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COMPUTATIONAL FLUID DYNAMICS STUDY ON TWO-PHASE CO_2 DISPERSION IN A NEUTRAL ATMOSPHERE

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Abstract: A large release of Carbon Dioxide (CO_2) is modelled with Computational Fluid Dynamics (CFD), (Fluent v12.1). Special attention is given to the modelling of a neutral atmospheric boundary layer (ABL) with gravity. Both the presence of non-vapour CO_2 and the high density of CO_2 require that the effect of gravity is taken into account. The ABL describes the velocity and turbulence properties as a function of height, these strongly influence the mixing and dispersion of the hazardous substance with the surrounding air. Profiles for the ABL are obtained which are constant over the length of the calculation domain. The CO_2 release is modelled as both a gas release as a two-phase release.

The results are compared and the effects of the ABL and the single/two phase flow are discussed. In addition the results are compared to results obtained by another CFD code (CFX) and by a Gaussian method. Unfortunately no experiments with CO_2 are available yet to validate the developed model. However, the results from the verification are encouraging to continue the CFD study on CO_2, with obstacles present. This advanced knowledge of CO_2 release behaviour could be applied to envisage stepwise a virtual accidental release in existing urban or industrial areas.

Key words: *CFD, CO_2, safety, dispersion, two-phase flow.*

INTRODUCTION

CO_2 dispersion modelling for accidental releases has become more and more interesting with the rise of CCS (Carbon Capture and Storage) projects in which CO_2 will be transported over long distances from the industrial source to the location of storage. Typically, the CO_2 will be transported as a liquid at high pressure (100-150 bar) and ambient temperature. One means of studying the consequences of accidental release and dispersion of CO_2 is by modelling this process using CFD.

Despite the fact that CO_2 is part of the air we breath out, it is not a harmless substance. As is shown in table 1, above 5% CO_2 will have adverse effects and can even lead to death for exposure times over 1 hour.

Table 1 Toxicity properties of CO_2 (Connolly, S. and L. Cusco, 2007).

Exposure time (min)	1% lethality (vol% CO_2)	50% lethality (vol% CO_2)
1	11	15
10	8	11
30	7	9
60	6	7

Modelling the release of CO_2 has challenging features. As the transport will be under high pressures an accidental release will most likely be two-phase. For this reason a two-phase model should be used. CO_2 is special in a way that its triple point pressure is above ambient pressure. As a result the two phases are vapour and solid instead of vapour and liquid. In addition, CO_2 vapour has a higher density than air, which requires the incorporation of gravity in the calculations. This influences the modelling of the atmospheric boundary layer.

The first part of this paper shows a preliminary study of which factors have a large influence on the results of CFD calculation on a two-phase release of CO_2. The second part shows a comparison with a study found in literature. For both sets of calculations Fluent (v12.1) is used. This is not an ideal way of validating a model, however, very little experimental data are available on the release and dispersion of CO_2.

CASE DEFINITIONS

General case

Before studying an actual situation, a sensitivity study is performed to investigate which factors are important for calculating the dispersion of CO_2 in the atmosphere. The studied parameters include: inflow conditions for the CO_2 source (1 or 2 phase, temperature, vapour/solid fraction), particle size, gravity, atmospheric boundary layer (ABL). The different inflow conditions for the source are shown in table 2. For the other variations (particle size, gravity, and ABL) case f with the highest solid mass fraction is taken.

The described situation is a full bore rupture of a 5 cm diameter pipeline. The inflow conditions are based on a pipeline with liquid CO_2 at a pressure of 100 bar and at 15°C. The resulting mass flow is calculated with Effects (v7.5) (Effects-information). The calculated mass flow rate is 33 kg s^{-1}, this value is used as input for the CFD calculation. The outflow is modelled at 1 m height. The computational domain is 300mx100mx50m. (length, width, height)

Table 2 Overview of input for the CO_2 for the general case. 195 K is the sublimation temperature of CO_2.

	Type or release	T(K)	% mass solid
(a)	Gas	293	-
(b)	Gas	250	-
(c)	Gas	195	-
(d)	Gas + Solid	195	1
(e)	Gas + Solid	195	10
(f)	Gas + Solid	195	50

Validation case

After studying the important parameters, the method is used for verification with a situation from literature (case 3 in (Hill, T.A., et al., 2010)). Release from a full bore rupture (0.5m) with starting conditions: 150 bar, 20 °C, constant enthalpy release. The CO_2 inflow conditions become: 5628 kg s^{-1} at 195 K, the vapour mass fraction is taken as 0.644 and 1, the equilibrium radius is 1.490 m. The atmospheric boundary layer is taken as D5, i.e. neutral stability class with 5 m s^{-1} wind velocity at 10 m height.

CFD SET-UP

The release of CO_2 starting from 150 bar and 20 °C results in a two phase flow: vapour and solid. Due to its high triple point pressure, CO_2 does not form droplets at ambient temperatures, instead solid particle are formed. For the studied situations shown in this paper it is assumed that the behaviour of particles can be described by the same equations as the behaviour of droplets.

For the two phase flow the DPM (discrete phase model) is used. This is a Langrangian particle tracking method. CO_2 particles are modelled as 'droplets', because for this setting evaporation (or sublimation in case of CO_2) is included. There is a two-way coupling of mass, momentum, energy, and species between the particles and the flow. As the volume fraction of non-vapour is small no VOF (volume of fluid) method is needed for the calculations.

The ABL is included based on the method described by (Tang, W., et al., 2006). The resulting profiles for velocity and turbulent kinetic energy for a D5 atmosphere are shown in figures 1(a) and (b), respectively. The profiles on inlet and outlet are very similar and correspond very well to the theoretical profiles. This allows it to be used as a tool in dispersion calculations.

The properties of CO_2 are based on the properties from the DIPPR database (DIPPR-database), which are also available within Effects. The used material properties are temperature dependent. For temperatures below the triple point temperature, the solid properties are used.

For the particles the boundary condition *trap* is chosen. This means that when a particle reaches the ground, its mass will immediately be added to the vapour phase. This mimics the situation of the formation of an evaporating pool. The difference is that in the model the vapour release is immediately and in real life the evaporation of a pool will be delayed in time with respect to the dispersion of the jet. Some other options for the particle boundary conditions at walls are: *escape* and *film*. In the first option the particles simply disappear from the domain when they reach the wall, in the second option the droplets have interaction with the wall, forming a film and smaller droplets. This boundary condition only influences particles that do indeed reach the ground.

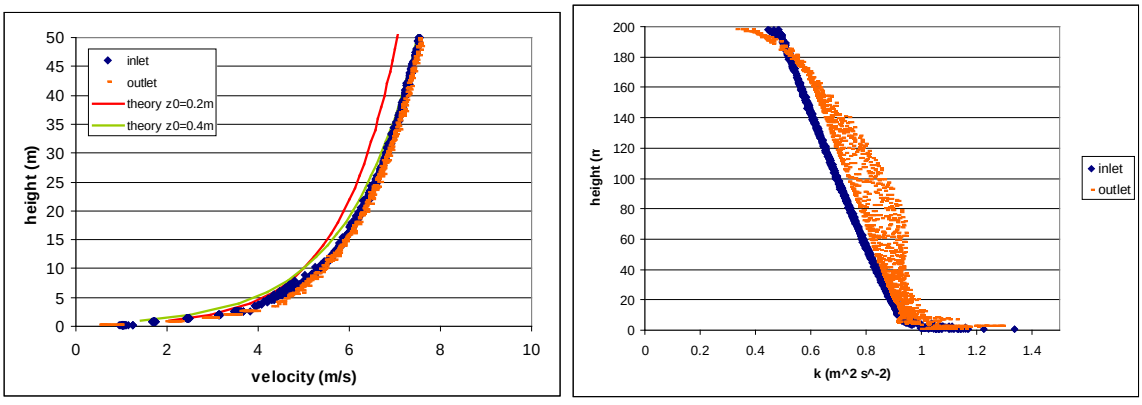

Figure 1 Results for the D5 ABL: (a) velocity profiles: theoretical and calculated; (b) turbulence profiles at inlet and outlet of domain.

RESULTS

General case

For the cases (a) to (f), table 2, the resulting mole fraction CO_2 is plotted at the horizontal line through the centre of the CO_2 source plane in the direction of the flow (central line) in figure 2 (a). All cases have been calculated with 500 µm particles without the presence of a correct ABL. Only a uniform velocity and turbulence profile was applied at the inlet.

All cases show very similar results for concentration as a function of distance. Only case (f) with 50% mass fraction solid CO_2 at the inlet boundary condition shows a different concentration profile. At a distance of about 30m the particles in case (f) reach the ground and the mass is released into the vapour phase. As the initial amount of solid is high, there is a large effect on the CO_2 concentration. For case (d) and (e) the particles also reach the ground, however, the effect is much smaller because of the lower mass fraction solid at the inlet.

Figure 2 (b) shows the CO_2 mole fraction at the central line for case (f) with several particle sizes. For both 500 µm and 250 µm diameter, the particles fall on the ground, releasing all of their mass instantaneously. This leads to a sudden increase in the mole fraction. For 100 µm diameter the particles sublimate before reaching the ground and no sudden increase in concentration is observed and the concentration decreases monotonically.

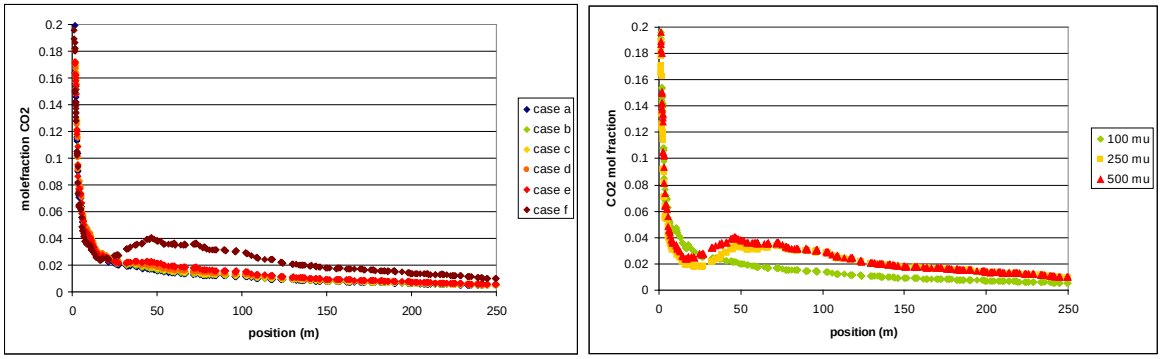

Figure 2 Results on mole fraction over central line for general case: (a) for several initial conditions from table 2; (b) for case (f) with several particle sizes.

The results shown so far were all obtained with a constant velocity (5 m s^{-1}) at the inlet of the domain. Case (f) has also been calculated with a uniform velocity profile at the inlet of the domain and with a ABL profile. The resulting mole fraction at the central line is plotted in figure 3. It can be observed that implementation of the ABL profile leads to lower mole fraction due to increased mixing by the atmospheric turbulence.

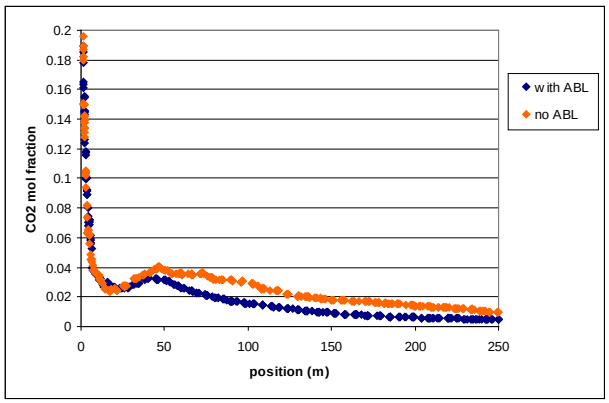

Figure 3 CO_2 mole fraction over central line for case (f), with and without ABL.

The results shown above indicate important factors for CFD modelling of releases. Important factors to take into account for accidental releases are:

- ABL
- Gravity
- Particle size (source term)

Validation case

The validation case that is introduced above is modelled with several tools: Gaussian modelling and two CFD methods. In many situations Gaussian modelling is considered as a standard way of modelling releases. For this reason it is taken as the reference. Gaussian modelling has its shortcomings in that it is not able to model correctly the effect of obstacles in the flow; however, in the study presented here no obstacles are present. For this situation these models have generally been validated. And to compare the CFD results in this situation with a Gaussian method may give information about the accuracy of the CFD model. Phast uses an example of these methods and has been used as a reference for this study.

The results from two CFD codes (Fluent and CFX) and the Gaussian method (Phast) are shown in table 3. The mole fractions at certain distances over the central line are reported. For the CFD codes two situations are calculated: only vapour and vapour with particles (0.356 mass fraction). From Table 3 it is clear that the calculation with CFX always overestimates the CO_2 mole fraction, with up to 7.3% absolute deviation. Further from the source this difference decreases. The results from

the Fluent calculations show results much closer to the Phast data, with approximately 1% absolute deviation. This deviation is nearly constant over distance. The Fluent results best resemble the Gaussian results taken as the standard.

Table 3 Results of CO2 mol fraction at central line for several calculation methods. The Phast and CFX results are taken from (Hill, T.A., et al., 2010).

	Phast	CFX	CFX	Fluent	Fluent
		Vapour	50-150 μm (0.356 solid fraction)	Vapour	150 μm (0.356 solid fraction)
200m	11.3 %	15.5 %	18.6 %	8.9 %	10.4 %
300m	8.1	11.0	12.1	6.6	7.1
400m	6.4	8.2	8.1	5.2	5.3

DISCUSSION

Before discussing the different results from the two CFD methods, it is interesting to see whether these differences are significant. The maximum difference between the two methods is obtained at 200m: 18.6% for CFX, and 10.4% for Fluent. This gives a difference of 8.2% .In Table 1 the toxicity values of CO_2 are mentioned. For an exposure time of 1 minute 11% vol CO_2 results in 1% lethality. According to CFX at 200m this value is exceeded with 7.6% whereas according to Fluent this value is not exceeded at this position. In order to obtain a correct statement on the effects of the CO_2 concentration at that point it is important to improve the CFD modelling and validate it with experiments.

Comparing the two CFD methods may give insights into which parts of the modelling are essential for the accuracy of the results. Some options will be discussed here. The first option is the modelling of the atmospheric boundary layer. This means having a correct logarithmic velocity profile over the entire domain and also a correct description of the turbulence levels over the height of the domain. In the Fluent case described in this paper the boundary layer profile is sustained over the whole length of the domain and is consistent with theoretical profiles. In (Hill, T.A., et al., 2010) the neutral atmospheric boundary is mentioned, however, it is not mentioned how it is applied or how well it is preserved. When no special care is taken it is known that an applied logarithmic velocity profile at the inlet will change over the computational domain (Blocken, B., et al., 2007). In figure 3 it has been shown that inclusion of the boundary layer increases the mixing and in this way decreases the mole fraction CO_2 found at a certain distance. More information on the treatment of the ABL by (Hill, T.A., et al., 2010) would help to interpret the significance of a correct boundary layer in the described situation.

A second option is the modelled droplet size. The CFX calculations use a droplet size distribution between 50 and 150 μm, the Fluent calculations use only droplets of 150 μm. Hill, T.A., et al. (2010) show that results are not very sensitive to droplet size. If there is any effect, it would be that larger droplets result in higher concentrations. Following this line, the Fluent results should give higher concentrations than the CFX results because of the larger droplets that are used. This is opposite what is shown in Table 3 where the TNO results give lower concentrations than the values presented by Hill, T.A., et al. (2010). The factor droplet size does not seem to be the source of the difference in the described case.

Other possible differences are: the level of turbulence in the jet flow or the atmosphere, implementation of gravity. Unfortunately very little information on these subjects is available from (Hill, T.A., et al., 2010). This prohibits a more detailed comparison.

The fact that the Fluent results closely resemble the Gaussian models which are usually taken for calculations without obstacles is very encouraging. Apparently, the developed CFD model is able to describe the dispersion in an empty domain well, when compared to a Gaussian model. Now this has been established, it is possible to use the CFD model also in more complex geometries. This is where CFD is truly beneficial over other methods.

In addition, to really validate all the numerical results shown in this paper, experimental data are required. At the moment no such data is openly available. Several programs are currently under development to perform (large scale) release experiments with CO_2, however, no results are available yet for validation.

CONCLUSIONS

A method for performing two-phase CFD calculations has been described. For the described CO_2 releases the volume fraction non-vapour remains sufficiently low to use the Discrete Phase Model. The results show that it is important to correctly model the ABL and particle size, and include the effects of gravity.

A release of CO_2 was modelled with Fluent and compared to calculations with a Gaussian model: Phast and another CFD code: CFX. The Fluent results from this work are close to the values obtained by the Gaussian model. This is good as the calculations are performed in an empty domain. In general Gaussian models have been developed for these situations. This gives confidence to also start using CFD in more complex geometries. For an actual validation of the models for CO_2 release experimental data should become available.

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