-5}$ kg/ms for the ambient air. Simulations were carried out with the pressure jump at the 2nd, 3rd, 4th and 5th computation second. Thus, in the first seconds the jet expansion of a high pressurized release was simulated, and after the pressure jump the plume dispersion was calculated for a longer time period to capture the raining down phenomena of the pollutant.

For simplicity of mesh generation the computational domain is considered to be hexahedral and the leakage hole is taken to be squared by having the leak size $\ell = 0.06$ m. In the first few simulation seconds, when the jet is released at high pressure, a high-resolution mesh in the leakage vicinity is required. Therefore, the computational grid is built, as shown in Fig. 10 (a), from hierarchical blocks with decreasing refinement degree by starting from the bottom central region where the exit hole exists. The grid size in and around the leakage hole is at least $\ell/6$. When the jump condition is adopted, the flow fields at the corresponding time step are projected on a homogeneous mesh, as shown in Fig. 10 (b), and the simulation is continued up to 200 seconds. This projection is justified by the fact that after the pressure jump the plume dispersion phenomena obtains priority compared to the initial jetting flow. Also, due to the plume expansion the computational domain is to be considered larger for including the plume over the whole simulation time. Even though the sidewise and upward boundary conditions allow the plume to cross over the domain boundaries, but this is undesirable due to the loss of information about the plume dispersion.

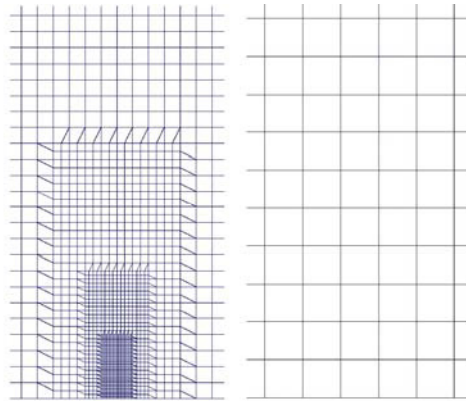


Fig. 1. Types of meshes used for the computations (a) hierarchical mesh; (b) homogeneous mesh.

Thus, after the pressure jump the computational domain is considered to have an extent of 70 m in the horizontal directions and the height of 70 m. Grid sensitivity tests were made for grid sizes in all three spatial directions of 1.5 mm, 1 mm, 0.5mm and 0.33 mm leading to meshes of approx $5 \cdot 10^4$, $1.75 \cdot 10^5$, $1.4 \cdot 10^6$ and $4.7 \cdot 10^6$ cells, respectively. The computation results on the coarsest mesh were shown not to agree with those realised on the other three finer meshes, whereas the computations on the finest mesh were too much time consuming. Thus, the mesh with a grid size of 0.5 mm was considered for further simulations.

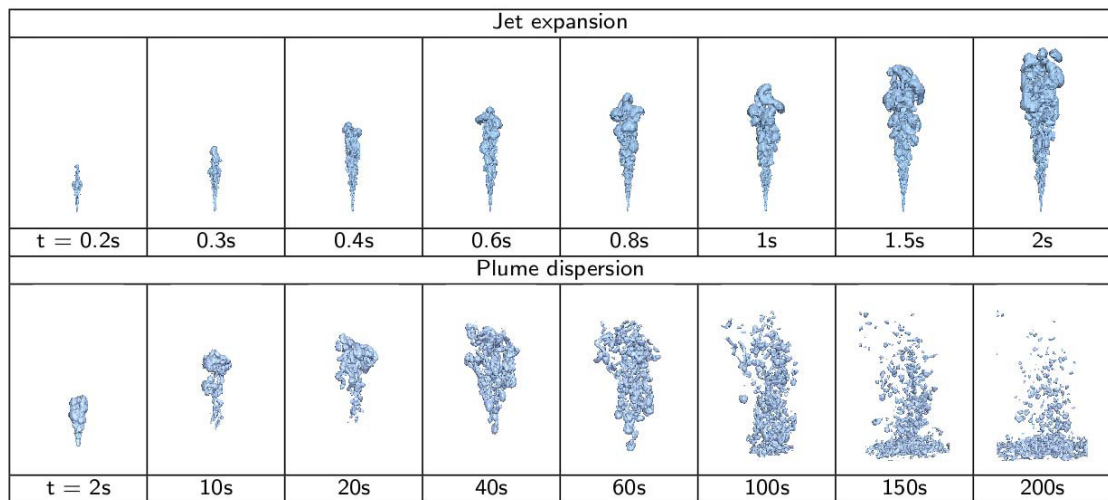


Fig. 2. Snapshots of a concentration isosurface. (top) Jet expansion in the first 2 seconds of the pressurized release, pictures height corresponds to 27 m; (bottom) Plume dispersion after the pressure jump at t=2s, pictures height corresponds to 65 m.

In the upper line of Fig. 2 snapshots of the jet expansion in the first 2 seconds are shown by means of concentration isosurfaces at different time steps. One can observe the growth of the jet in height, the lateral expansion and also the pollutant mixing with air and dispersion by building a plume. After the pressure jump at $t=2s$, the plume follows to disperse, to lift up and to grow due to the large inertial forces which overtop the gravity. When a maximum height is reached, the plume starts to rain down continuing so until the earth surface, see Fig 2 bottom line. That is explained by the higher density of the CO_2 compared to air.

To visualise the raining down of the pollutant, some snapshots of the CO_2 concentration in the horizontal plane at a height of $z = 1m$ are shown in Fig. 3. After the pressurized release the plume is uplifted and only after nearly 60 seconds in the raining down period the pollutant is reaching again this plane. The raining down continues and in the chosen horizontal plane more and more amount of pollutant exists over larger distances.

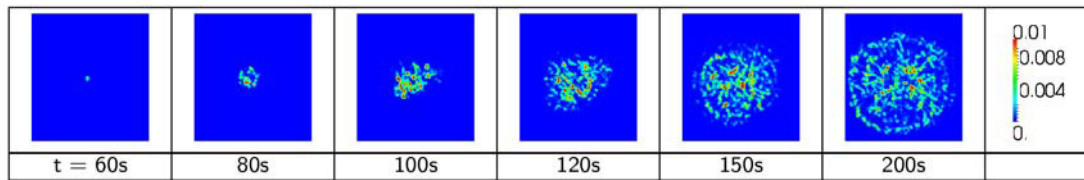


Fig. 3. Snapshots of the concentration field in the horizontal plane $z = 1m$, pictures dimensions correspond to $70 \times 70 m^2$.

Quantitative characterization of the gaseous plume dispersion is given by means of the maximal reached height and horizontal distance from the leak orifice midpoint to a certain concentration level. A guide of CO_2 concentration levels is given in Vendrig et al. [9], namely, the tolerable exposure level for humans is 0.2%, the Long-Time Exposure Limit (LTE) is 0.5%, the Short-Time Exposure Limit (STEL) is 1.5%, whereas at 2% headache and dyspnoea occur and 10% is the upper concentration level where unconsciousness, dizziness appear. These levels will be considered in the analysis of CO_2 concentration distribution as a function of the spatial coordinates and time.

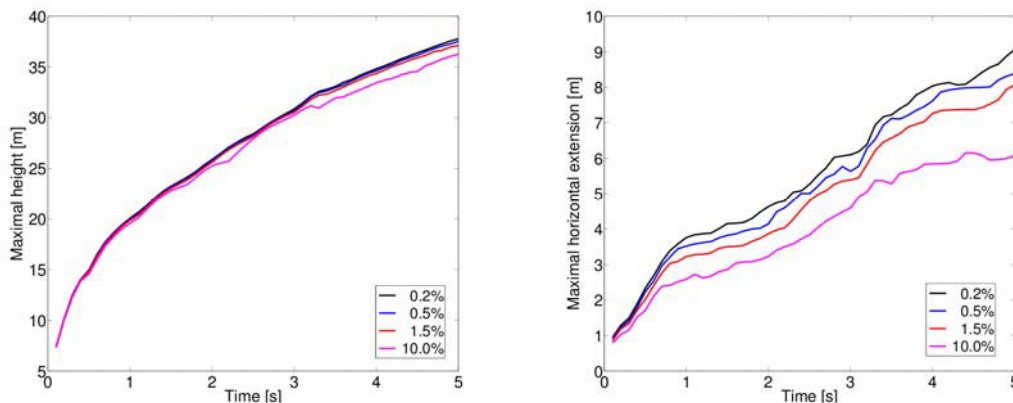


Fig. 4. Time evolution of the pressurized jet released through the leakage hole (a) maximal height; (b) maximal horizontal extent.

During the pressurized release of 5 seconds the expansion of different concentration levels is given in Fig. 4. The time evolution of the maximal height (Fig. 4a) and horizontal distance (Fig. 4b) show that the CO₂ jet expands, while lower concentrations reach higher distances than higher one. However, the maximal reached distances of the tolerable exposure level and the STEL do not differ so much, only up to 1m. The plume dispersion and raining down were further simulated when the pressure jump is adopted at the 2nd, 3rd, 4th and 5th second of the computational time. A comparison of the long time evolution of the CO₂ plume concentrations 0.2%, 1% and 2.25% is given by means of maximal reached height and horizontal distance in Fig. 5. The diagrams in the left column show the continuous increase of the reached plume height in the first dispersion period when the inertial forces still dominate. After a maximum height was achieved the gravitational forces becomes dominant because the pollutant is heavier than air, and the plume rains down. That can be earlier observed for larger concentration levels, e.g. the level of 2.25% reaches the ground starting at 100s and continue to remain on the ground. Much higher concentration levels disappear due to the plume dilution, e.g. if the pressure jump occurs at 2s then the level 10% disappear at about 50s. Concerning the maximal reached horizontal distance, right column of Fig. 5, it increases in time demonstrating the lateral expansion of the plume. After a concentration level is reaching the ground the lateral expansion is almost ceased (e.g. for concentration 2.25%). The zigzag course of the time evolution curves, evident at larger concentration levels, is due to the reached maximal distance at different plume cloud parts.

4. Conclusions and future work

A two-component turbulent CFD method was used to determine the time evolution of dense gaseous carbon dioxide plume in ambient air. After the CO₂ jet was released through a pipeline leakage hole of idealized square shape, a pressure jump was applied at certain time steps. A package of simulation results was generated to characterize the jetting expansion of the pollutant and the dispersion of the out-coming plume. It was found that, as long as the inertial forces dominates, the plume height increases up to a maximum height was reached, after which the raining-down of the dense gas cloud occurs under the gravity action. Also the time evolution of the maximal reached horizontal distance of different concentration levels has demonstrated the plume expansion. These numerical findings can provide qualitative and quantitative information for risk assessment purposes of pipeline transportation in the frame of the CCS-technology and for hazard analysis. No wind action or topographical roughness was taken into account. Future work will investigate the dispersion of CO₂ under variation of atmospheric conditions, wind velocity and direction and topographical unevenness. It is also planned to study the gases compressibility influence on the plume expansion.

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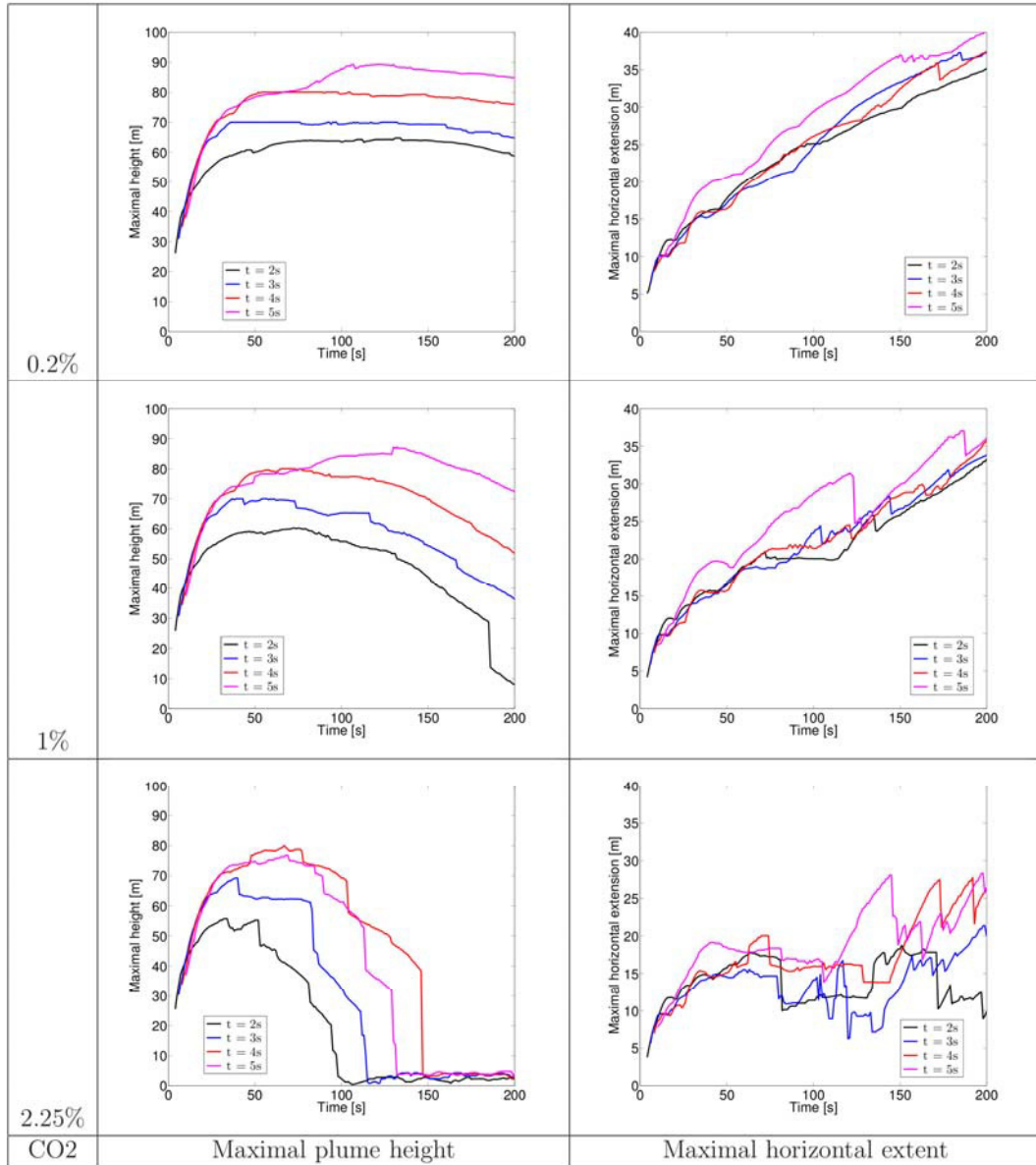


Fig. 5. Comparison of the long time evolution of the CO₂ plume concentrations 0.2%, 0.5% and 1.5% when the jet pressure jump is adopted at different time step (a) maximal height; (b) maximal horizontal extent.

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