CFD MODELLING OF ACCIDENTAL HYDROGEN RELEASE FROM PIPELINES

Wilkening, H.[1] and Baraldi, D.[1]
[1]European Commission, DG Joint Research Centre, Institute for Energy, Nuclear Safety Unit, Westerduingweg 3, Pb2, 1755 ZG, Petten, The Netherlands

ABSTRACT

Although today hydrogen is distributed mainly by trailers, in the long terms pipeline distribution will be more suitable if large amounts of hydrogen are produced on industrial scale. Therefore from the safety point of view it is essential to compare hydrogen pipelines to natural gas pipelines, which are well established today. Within the paper we compare safety implications in accidental situations. We do not look into technological aspects such as compressors or seals.

Using a CFD (Computational Fluid Dynamics) tool, it is possible to investigate the effects of different properties (density, diffusivity, viscosity and flammability limits) of hydrogen and methane on the dispersion process. In addition CFD tools allow studying the influence of different release scenarios, geometrical configurations and atmospheric conditions. An accidental release from a pipeline is modelled. The release is simulated as a flow though a small hole between the high-pressure pipeline and the environment. A part of the pipeline is included in the simulations as high-pressure reservoir. Due to the large pressure difference between the pipeline and the environment, the flow conditions at the release become critical.

For the assumed scenarios larger amount of flammable mixture could be observed in case of hydrogen release. On the other hand, because of buoyancy and a higher sonic speed at the release, the hydrogen clouds are farther from the ground level or buildings than in case of the methane clouds, decreasing the probability of ignition and reducing the flame acceleration due to obstacles in case of ignition. Results on the effect of wind in the release scenarios are also described.

1 INTRODUCTION

On July 30th 2004, 15 people were killed in a severe accident in Ghislenghien, Belgium. Construction workers pierced a major underground gas distribution line causing a release of large amounts of methane. A gas explosion occurred followed by a large fire. Projectiles from the explosion were found within a distance of some hundreds of meters away from the ignition point [1]. Such events are extremely rare but the consequences could be potentially devastating. The amount of energy stored in such pipelines is large because these pipelines are operated at pressures up to about 70 bars and have a diameter of up to 2 m [2]. Because of the large pressure ratio between the pipelines and the outside environment at atmospheric pressure, critical conditions occur at the leak. Therefore the flow becomes sonic in the smallest cross-section. Due to the critical flow conditions, release rates are large reaching values as high as several GW thermal equivalent.

In the future the use of hydrogen will increase in the context of the so-called hydrogen economy. For economical reasons large amounts of the hydrogen will be produced in large scale facilities and distributed via pipeline networks. That distribution configuration is very different from today's situation where the smaller quantities of hydrogen are either produced on-site or delivered by road tanker [3]. Such type of new technology is acceptable to the society only if it does not introduce any additional risk to the population. One method of proving the lack of additional risk is by comparing the new technology to well established technologies in the same area such as natural gas pipelines. In this context it is useful to study accidental releases from large pipelines for methane and hydrogen under similar conditions. Since the experimental approach is not feasible because of unaffordable costs, numerical simulation tools can be used alternatively.

The main aim of this work is to investigate realistic accident scenarios from the numerical point of view, identifying relevant tendencies in the results mainly about the potential consequences of explosions. Although some considerations on ignition probability are included in the paper, it must be emphasized that it is not among the intentions of this work to perform a risk analysis. In section 2 we describe the CFD (Computational Fluid Dynamics) code CFD-ACE. In section 3 we describe a 2-D CFD study for 4 cases where we compare methane and hydrogen in two different scenarios. In one scenario wind is blowing with a speed of 10 m/s while in the other scenario a no-wind situation is investigated. The results obtained are discussed in section 4. In section 5 a comparison between 2-D simulations and a 3-D simulation is shown. In section 6 the conclusions are drawn.

2 CODE DESCRIPTION OF CFD-ACE

The commercial CFD (Computational Fluid Dynamics) code CFD-ACE has been used for the numerical investigation. CFD-ACE solves the governing equations for mass, momentum, energy and species mass fraction on an arbitrary grid using an implicit finite volume method. Depending on the physical problem simulations can be either steady-state or transient. Species densities are calculated using the ideal gas law. Viscosity, molecular diffusivity and thermal conductivity are calculated by the kinetic theory. Heat capacities are calculated from two polynomial temperature curve fits from the JANAF tables for two temperature ranges. Further details about the code can be found in the documentation [4]. Although CFD-ACE is an implicit code allowing arbitrary time step size, rather small timesteps had to be used due to the critical high-speed flow condition in the release zone. Although the code is used by many users and has been validated against various types of problems, we still performed our own validation simulation related to gas dispersion. This validation has been documented in [5].

3 2-D RELEASE SIMULATIONS

According to the conditions of the accident in Ghislenghien, a study of accidental gas release from a natural gas and from a hydrogen pipeline into the open atmosphere has been performed. In order to reduce the computer-time and to allow straightforward simulations as well as an easy and fast setup, simulations have been performed initially in 2-D. In the simulations high-pressure release and the influence of different wind conditions have been investigated.

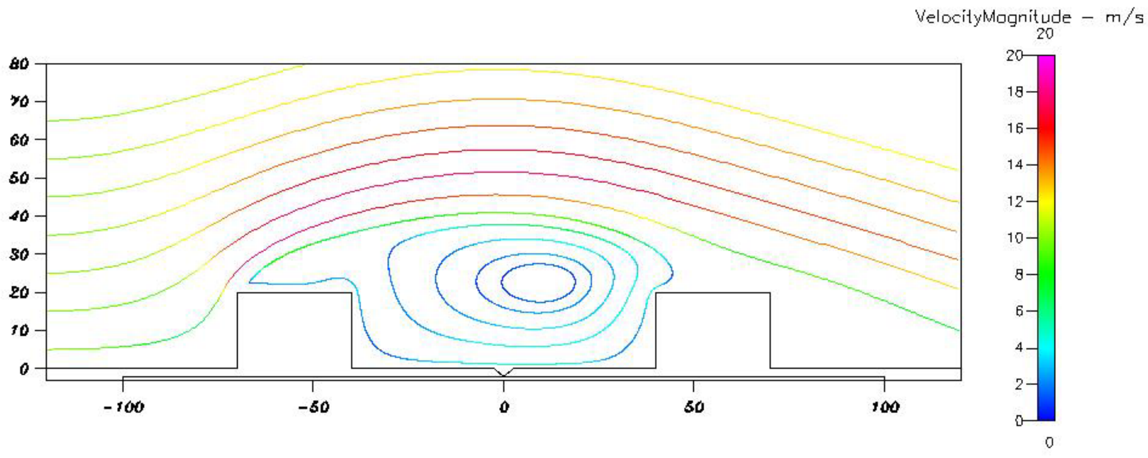

Figure 1: Streamlines of a steady-state flow field around buildings, generated by wind at 10 m/s blowing from left to right.

The initial geometry is an environmental area 240 m wide and 80 m high as shown in Figure 1. Two 30 m wide and 20 m high buildings representing factory buildings are placed in the domain. Below the ground level, a part of a pipeline is modelled as source for the dynamic release simulation. The 1 m diameter pipeline is filled with either methane or hydrogen at a pressure of 11 bars (today natural gas pipelines operate at pressures from 50 mbar to 80 bars and have a diameter up to 2 m). The underground pipeline is illustrated in the Figure 1 in the region with x between –100 and +100 m. A dug hole in the ground is shown in the figure at the coordinate x = 0 m. The leak in the pipeline is located at x = 0 m at the same position of the dug hole. The release is modelled as a flow through a 20 cm wide hole between the pipeline and the external environment. The computational grid has a total of 71300 cells with a minimum spacing of 1cm at the release position and 1.5 m at the far-field boundaries. No-slip conditions are applied to the ground and to walls.

In the cases with wind, preliminary steady simulations without any release have been performed in order to evaluate the flow-field generated by the wind itself. For the inlet, a wind-profile from 0 to 10 m/s is imposed. Hydrostatic atmospheric pressure distribution is assumed at the outlets. That flow-field has been subsequently employed as initial conditions for the release simulations. Figure 1 shows the flow field around the buildings before the release occurred in the case with wind. In the wake of the left building, a large recirculation zone has developed. When the release begins, a jet is formed just at the pipeline opening to the environment (Figure 1). As the pressure ratio between pipeline and the environment is by far critical, the flow conditions become sonic (420 m/s for methane and 1340 m/s for hydrogen) in the smallest cross-section of 20 cm.

3.1 Methane Release

The initial methane release rate is ca. 342 kg/(sm) - the unit kg/(sm) is due to 2 dimensional simulations, where the third direction is not specified, being the simulation 2-D only. Due to the high upward velocity in the release cross-section, an expanding jet is formed over the dug-hole. The jet has enough impulse to penetrate into to environment quite high up. This can be seen in the case of methane release from the streamlines shown in Figure 2. The time plotted (1s) is within early release phase. The jet reaches as high up as 40 m. This height is an overestimate due the fact that the simulation was done only in 2-D, which virtually reduces the overall friction between the jet and the surrounding environment. Next to the jet two major recirculation regions are formed causing a lot of entrainment. This is the major mechanism for mixing between the released methane and the surrounding air.

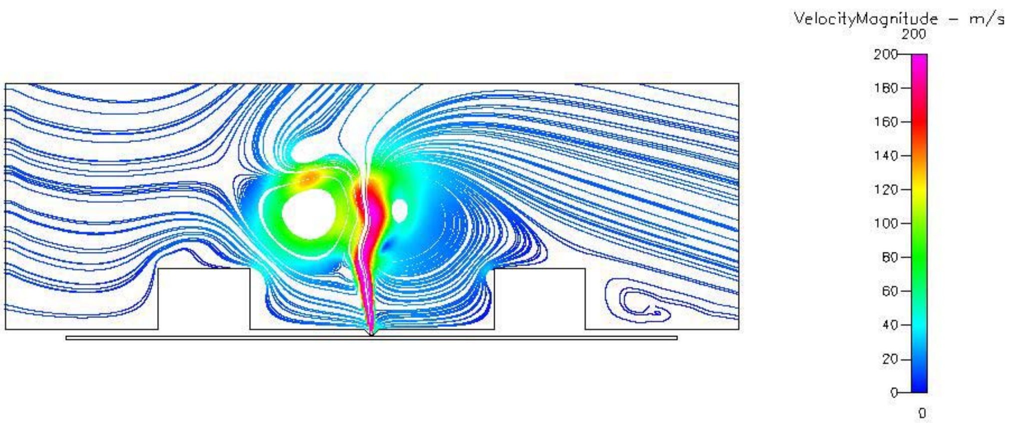

Figure 2: Streamlines just after 1 s of high-pressure release from the pipeline. Wind at 10 m/s blowing from left to right.

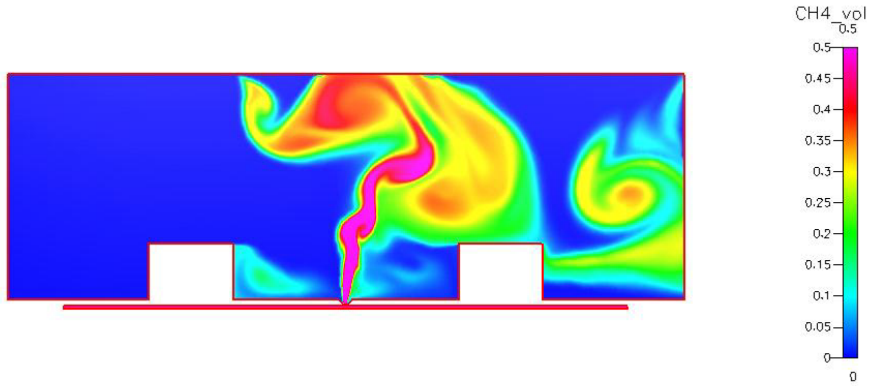

Figure 3: Methane volume concentrations after 7.5 s of high-pressure release from the pipeline and wind at 10 m/s from left to right.

Figure 3 shows methane concentrations at 7.5 s after the release started. At this time the jet has reached its maximum height in the simulation. Its impulse is not strong enough to go higher up and the flow becomes driven by the wind and by buoyancy. Inside several recirculation zones larger amounts of methane are trapped. This is e.g. the case for the recirculation zone behind the left building. Although the methane concentration is in this region only about 10% vol., it is well within the flammability limits of a methane-air mixture, which is 5.3 to 15% methane in air. In many other regions the mixture is not flammable as the methane concentrations are either too low or too high. Due to the wind a large amount of methane is transported downstream (to the right). The wind has also a stabilizing effect on the jet: the big recirculation zone above the building stays always on the right hand side as opposed to the case without wind when this regions oscillates from one side to the other. In the case with wind, the conditions within the calculation domain are nearly constant within the calculation domain at this time (7.5 s after the beginning of the release).

The second case taken into consideration is a no wind scenario with all other conditions unchanged. Figure 4 shows methane concentrations 30 s after the release started. Because of the lack of wind, methane is not as much transported sideways as in the other case. In this case buoyancy forces are more important than in the case with wind. Moreover without wind the jet develops some own recirculation, which is able to trap some methane near one of the buildings. It must be emphasized that without wind there is no real stabilizing effect since the jet inclination changes from left to right all the time (compare Figure 4 and Figure 5-right). As a result the concentration distribution changes with time on larger scale.

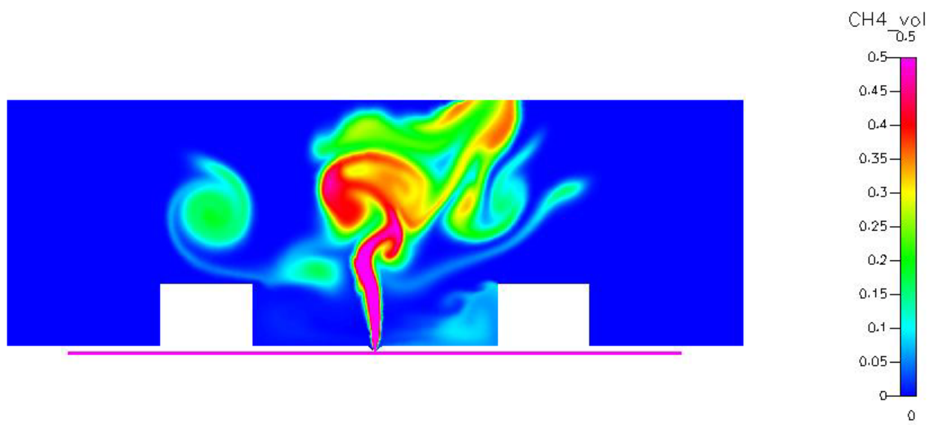

Figure 4: Methane volume concentrations after 30 s of high-pressure release from the pipeline with no wind.

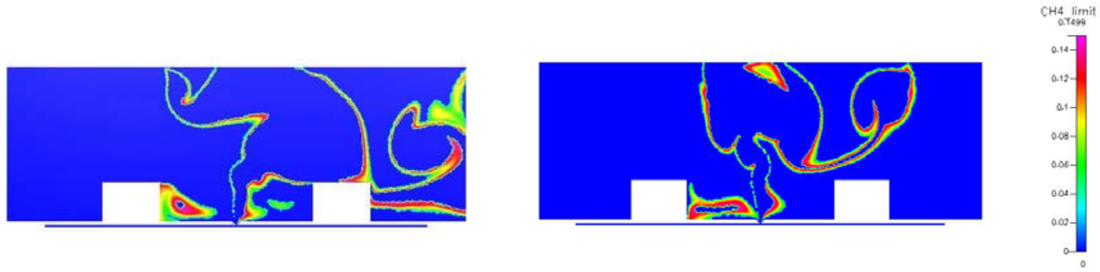

Figure 5: Methane molar concentrations for the wind (left) and no-wind (right) case both 7.5 s after the high-pressure release starts. Only regions with concentrations within the flammability limit are shown between 5.3 and 15 %. All other concentrations are set to 0 % to highlight only the flammable regions.

In Figure 5 the regions outside the flammability limits are coloured in blue both for the wind case and for the no-wind case. Flammable mixtures can be observed in two regions: within a narrow band between the jets rich mixture and the outside lean mixture, and in several recirculation zones e.g. next to the left building. Due to the narrow flammability limits of methane most of the released methane is outside the flammability limits. As recirculation zones are more stable and the flammable mixture area is much larger due to the mixture entrapped in the recirculation zones, the probability of an accidental ignition causing a large fire or even an explosion is larger in the wind case than without wind.

3.2 Hydrogen Release

For the hydrogen pipeline release scenario the same conditions have been applied as in the methane case. The same high-pressure release from a pipeline at 11 bars is assumed. In the case with wind, the simulation has been started from a steady-state simulation without release using the same grid as in the methane scenarios. In the subsequent release simulation, the release rate is ca. 115 kg/(sm) hydrogen.

Figure 6 shows hydrogen concentrations 4 s after the beginning of the release with a wind of 10 m/s blowing from left to right. At this time the jet has reached its maximum height of ca. 40 m. Its impulse is not strong enough to go higher up and the flow becomes wind and buoyancy dominated. Inside several recirculation zones larger amounts of hydrogen are trapped. This is e.g. the case for the recirculation zone on top of the right building. The hydrogen concentration is here only about 30% but well within the flammability limits of a hydrogen-air mixture, which is 4 to ca. 74 % hydrogen in air. Due to the higher velocities and the larger buoyancy force compared to the methane case, very little hydrogen can be found in the close vicinity of the ground, where there is a higher probability of ignition. This configuration makes ignition more unlikely and, in case of ignition, it reduces the risk for effective flame acceleration because of the lack of obstacles that are normally located at ground level. It is well known that obstacles can increase the turbulence-combustion interaction, producing significant acceleration of the flame.

The second hydrogen case is a no wind scenario with all other conditions unchanged. Figure 7 shows hydrogen concentrations 4 s after the beginning of release. Without wind hydrogen is transported upwards only by forces due to impulse of the jet flow and due to buoyancy. Also in this case the jet develops some own recirculation, which is able to trap some hydrogen. This effect is reduced compared to the methane scenarios due to the higher jet velocities and the larger buoyancy in the hydrogen cases. The amount of hydrogen close to the ground or to buildings is rather small compared with the methane cases.

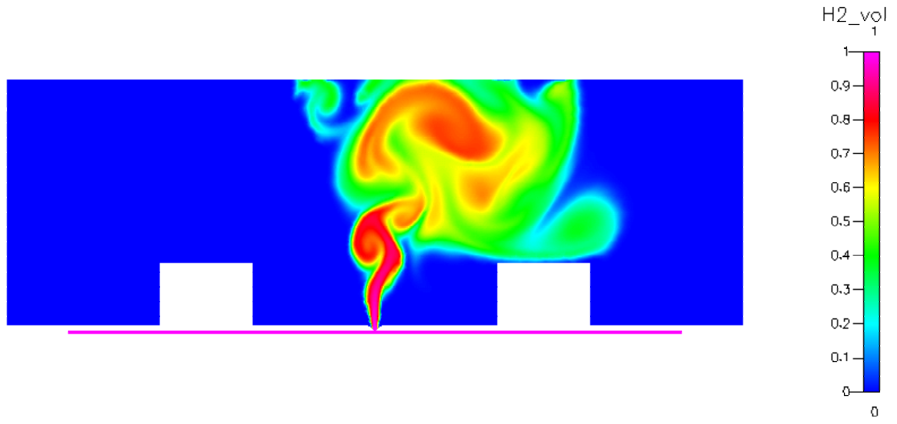

Figure 6: Hydrogen volume concentrations after 4 s of high-pressure release from the pipeline and wind at 10 m/s from left to right.

In Figure 8 the regions outside the flammability limits are coloured in blue both for the wind case and for the no-wind case. Similar to the methane cases, flammable mixtures can be observed in the two same situations. In this case, the flammable band between the jet rich mixture and the outside lean mixture is wider than for methane. On the contrary, the recirculation zones (e.g. on top of the right building) are in general smaller than for methane. The situation differs from the methane cases because most of the released hydrogen is within the flammability range due to the wider flammability limits of hydrogen.

4 DISCUSSION

The results presented in section 3 provide only a qualitative overview. Methane and hydrogen have very different properties that may affect an explosion event such as the one in the Ghislenghien disaster. Some important properties concerning combustion are summarized in Table 1.

The major difference between methane and hydrogen is the 7 times wider flammability range of hydrogen. The 8 times lower density of hydrogen is partially compensated by it's higher heating value in the calculation of the global thermal energy. Therefore in Figure 9 and Figure 10 released thermal chemical energy is plotted rather than mass. Such normalization allows easier comparison of hydrogen and methane. (Simple division with the lower heating value of the gases would result in masses.) The unit GJ/m is still due to 2 dimensional simulations. The simulation has been stopped in all cases, when no more significant changes were observed when watching the animated results.

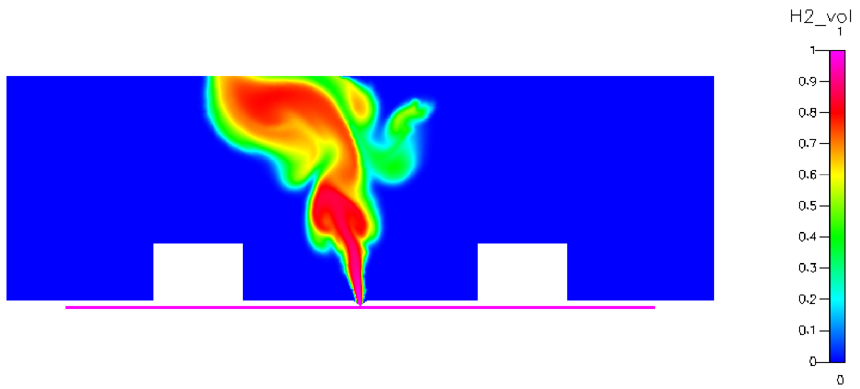

Figure 7: Hydrogen volume concentrations after 4 s of high-pressure release from the pipeline with no wind.

Figure 8: Hydrogen volume concentrations for the wind (left) and no-wind (right) case both 4 s after the high-pressure release starts. Concentrations within the flammability limit are shown, that is between 4 and 74 %. All other concentrations are set to 0 %.

In Figure 9 within the first second of release no significant difference among all four cases are observed. The higher critical flow velocity (ca. 3 times higher for hydrogen) in the release of hydrogen is compensated by the higher density of methane (8 times higher than hydrogen) and by the higher heating value of hydrogen. From ca. 1 s onwards, some gas is leaving the calculation domain via the boundary, first hydrogen (due to the larger critical velocity) and later methane at ca. 1.5 s. Generally larger amount of methane is accumulated in the calculation domain than hydrogen because of the lower buoyancy of methane and the smaller impulse of the methane released jet. Larger amounts of methane and hydrogen are accumulated within the computational domain for the wind cases than for the no-wind cases. The wind transports methane and hydrogen sideways and therefore keeps them in the computational domain rather than let the gases escape through the top boundary of the domain. Moreover the gases are trapped in the recirculation zones generated by the wind itself.

	Hydrogen	Methane
Density [kg/m3] (NTP) and relative to air [-]	0.0838, 14 times lighter than air	0.6512, 1.8 times lighter than air
Lower heating value [kJ/kg] (chemical thermal energy)	119 972	50 020
flammability limits [vol. %]	4 – 74	5.3 –15
max. laminar burning velocity [m/s]	3.25	0.44
relative radiative heat transfer [%]	5 –10	10 –33

Table 1: Mean combustion properties of hydrogen and methane.

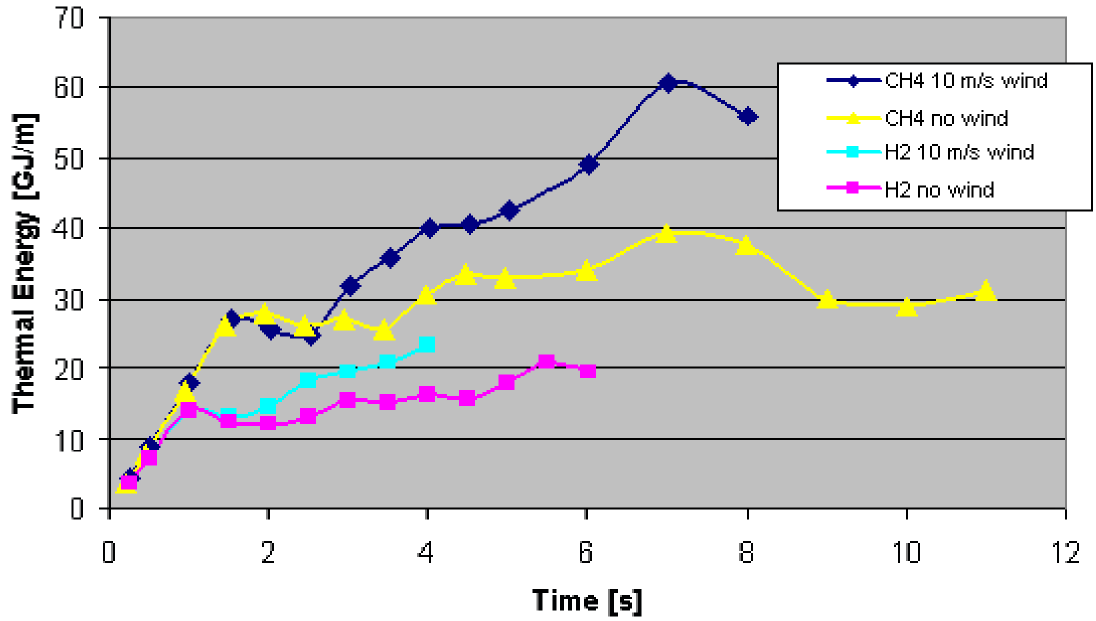

Figure 9: Comparison of integrated chemical thermal energy within the environment (computation domain only) for methane and hydrogen - wind and no wind case.

Figure 10 shows the flammable part of the gases released into environment within the calculation domain in terms of thermal energy. The situation is reversed compared to Figure 9. The flammable part of hydrogen is much larger than the one of methane due to the much wider flammability limits of hydrogen (see Table 1). In general the ratio between flammable and total energy (or mass) is about 10 to 15 % for methane and 60 to 80 % for hydrogen. As the total release energy within the flammability limits is much larger for hydrogen, a possible hydrogen explosion might be worse compared to methane especially taking into account the higher chemical reactivity for hydrogen (see laminar flame speeds Table 1). It must be emphasized that most of the flammable hydrogen is far away from the ground or building making such events less likely.

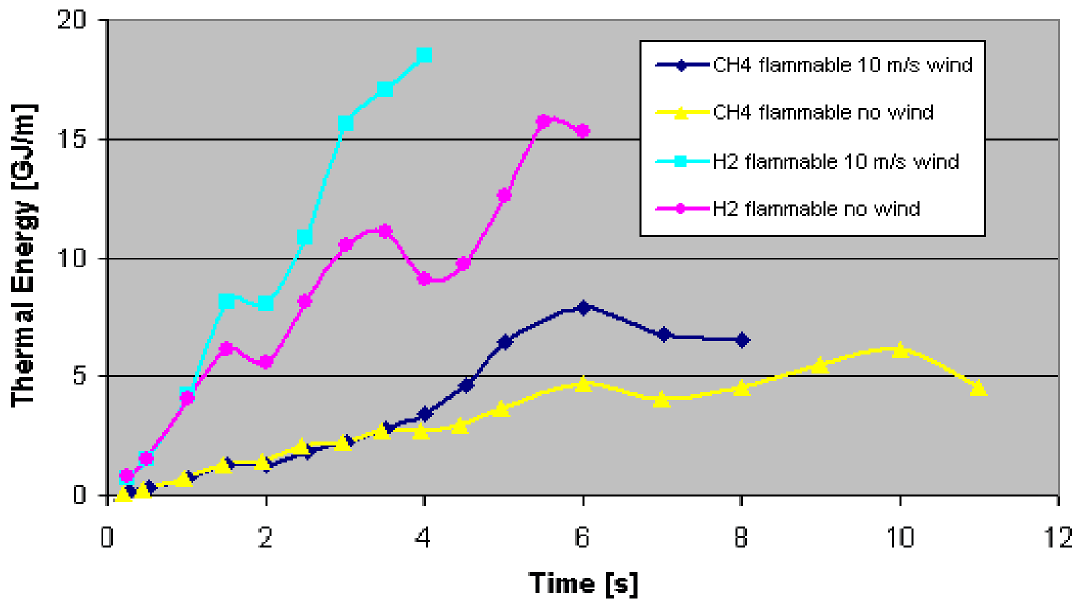

Figure 10: Comparison of integrated thermal flammable energy within the environment (computation domain only) for methane and hydrogen - wind and no wind case.

5 COMPARISON BETWEEN A 2-D AND 3-D SCENARIO

In sections 3 and 4, the results from 2-D simulations were presented and discussed. These simulations quasi assumed an indefinite wide jet in the third non-modelled dimension. This approach is capable to save computing time and resources, which typically increase in 3-D by at least one to two orders of magnitude. A 3-D calculation has been performed in order to show similarities between 2-D and 3-D simulations.

Figure 11 shows an outline of 3-D geometry similar to the 2-D geometry used in section 3. The buildings are 8, 10 and 15 m high, 30 and 40 m wide and 60 and 70 m long. Also a part of the pipeline is modelled as in the 2-D case (pipeline pressure 11 bar). The release is modelled as a flow through a circular hole of 30 cm diameter between pipeline and environment. The computational domain is about 130 m high, 260 m wide and 400 m long and was meshed with about 3.5 millions cells. The grid is a so-called hybrid grid since cells are hexahedrons, prisms, pyramids or tetrahedrons. The computation has been performed on high performance computing cluster on 16 CPU's in parallel. For comparison the hydrogen release case with 10 m/s wind was chosen.

In Figure 11 the 4 vol. % hydrogen (lower flammability limit) iso-surface is shown 3.92 s after the high-pressure release starts. The release rate is about 42 kg/s hydrogen. In the lower part of the plume the outer part of the narrow jet can be observed. In the upper part the transition from jet dominated to wind and buoyancy dominated convective transport is illustrated. The jet did not reach up as high as in the 2-D case as it could expand horizontally in two directions rather than one as in the 2-D simulation. Also viscous effects slow down the jet more in 3-D than in 2-D because the surface to volume ratio of the jet is larger in 3-D than in 2-D. In fact in reality the jet in the 3-D simulation is for large parts nearly axisymmetric rather than plain as assumed in the 2-D simulations. Nevertheless axisymmetric simulations would not allow studying the effect of wind.

Figure 12 shows a vertical section through the jet. The jet is much more narrow than in the 2-D simulations. A wide flammable area is formed between the jet rich mixture and the outside lean mixture as in the 2-D case (see Figure 8).

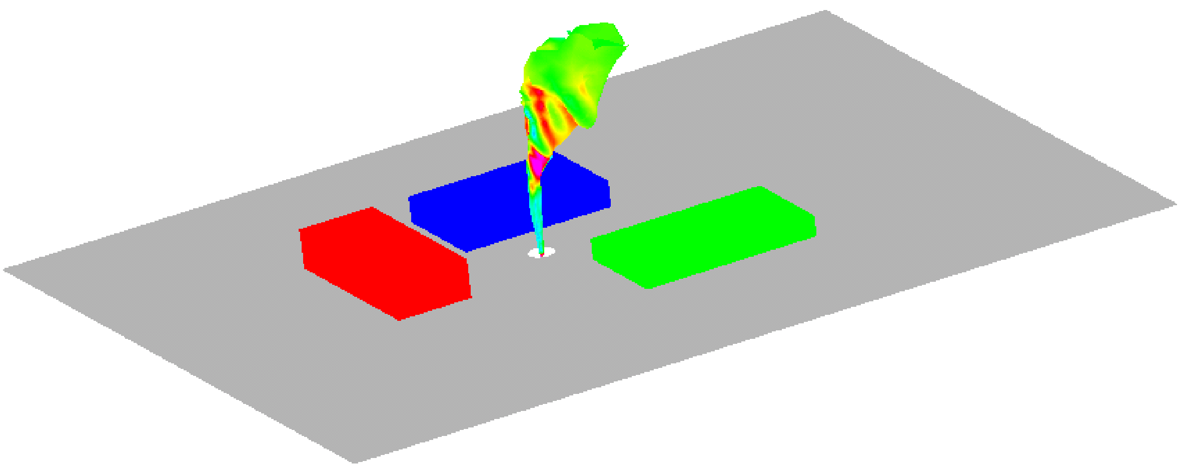

Figure 11: 3-D hydrogen release simulation, shown is a 4 vol. % hydrogen isosurface colored with velocity magnitude (0-25 m/s from blue to pink) 3.92 s after the high-pressure release starts. Wind at 10 m/s blowing from left to right.

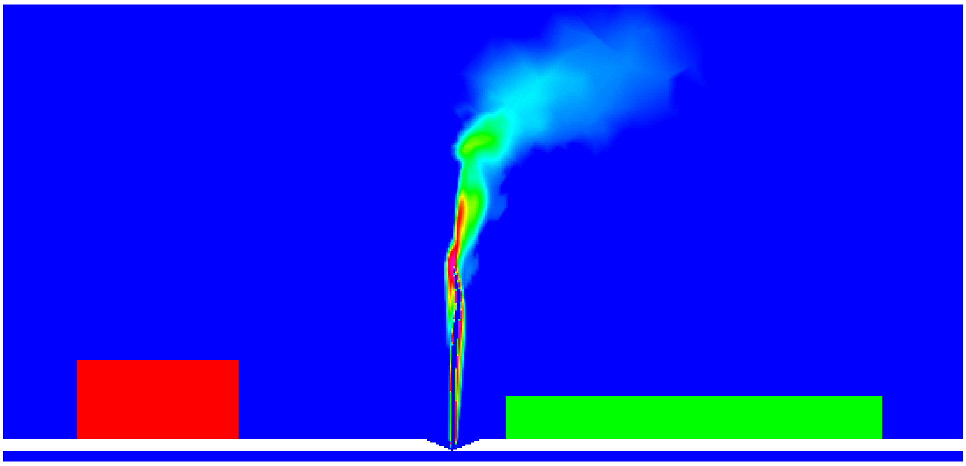

Figure 12: 2-D vertical cut of the 3-D release simulation. Hydrogen volume concentrations 3.92 s after the high-pressure release starts. Shown are only those concentrations within the flammability limit.

The jet behaviour is partially different in 3-D than in 2-D as can be seen from Figure 6, Figure 8, Figure 11 and Figure 12. This is due to the stronger and more realistic mixing in 3-D than in 2-D simulations. Nevertheless 2-D results are still useful. This can be seen from Figure 13 comparing it to Figure 9 and Figure 10.

Figure 13 shows the integrated hydrogen mass, within the environment. The total hydrogen mass and the mass of hydrogen within the flammability limits are compared. Since no hydrogen has left the computational domain within the simulated time, the total mass refers to a nearly straight line where the slope indicates the hydrogen release rate into the environment. In addition the amount of hydrogen within the flammability limits is plotted. The ratio between flammable and total mass varies between 60 to 80 %. These values are similar to those observed in the 2-D simulations.

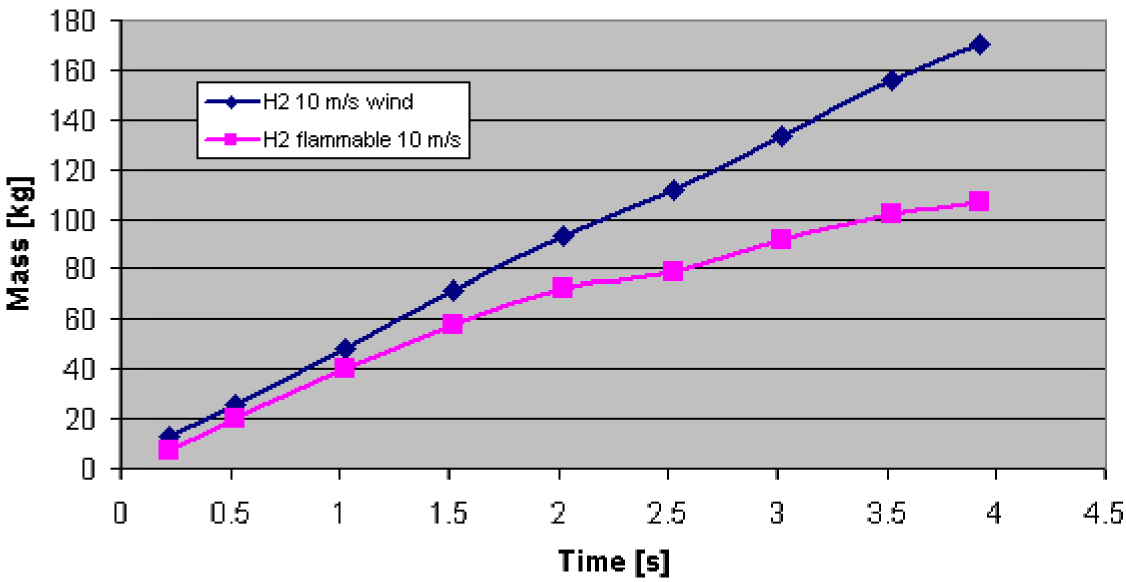

Figure 13: Total and flammable hydrogen mass within the environment for the 3-D simulation with 10 m/s wind blowing.

6 CONCLUSIONS

In this paper 2-D and 3-D CFD simulations from accidental methane and hydrogen releases from pipelines have been presented. By comparing 2-D to 3-D results it was shown that some useful results could be obtained also from 2-D simulations. The 2-D approach was followed because of the prohibitive computer run-time of a fully 3-D simulation. With 2-D calculations, it was possible to investigate different configurations such as environments with and without wind.

Especially in case of methane release, the configuration with wind could be more serious than without wind, since some flammable mixture might be accumulated in larger recirculation zones behind buildings. As these zones are rather stable and close to the ground and buildings, ignition is possible for such kind of scenarios.

The total amount of thermal energy of methane and hydrogen is almost the same when the pipeline operating pressure (pipeline pressure larger than critical pressure) and hole size are the same. The amount of flammable mixture is much larger in the case of hydrogen release, as the flammability range is much wider for hydrogen than for methane. Because of the different density, buoyancy effects are stronger for hydrogen than for methane. Moreover the sonic speed of hydrogen is much larger than that of methane. These two physical properties cause a smaller accumulation of hydrogen than methane in the regions close to the ground level. At ground level or close to buildings, ignition is more likely. Moreover if an explosion occurs, the presence of obstacles near the ground can increase the flame acceleration.

Because of the limited number of simulations performed, it was not possible to evaluate if the larger amount of flammable hydrogen is compensated by the fact that hydrogen tends to escape more quickly from the ground level than methane. Further investigations are required. In order to assess whether hydrogen pipelines could cause a higher risk of explosions than methane pipelines, a risk analysis is necessary and that goes beyond the scope of the paper.

REFERENCES

1. Fifteen die in Belgium gas blast, BBC NEWS, http://news.bbc.co.uk/2/hi/europe/3939087.stm
2. Geiger, J., Was für’ne lange Leitung, Energie Waldeck-Frankenberg GmbH, http://www.vew-korbach.de/aktuelles/ewfdirekt/lange-leitung.htm
3. Ogden, J.M., Steinbugler, M.M. and Kreutz, T., A comparison of hydrogen, methanol and gasoline as fuels for fuel cell vehicles: implications for vehicle design and infrastructure development, Journal of Power Sources, Vol. 79, 1999, pp. 143–168.
4. CFD-ACE, 2004, User Documentation, ESI Group, Paris, France.
5. Heitsch, M., Wilkening, H. and Baraldi, D., CFD-modelling of gas-transport and mixing phenomena in the Battelle experimental facility for nuclear safety applications, 7th World Congress of Chemical Engineering, 10 - 14 July 2005, Glasgow, in print.