Interpretation of geometrical effects in consequence modelling. Comparison study between the commercial consequence assessment tools FLACS and PHAST for flammable gas dispersion

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Preface

This master thesis marks the final part of a two year master`s degree in process safety at the University of Bergen (UoB).

The main work of the thesis has been performed as a collaboration between the University of Bergen and GexCon AS. The objective was to understand differences seen in results given by more or less advanced tools for modelling the flammable gas dispersion phenomena. Computer simulations, using FLACS and PHAST tools have been performed at the GexCon AS Fantoft office in Bergen.

Thanks to;

- Bjørn J. Arntzen at University of Bergen, for arranging and helping me, getting started with the work.
- Vincent Van den Hoogenband for originating the idea of the thesis work.
- Jorunn Gulbrandsen and Aibel AS for allowing me to finish my thesis by reducing my working hours. I would also like to thank good Aibel-colleagues at the technical safety department for the cheerful and good working environment.
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I especially would like to thank and express my appreciation to my supervisor at GexCon Nicolas Salaün for his patience, encouragement and great support throughout the thesis work. You were just as much a friend as you were my supervisor.

I finally will also thank my Silje for making it possible for me to finish my master`s thesis. Thank you for taking such good care of Agnes (both day and night) so I could finish the thesis work. I look forward to spending more time with you and Agnes in the near future. The upcoming weekends are from now on sacred.

Eivind N. Ekerold
April 2. 2014

Abstract

Computational fluid dynamics and integral consequence modeling is today a crucial part of safety assessments worldwide. The models are widely used to predict the effects of ventilation patterns, hazardous gas dispersion, flammable potential, toxic exposure or fire and explosion loads. In addition, the consequence assessment is combined with likelihood considerations in order to build-up risk assessment and hence to compare to risk-acceptance criteria. All these aspects are one way or another analyzed and open for optimization when considering consequence or risk based design of industrial facilities.

Implicitly, discharge considerations (prior to dispersion) and explosion modeling aspects (subsequent to flammable gas dispersion in case of ignition) are kept in mind when analyzing the comparisons performed since the consequence assessment cannot only be related to gas dispersion and must be seen as a complete threats identification process.

Of course, it is recognized that there are significant differences between an integral model and a CFD approach. Simplified integral approaches (like the one included in the DNV PHAST tools but also like the ones promoted in the TNO Yellow Books [9] or in other commercial packages for safety assessment) consider simplifications and empirical assumptions. Mainly, they do not include a straightforward way of dealing with a detailed and complex geometry (influence of vessels, piping, walls etc…) nor they can consider terrain and topography. The integral approaches require less computational time, are easier to handle and are much more cost efficient (considering use within the range of applicability…), thus by all means, less labor intensive but thus also less case specific.

On the other hand, CFD codes (like FLACS, CFX, KFX…) are taking into account the effects of complex geometries within the dispersion simulation process. CFD modelling requires significant additional efforts in terms of simulation time, hardware capabilities, skills, man-hours… and thus overall cost.

The optimal goal of the safety engineer is to use an approach that is suited for the problem to be solved. Also, and by all means, not only accuracy but also conservatism are evaluated within safety engineering.
Subsequently, and despite the intrinsic differences listed above, CFD tools (like FLACS) and simplified tools (like PHAST) are observed to serve the same purposes in consequence analysis within the industry.

Practically, this study progressively examines and compares the results given by the CFD model FLACS version 10 and the integral model PHAST version 6.6 for a set of various hazardous gas dispersion scenarios. The following aspects have been analyzed;

- An academic investigation has primarily been performed: ideal steady state free field gaseous jets have been simulated within PHAST and FLACS in a range of conditions where both tools should perform well.
- Experiments from the large scale Kit Fox trials have subsequently been simulated with both the models for the trial 0604, making it possible to compare the tools with real scale releases.
- Following this, one has tried to represent / simulate impinging jets and releases into a congested geometry consisting of pipes resembling a ventilated offshore module, moving slightly away from the theoretical range of applicability (but nevertheless sticking to what is observed in the industry). Attempts to represent the geometrical effects in PHAST have been made. A set of various flow rates and resulting gas clouds have been considered and analyzed.

- Eventually, releases in a realistic process module have been simulated.

Among all the previously described cases, comparison of the centerline concentration decays and resulting flammable potential (as the flammable mass within the gas cloud) have been assessed with varying mass flows and wind conditions.

The initial simulations for free field jets in FLACS and PHAST gave overall good agreement between the models in terms of concentration decay along a centerline profile and for flammable mass. The effect of ground has been studied including releases at 10 meters and at 1.5 to 2 meters above ground level. The dispersion model in PHAST (when user defined discharge was used in PHAST) was most comparable with the FLACS results for concentration decay along a centerline profile. The results were within 20% deviation for almost all cases for centerline profile concentration decay. However, simulations run by the FLACS model gave the largest flammable plumes for most of the scenarios run. The comparison effort concludes that the free jets are within a range that may give the same risk assessment for the open free field flammable scenarios.

To comfort this initial statement and to move slightly towards some concepts of introducing effects of geometry over dispersion, an experimentation used in the two tools validation framework was also analyzed in order to give more robustness of the comparison and also to get insight of the "validation range" concepts. For the particular studied case, FLACS performed very well in both near and far field, on the conservative side. PHAST was still in relatively good agreement with the experiments while very close to the +/-30 % deviation threshold.

Subsequently, the level of congestion in which the gas cloud disperses was slightly increased. Jets impinging into pipework were run at a relatively low mass flow rate (0.59 kg/s, high likelihood) and at a relative large mass flow rate (9.48 kg/s, lower likelihood). Observations show that small releases are quite dependent of their immediate environment as the impingement may fully control the behavior of the jet (a tunneling and an obstruction effect were seen). The large jet (9.48 kg/s) completely filled the geometry and thus represented a different phenomenon. However, even though the geometrical effect influences the gas cloud shape for the smaller release, the contour of the potential consequences were not that different at a consequence assessment level and neither was the flammable mass. For the largest flow rate interacting strongly with the geometry, three times as high flammable mass was observed in FLACS compared to the PHAST model, indicating different consequences assessments by the models and a large violation of the threshold for the use of the tool outside its main range of application.

The thesis is written down as a technical safety scientist would perceive the situation at hand. Advanced details of the chosen models are therefore ruled out of the thesis scope. The focus will be on applicability and the domain where the different models give comparable results. Recommendations on optimized use of the tools available are eventually suggested.

Nomenclature

ALARP	As Low As Reasonably Practicable
CASD	Computer Aided Scenario Design, FLACS Preprocessor Tool
CFD	Computational Fluid Dynamics
CMR	Christian Michelsen Research
DAL	Design Accidental Load
DNV	Det Norske Veritas
DNS	Direct Numerical Simulation
ER	Equivalence Ratio
ERP	Equivalence Rougness Pattern
FDS	Fire Dynamics Simulator
FEED	Front End Engineering
FLACS	Former denomination of Flame acceleration simulator, only FLACS used now for the software product (note in capital letters; flacs is the name of the numerical solver)
FLOWVIS	Flow Visualization Tool, FLACS Post Processing Tool
KFX	Kamelon FireEX
LFL	Lower Flammability Level
LES	Large Eddy Simulation
LNG	Liquefied Natural Gas
NORSOK	Norsk Sokkels Konkurranseposisjon
OAT	One at a Time
PPM	Parts Per Million
PFD	Process Flow Diagram
PHAST	Process Hazard Analysis Simulation Tool
RANS	Reynolds averaged Navier Stokes
UDM	Unified Dispersion Model
UFL	Upper Flammability Level
UoB	University of Bergen
UK	United Kingdom
URP	Unified Roughness Pattern

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1 Introduction

1.1 Motivation

In the process, petro-chemical, nuclear … or other industries, processing flammable and explosive volatile substances creates a risk of unwanted releases from process containment with subsequent fire and or vapor cloud explosion as a result. The Buncefield accident in December 2005 clearly challenged the existing knowledge of vapor cloud explosions and showed that the need for developing better risk assessments is necessary in terms of limiting the probability of such incidents and mitigating the possible consequences [27]. The same concerns exist with potential toxic releases in the chemical industry or even within the oil & gas industry (H_2S, SO_2, NO_2… are examples). A significant record of accidents from the past is easily obtained in the literature (Bhopal, …).

The Norwegian oil and gas industry has been spared for large-scale incidents over the last twenty years since the Alexander Kielland accident. However, the Norwegian oil and gas sector has not been spared for incidents that may have resulted in severe consequences. The yearly report Risiko i Norsk Petroleumsvirksomhet [10] gives an updated risk picture of the risk level at the Norwegian sector.

Subsequent Figure 1-1 shows the amount of reported gas leakages over the last twelve years.

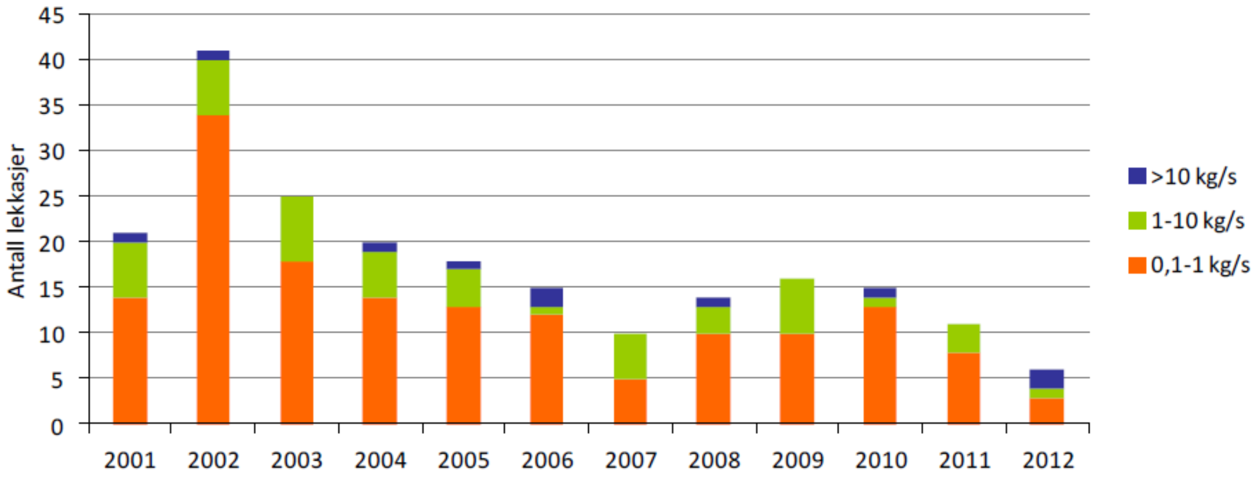


Figure 1-1 *Gas leakages on Norwegian sector with distribution of magnitudes from 2001-2012 [10]*

A potential leakage will, depending on the chemical at hand, wind conditions, leakage rate etc., disperse and generate an explosive or toxic gas cloud. Ignition of this cloud may cause severe damage to personnel, environment and material assets within a given perimeter. It would therefore be an obvious goal for any safety scientist or personnel working in the industry to reduce the likelihood for an accidental leakage and/or the consequences of an ignition of this leakage.

Eventually, designing facilities that are able to withstand the consequence loads is also an option.

A typical consequence tree is illustrated below in Figure 1-2. It depicts the events following a release of a flammable substance.

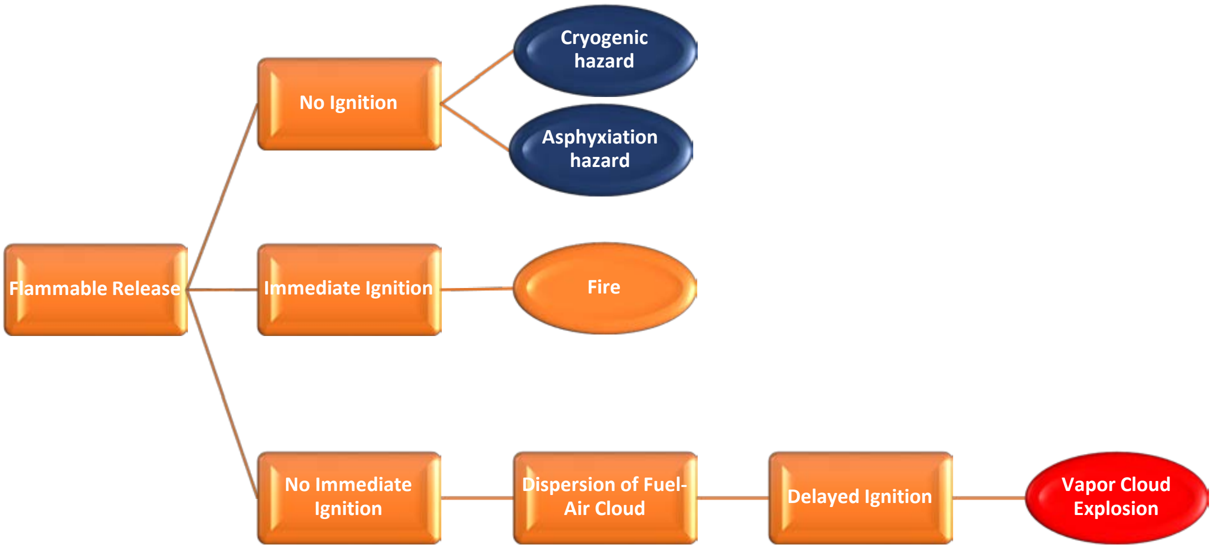


Figure 1-2 *Event tree showing the sequence of events leading to a hazardous scenario.*

Today, numerous different computer models simulate hazardous events such as material discharge, gas or two-phase dispersion in air, fire and/or explosion loads with time.
There are however large differences between the models in terms of methodologies and applicability of the different software packages.
At this point in time, it doesn't exist any univocal methodology describing what kind of model should be chosen for a particular kind of hazardous scenario. The safety engineer has thus a wide choice of computer software to cope with for each particular problem and it is its responsibility to get insight of what these tools contain in order to make a selection that promote as much accuracy as possible.

This statement is driving the content of this thesis.

1.2 Objective

Studying hazardous gas dispersion is today an important and central part of risk assessment. Quantitative results used for decision making is a critical aspect of the evaluation of risks associated with a specific process design. Hazardous gas dispersion simulations by CFD can today be used for evaluating positioning of gas detectors, evaluating gas spread with potential accumulation and by that giving an indication of the explosion risk, thereby aiding engineers in a safer design and to improve mitigation measures. The dispersion simulations also gives information regarding the dimensioning gas cloud through probabilistic analysis summarized in the DAL report for each installation [18]. CFD dispersion models can also be used to simulate exhaust stacks releases, aid in accident investigation, perform wind chill analysis…, to mention a few areas.

Several other quantitative tools are used for hazardous gas dispersion assessment. Simpler empirical codes like PHAST and TRACE also exist on the market. These codes are cheaper and less labor intensive compared to CFD codes which requires detailed knowledge and analyst skill to perform simulations.

If, and when a simple model compared to a CFD code can equally well represent the risk picture, the simpler model would be preferred due to time constraints for projects and the model's low cost compared to the CFD models.

On the other hand, a quicker access to a result shall not corrupt the representatively of the results and lead to a wrong / partial perception of the risk picture.

The simpler codes do not have the inherent ability to represent the environment where the dispersion takes place. The geometrical impact may be segregating walls, building, pipes or valves in the domain of the simulation, often related to mitigation purposes. The CFD codes can match this complexity of almost all environments where any form of congestion / obstacles affects the flows. This is seen for instance in an offshore installation and is widely used for this purpose. Many have therefore drawn the conclusion that simpler models should not be used for risk assessment in environments that consists of any form of geometry. Despite this observation, empirical and simplistic assessments are also often observed in dense geometries.

Many of the simpler models have been validated against large scale experiments and have shown good agreement with these experimental results for open field situations with some topographical effects of vegetation, or objects in the domain of the dispersion, [1, 6 , 14]. Some of the simpler models are also used in risk analysis for both on and offshore plants within the industry.

The objective of the study is to identify the most suitable approach for dispersion modelling for a given scenario, depending on the configuration where it takes place.

In short, this report will try to define the domains where the studied models give comparable results, where the results differ reasonably and where the results are strongly different. Causes leading to these observations will be discussed and recommendations over the use of such or such approach will be stated.
Further on, the main objective of this thesis is to establish some guidelines that define the appropriate use of the simulation tools for different simulation scenarios if possible, with different environments ranging from what will be defined as low congestion to highly congested and then finally realistic release scenarios. The main focus-area will be to see the effects of external wind and / or congestion on simulations done in FLACS and to see how PHAST can be used to represent this added congestion and cope with inherent limitations. The focus will also be to discover how we can match the complexity of the scenario by the complexity of the chosen simulation model. Some scenarios might not need a complex simulation tool to fully describe the associated hazards. The simulations performed as part of this report have been performed in the user perspective. For a safety scientist it would be favorable to know what kind of model that is applicable for simple or complex scenarios. Is a simple integral approach sufficient or is it necessary to employ a fully 3D CFD approach?

1.3 Overview of the content of the thesis

The study is structured as described below.

- Theory and background is given in chapter 1 to 4.
- Chapter 0 compares FLACS and PHAST for free field jets: jet releases at 10 meters above ground (without ground effect and boundary layer / wall function interaction) to 1.5-2 meters close to ground level are studied. This corresponds to an academic case.
- Chapter 6 deals with the comparison of simulations from FLACS and PHAST against the large scale KIT FOX experiment. This enlarges the scope of the previous academic case to a more realistic experiment including some introduction of basic mean to cope with interaction with objects in the empirical models (ground roughness).
- Chapter 7 covers the study of geometrical objects in the flow path in FLACS and by using parameters within the PHAST model to attempt to reproduce the same effects.
- Chapter 8 shows a realistic case and compares the results for consequence assessment in a real offshore module by using first FLACS and then tries to model the same scenario in PHAST.

Eventually, sections 9 and 10 discuss and conclude the current work.

The complete workflow is described in following Figure 1-3 progressing forward from open field scenarios into more and more congested scenarios

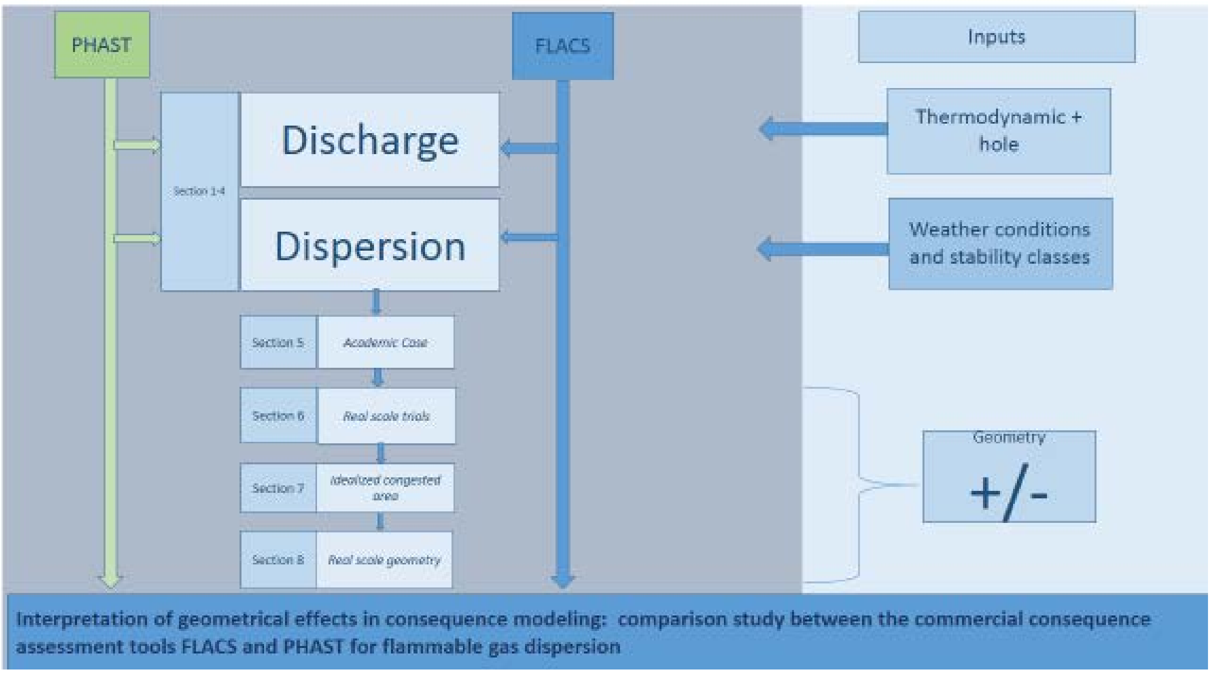


Figure 1-3 *Description of scope of work for comparison study.*

1.4 Overview of past research

A literature survey was performed at the start of the study in order to find relevant research on comparing CFD with integral models. No official releases comparing only FLACS and PHAST was found, but several articles addresses the differences in the results given by different CFD models and integral models for free field and dispersion simulations and dispersion simulations influenced by geometry.

An in-house article [1] not officially released by GexCon concludes that FLACS and PHAST are comparable for releases in non-obstructed environments (verified for Jet releases). In congested environments, empirical tools are often used outside validity range and may therefore deviate from the conservative / representative pattern. However, no attempt was made to tune the PHAST model or discuss the ability to handle geometrical effect in any way.

In the article "Risk assessment of dangerous products release and dispersion" [6], a comparison between CFD and the integral model PHAST points to the fact that for free field open releases the results from CFD and integral model should be somewhat comparable. These simulations were also compared to the large scale outdoor Prairie Grass experiments and showed good agreement between the models and the experimental results. The same article also described the results for an increased congested environment with several wind conditions. The paper concludes that PHAST is unable to account for different wind directions and inaccurate results are seen.

In the article "Large scale outdoor flammable & toxic gas dispersion modeling in industrial environments" [4] a comparison of the HazRes CFD Gas Dispersion Model COMSOL with a widely used integral model for releases of methane in both a congested and open environment. Good agreement was seen for the models compared to the results from the large scale MUST experiment. A conclusion also given is that caution should be taken when using integral models for positioning of gas detectors in offshore plants. This in mainly because of differences in how the model treats the wind effects on the release.

Other CFD codes like FDS has also been validated against large scale trial. [15] Gives a description of the FDS code and its ability to model atmospheric dispersion.

When evaluating the research in the field of CFD and integral modeling the conclusion seem quite clear from the current research. CFD modeling should be preferred when the domain of the simulations is within a complex geometrical environment and comparison of CFD against integral model only shows good agreement in open field topography without geometrical complexity.

However, none of the research so far gives insight as to how far you can go into the complex environment before the results from CFD and integral model start to deviate from each other as such a degree that makes the integral model an inappropriate tool for the scenario.

2 Introduction to hazardous gas releases

2.1 Introduction

To understand releases of gaseous materials, the underlying physics involved in fluid discharge and subsequent compound dispersion need to be understood before being modeled in a correct manner.

Discharge is the initial stage where the storage / stagnation / process conditions in which the fluid is manipulated in nominal operating conditions play the lead role. The key parameter to assess the flow exit out an aperture / puncture / leakage will be pressure and temperature at stagnation conditions, material properties, and size of discharge orifice.
The discharge process will describe the evolution of the fluid and of the flow characteristics from this normal operating stagnation conditions, towards orifice conditions and eventually expanded atmospheric conditions, further away in space from the orifice.

The dispersion process takes place after the discharge process. Initial jet velocity, wind and ambient turbulence then dominate the dispersion process in correlation with air entrainment and air and fluid mixing. Usually, the gas dispersion process is defined as a combination of transport and dilution processes:

1. Transport bringing the fluid away from the source under the effect of initial velocity and / or wind velocity.
2. Dilution introducing more and more ambient air in the fluid due to turbulence of jet or atmosphere (also due to temperature driven mixing).

For both of the quantification steps, the behavior of the fluid is based on material / thermodynamic properties, as the release may be gaseous, liquid or two-phase. It is worth noting that for initially pressurized gas jet releases, the transition from storage conditions to ambient conditions comes along with a brutal drop of temperature (for hydrocarbons, not for hydrogen for example) and that initial state of the fluid at the dispersion level is depending on the discharge properties.

To understand releases of gaseous materials the underlying physics involved in discharge and subsequent dispersion needs to be understood and modeled in the correct manner.

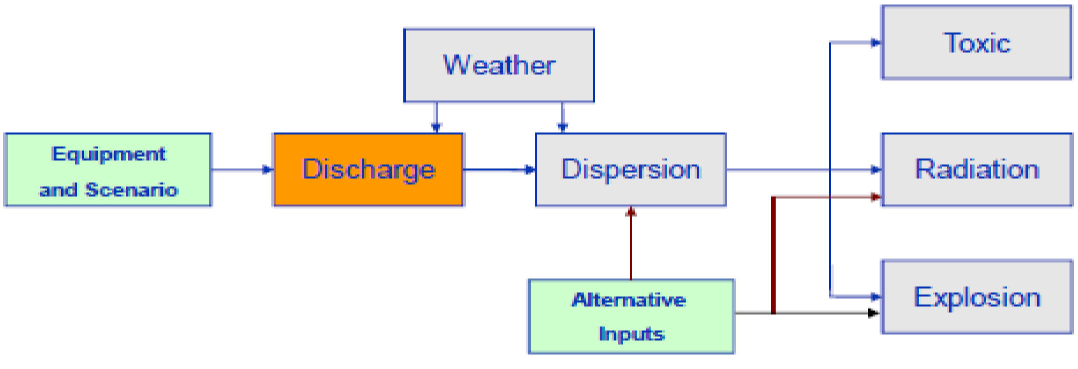


Figure 2-1 *Hazards posed by loss of containment of flammable, toxic or radiative material.*

For the safety scientist the most important parameters for a flammable gas cloud will always be the extent / size of cloud, the flammability regions and the amount of flammable mass. The safety engineer also needs to be aware of the factors that may influence the dispersion phenomena and to make conservative predictions. Figure 2-1 gives a description the hazards posed by loss of containment.

This next section divides the theoretical description of a pollutant release into several sub sections.

- The first part focuses on the source term calculation which is done differently within FLACS and PHAST
- The second part is the site characteristics, environment where the release and dispersion take place.
- The third part treats the meteorological aspects influencing the dispersion process.

The basics of theory of dispersion can be found in "*Lees Loss prevention in the process industries*" by Mannan [12], "*guidelines for use of vapor cloud dispersion models*" [3] and TNO the yellow book "*Methods for calculation of physical effects, due to releases of hazardous materials"* [9].

2.2 Discharge modelling

Source term calculations are of vital importance to make an estimate on amount of fluid released from process containment. It is the first critical step in an accurate estimation of downwind air concentrations resulting from this accidental release [3]. It is the foundations of the entire hazard assessment process either due to the intuitive choice of a key parameter like the leak size or because this calculation drives the input provided to the dispersion models and therefore, the hazard assessment.

The discharge rate is usually measured in kilograms per second (kg/s). Note that not only the release mass flow rate is of importance but also the final velocity (linked to air entrainment) and final expanded temperature (resulting in gas density) once the release is expanded from storage / stagnation / orifice to atmospheric conditions.

The release mass flow has to be distinguished from the nominal process flow within the nominal process conditions. The drop of pressure from the nominal conditions towards atmospheric conditions can be associated as a depressurization and hence is influenced by a "suction" effect. Unless particular cases where specific mitigation measure are present, the leakage flow rate is always largely superior than the nominal process flow rate.

Prior to assess the characteristics of the release, the most important data required are the following ones:

- Composition of the release fluid,
- Thermodynamic state of the fluid in the storage, stagnation condition in nominal operation,
- Leakage orifice size and shape
- Segment size/leak duration

From there, more or less advanced methodologies are available to characterize the flow properties during the discharge phase in terms of mass flow rate, final state when expanded to atmospheric conditions, phases (in general, can be gaseous, 2 phases or pure liquid).

The available approaches are often sorted depending on the initial state of the fluid in the containment prior to the release.

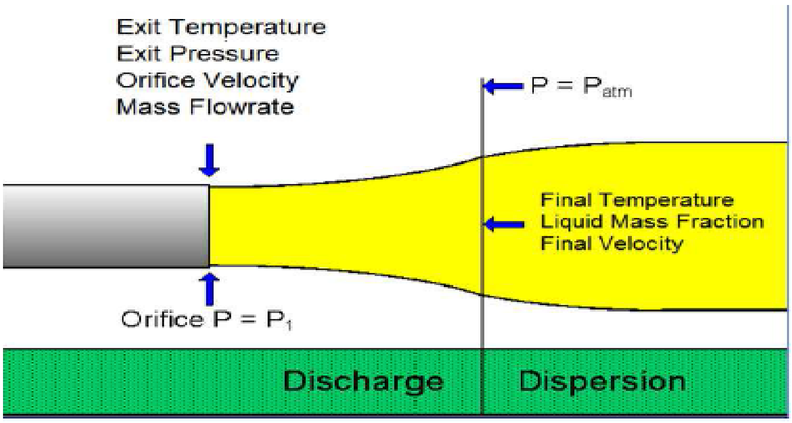


Figure 2-2 *Illustration of discharge/dispersion phenomena*, *[23].*

The final output of the discharge calculations are then incorporated within the dispersion models, as input.

Emission rate from these ideal gas jet releases can be calculated analytically, described in [3]. The following formulas for calculating a jet release of pressurized gas, assuming that the gas will be release through a small hole or puncture at a choked condition at the leakage orifice. A simple order of magnitude considers that the flow is chocked as soon as the storage pressure is twice the atmospheric pressure, for common hydrocarbon gas following the ideal gas law.

$$\frac{p}{pa} \geq \left(\frac{\Upsilon + 1}{2}\right)^{\frac{\Upsilon}{\Upsilon+1}}$$

p=absolute tank pressure (Nm^{-2})
p_a=absolute atmospheric pressure (Nm^{-2})
Υ=gas specific heat ratio

Equation 2-1

$$Q = \mathrm{CoAh}\left(\mathrm{p\rho0\Upsilon}\left(\frac{2}{\Upsilon + 1}\right)^{\frac{\Upsilon+1}{\Upsilon-1}}\right)^{\frac{1}{2}}$$

Q=time-dependent gas mass emission rate ($\frac{kg}{s}$)
C_o= discharge coefficient for the orifice/hole
ρ_0=density of gas in the containment ($\frac{kg}{m3}$)
A_h= orifice area (m^2)

Equation 2-2

Choked flow means that the gas is moving through the hole or orifice at its highest possible speed, the speed of sound in the gas [3]. If containment pressure is twice the atmospheric pressure the results will be a choked flow of the leaking gas. Equation 2-1 gives the mass flow rate of the leakage in the choked domain for isentropic conditions.

The flow will become subcritical when the pressure inside containment will be equal to the atmospheric pressure and there is no longer a strong enough pressure gradient to propel the leakage as a jet.

In light of this report, the source term calculations are treated widely differently in FLACS and in PHAST. Both use conservation equation for mass, momentum and energy with slight deviations on the energy considerations. Furthermore, the expansion phase is treated differently. For pure gas releases FLACS treats the release as a shock, utilizing Rankine-Hugoniot relations, while PHAST uses thermodynamics properties to describe the release. These differences result in distinct characterization of the expanded jet before the dispersion process starts.

Most risk analysis or safety studies utilizes different regimes in their analysis to fully show the behavior of different magnitudes of releases in the analysis. This is often based on the NORSOK Z-013 [18] standard section G.2.1.1, which segregates the leakage rates that should be assessed during probabilistic explosion analysis. For this report the leakage rates given in Table 2-1 was used.

Most leakages that occur on the Norwegian oil sector offshore are estimated to be in the magnitude of 0.1-1 kg/s [10].

Table 2-1 *Leakage regimes analyzed in this report.*

Small leak	**<1 kg/s**
Medium leak	**1 kg/s to 5.0 kg/s**
Large leak	**>10.0 kg/s**

All the different regimes of gas leakages given in the will be examined in this report for both methane and propane releases. For this report only point source releases will be examined of pressurized gas from a containment of significant higher pressure than the surrounding atmosphere, so liquid or to-phase spills are ruled out of the scope of work. The Kit Fox experiment is in this context an exception as this was simulated as a diffuse release.

2.3 Dispersion fundamentals

In the context of this report dispersion is defined as the process by which an atmospheric expanded gas released from a pressurized containment is spread within the ambient atmosphere.

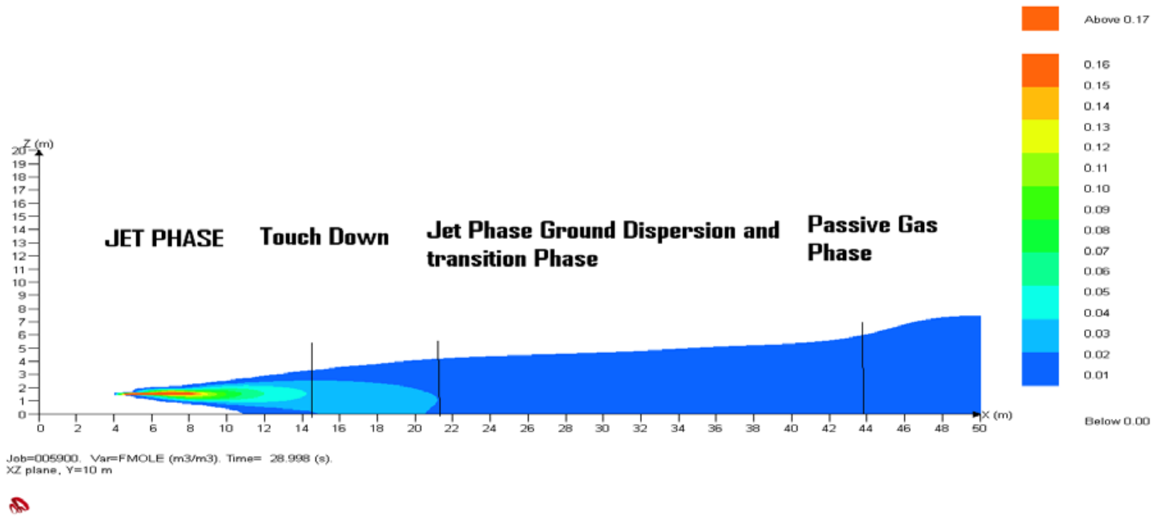


Figure 2-3 *Different phases of the gas dispersion phenomena. The Plot is showing concentration as function of downwind distance.*

The dispersion process is governed by several regimes and pollutant behaviors with respect to surrounding air. The initial phase is defined as a jet phase dominated by the high velocity / momentum of the release emerging from its point source. The jets velocity will be strongly influenced by the drag force exerted by the ambient air and will slow down the velocity of the jet. The velocity difference between the jet and the surrounding air generates small scale turbulence which causes the jet to spread sideways and suck air into the jet. The larger the difference between the jet and ambient air velocities, the larger the air entrainment. This increases mixing of the released material with the air.

A touch-down phase may follow for a gas release close to the ground. The ground will influence the jet and slow down the velocity before the jet comes into the passive gas regime. The characteristic behavior of the passive regime is that the velocity of the plume is comparable with the ambient air and is therefore dominated by the turbulence and flow pattern of this environment. In this regime the molecular weight of the gas plays a crucial role. Heavy gases tend to stay a ground level and light gases tend to rise upwards.

Throughout all of these phases, entrainment of ambient air will play an important role. The high velocity difference in the Jet phase will cause largest entrainment during the initial stage of dispersion.

Density is an important parameter when it comes to gas dispersion as it defines the buoyant character of the gas plume. The gas behavior after a leakage will always depend on the molecular weight of the gas. If the gas is lighter than air the gas will have positive buoyancy and tend to rise upwards. Negative buoyancy is when the gas will have a tendency to stay at the ground level. Heavy gases exhibit negative buoyancy while light gases exhibit positive buoyancy. The buoyancy is not seen strongly in the jet phase of horizontal gas leakages if the pressure of the leak is sufficiently strong. As the gas plume moves into the passive regime the buoyancy is seen more strong as the velocity of the plume is comparable with the external wind field. In this regime known as the passive gas regime the buoyancy is more relevant as the turbulence in the ambient atmosphere defines the movement of the plume.

A different class of releases is identified as diffuse releases. A diffuse release is a release without momentum. The release itself does not have enough energy to exert a significant force on the moving wind. The release will move with the velocity and direction of the ambient wind field. A typical diffuse release will be a spill of LNG. The LNG will in the ambient atmosphere flash into a vapor and move with the external wind field.

2.3.1 Flammable mass

As dispersion results from the preliminary discharge calculations, the dispersion simulation is a precursor for the explosion assessment. The flammable mass calculation given by the dispersion plume is therefore an important part of the risk assessment as it determines the chemical energy that is contained within the gas cloud. This information is essential as it may give an indication of the maximum explosion overpressures that the specific gas cloud may generate if ignited. In [16] a formula for explosion overpressure is given.

$$\boldsymbol{P \sim Vf^{\frac{5}{3}}}$$

Equation 2-3

P being the maximum explosion overpressure order of magnitude (barg) and V_f the stoichiometric gas cloud volume.

An accumulation of gas may also especially be important if gas leakages are expected to occur in a confinement or a congested environment consisting of segregating walls, piping and other process equipment that may prevent the dilution process of the gas/air mixture.

The equation Equation 2-3 given above also calls attention to the fact that the explosion overpressure in not linearly dependent on the flammable mass. Twice the flammable mass will not give twice the explosion overpressure, but will rise by a factor of 5/3 of the stoichiometric gas cloud volume.

No specific details is provided within this report, but the same distinctions between simplified and advanced CFD modeling of an explosion exists with respect to the dispersion topic discussed here. Simplified approaches or empirical methodologies can idealize the gas cloud and provide blast propagation assessment on the basis of empirical considerations while CFD tools models the flame propagation within an assembly of several small control volumes accounting for local effects, obstacles, and congestion.

2.3.2 Concentration and flammability

Concentration is a measure of the amount of one component in a mixture of other components. In process safety mindset this will be the amount of a hazardous gas mixed with the ambient air. Several different ways to define concentration can be found in the literature [2]. Concentration can be given by mass, volume or mole percentage. Most often the volumetric percentage (Vol %) of concentration in a mixture with air is used for representation of gas concentration. This way of representing gas concentration will be used throughout this report.

The flammability of a gas cloud is defined within certain concentration regions known as Lower flammability level (LFL) and upper flammability level (UFL), defined by gas explosion handbook [26]. According to [13] the flammability limits may scatter somewhat depending on the experimental methods chosen or with respect to temperature and pressure.

Methane has a flammable region between 4.4 and 16.5 % in volume in a mixture with air [26]. The Figure 2-5 below illustrates a jet with defined concentration regions up to LFL_2.

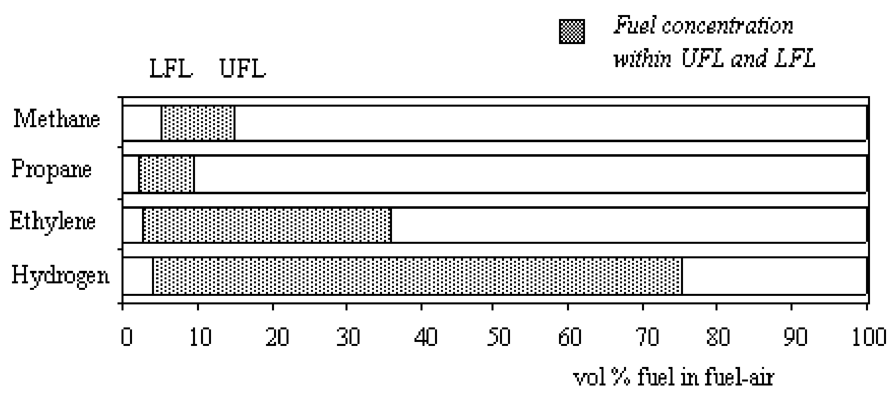


Figure 2-4 *Flammability limits. Taken from Gas explosion handbook [26] .Valid at 1atm pressure and 25°C*

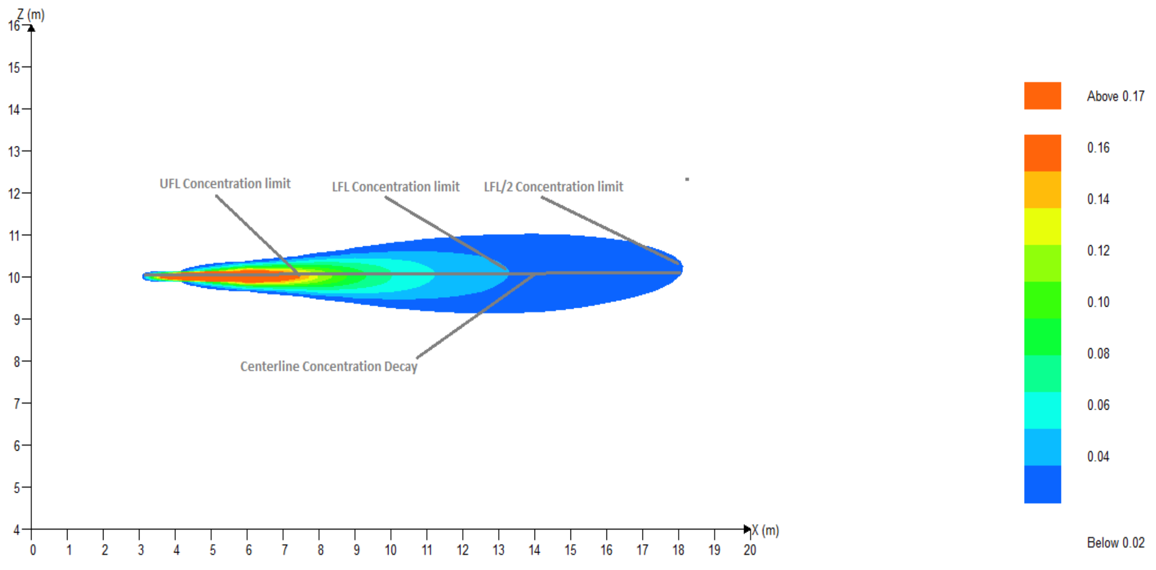


Figure 2-5 *FLACS jet showing the centerline concentration decay of a free jet and the flammable range.*

Outside the regions of UFL and LFL concentrations, the cloud will not be flammable and therefore cannot be ignited. It remains important to remember that once the cloud is ignited, complex combustion phenomenon occurs and additional dynamic mixing and transport with air is observed. Thus, a region that is initially in a concentration above the UFL may participate to the combustion eventually.

There is a concentration ratio for which the combustion of the fuel in air is optimal. This is the stoichiometric condition. At this particular condition, a laminar combustion will be optimal and both the reactivity and the speed of the flame in such a mixture will be at their highest. For methane this stoichiometric condition is close to 10 % concentration vol. in air.

2.4 Meteorological impacts on dispersion

The external wind field and ventilation conditions at a process facility will have implications on the gas release dispersion. In modeling, meteorological conditions are incorporated in the models as boundary conditions.

2.4.1 Wind and its implications on gas dispersion

Wind is generally generated by the Coriolis forces and large scale pressure differences in the atmosphere. The rough terrain, trees and buildings, or any type of congestion causes turbulence and result in lower wind speeds near the ground level. To a certain extent, this big picture is required to fully understand the specificities of the influence of the wind over a gas dispersion and formation of a plume. The effect of wind will slightly be different for a release at ground level compared to a chimney release or flare fumes dispersion at elevated height.

Intuitively wind also has strong implications on how far a gas leakage will move downstream of its leakage orifice. After the gas is released out of a pipe with sgnificant kinetic energy of the choked flow, there will be a drag force working on the gas, which makes it slow down, and eventually the gas becomes part of the external wind field, in what is defined as a passive regime.

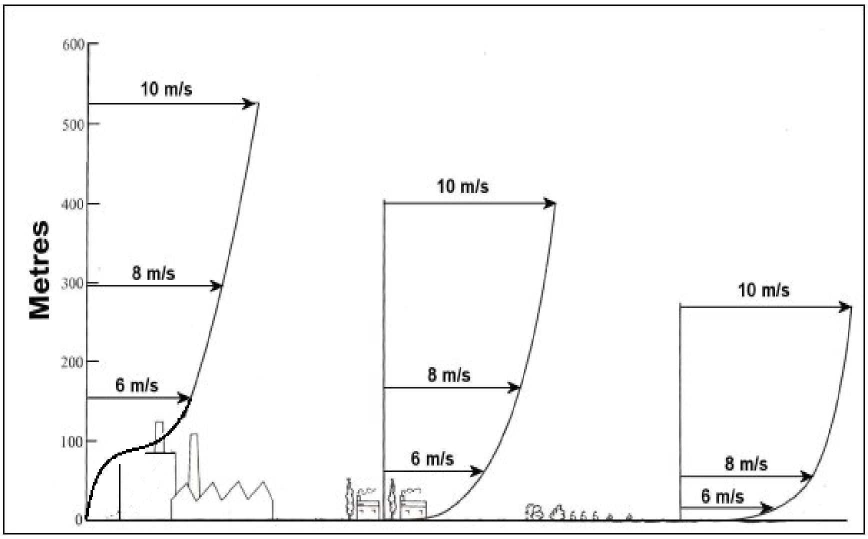


Figure 2-6 *Show the wind speed changes with surface roughness. The greater the roughness of the ground (e.g. city area), the steeper the wind gradient [12].*

This report will focus on how wind affects the dispersion simulations in terms of its implications on downwind concentrations and flammable mass. As this is the most important properties of the dispersion phenomena, different wind conditions were simulated for both FLACS and PHAST.

2.4.2 Stability classes

The turbulence in the ambient air will have a large impact upon the dispersion process, especially in the passive phase of the dispersion process. The turbulence in the atmosphere can be divided into defined increments or “stability classes”. These classes are differentiated based on how the atmosphere will enforce, accept or suppress the vertical motions. In the Handbook of atmospheric diffusion [17] three different classes’ of stability are defined into stable, neutral and unstable to account for atmospheric turbulence. The different classes have the following traits;

Unstable; Stability will be predominant when thermal convection drives the turbulence and wind shear effect is not as strong. This regime is often seen in sunny afternoons. The heat from the ground will heat up the air above it.

Neutral; Production of turbulence by wind will be large compared to heat from ground which will only have low contribution to. This will mainly be in the form of thermal radiation. This regime is seen expected on windy and cloudy days.

Stable; Thermal stratified flow is seen in this regime. This effect is driven by the cooling of the ground and will act as a sink for turbulent energy produced by the wind shear. This regime is most likely to be expected at nighttime.

The turbulence itself can be generated by a variety of factors such as wind flow over rough terrain or obstacles such as buildings or trees or any form of congestion. These factors again cause high and low pressure of the air masses and “fronts” that gives rise to wind flows. Thermal turbulence will also occur if rising currents of heat affects the air masses. On a sunny day the sun will warm up the air causing convection and turbulence in the ambient air.

In this report the stability classes F, D and B is used for the simulations in FLACS and PHAST.

Table 2-2 *Stability classes*

A	Very Unstable
B	Unstable
C	Slightly unstable
D	Neutral
E	Slightly stable
F	Stable

2.5 Site characteristics

Every safety scientist or personnel involved in process safety needs to be aware of the influence of specific site characteristic related to his or her facility of interest. For an offshore rig or platform, the personnel involved in safety assessments should know the wind rose and the most likely wind pattern through and around the platform.

2.5.1 Friction velocity and its implications on dispersion

There will always be a frictional force that is working between a surface and the fluid moving relative to the surface. The friction speed is a measure of friction force a surface exerts on a moving fluid. Typically, this can be a gas moving horizontally by the ground level. The friction velocity may also be used in dispersion models to give the rate of entrainment since the frictional stress exerted by the ground will have implication on the plume spread.

2.5.2 Roughness length/Surface roughness

Surface roughness or roughness length z is a description of how the ground influences to airflow above it, or how the roughness of the ground influences the mechanical mixing of the air above it. It is related to the averaged obstacle height. According to [3] the roughness length is approximately 10% of the obstacle height for typical surfaces. From the work on pipe roughness, the roughness length z_0 and the mean height ε for roughness elements are related approximately as follows.

$$z_{\circ} = \frac{\varepsilon}{30}$$ **Equation 2-4**

Z_0 = Roughness length or Ground Roughness.

ε = Average height of irregularities.

Numerical values for surface roughness will vary in the range of 0.01mm-3m. Ground roughness for sea topography is 0.2mm and for a city it will be 3 meter. The table below gives different types of roughness lengths defined in [3].

Table 2-3 Scales of surface roughness given in [3].

Roughness length (m)	Type of surface
1.0	Cities, Industrial complexes, forests
0.1	Residential areas, agricultural crops
0.01	Grass
0.001	Water, pavement surfaces

2.6 The impact of congestion on wind and dispersion

Most of the gas releases that occur on offshore or onshore facilities are in a congested environment. This congested environment can be made up of pipes, process equipment, segregating walls and so on. Local air movements and ventilation will therefore be different from a widely open terrain without any changes in elevation. Figure 2-7 illustrates this point. Here we can see the complex flow pattern of wind flowing through an onshore process facility, both wakes and recirculation zones is seen in the illustration.

For the comparison purposes the wind will play a crucial role as different wind conditions may give different dispersion plumes, especially for far field effects

The impact of obstruction in the flow path is not only related to the vertical and horizontal spreading of the gas plume. This effect also contributes to higher overpressure for a vapor cloud explosion. Pipes, segregating walls etc. adds to the initial turbulence and causes flames to accelerate.

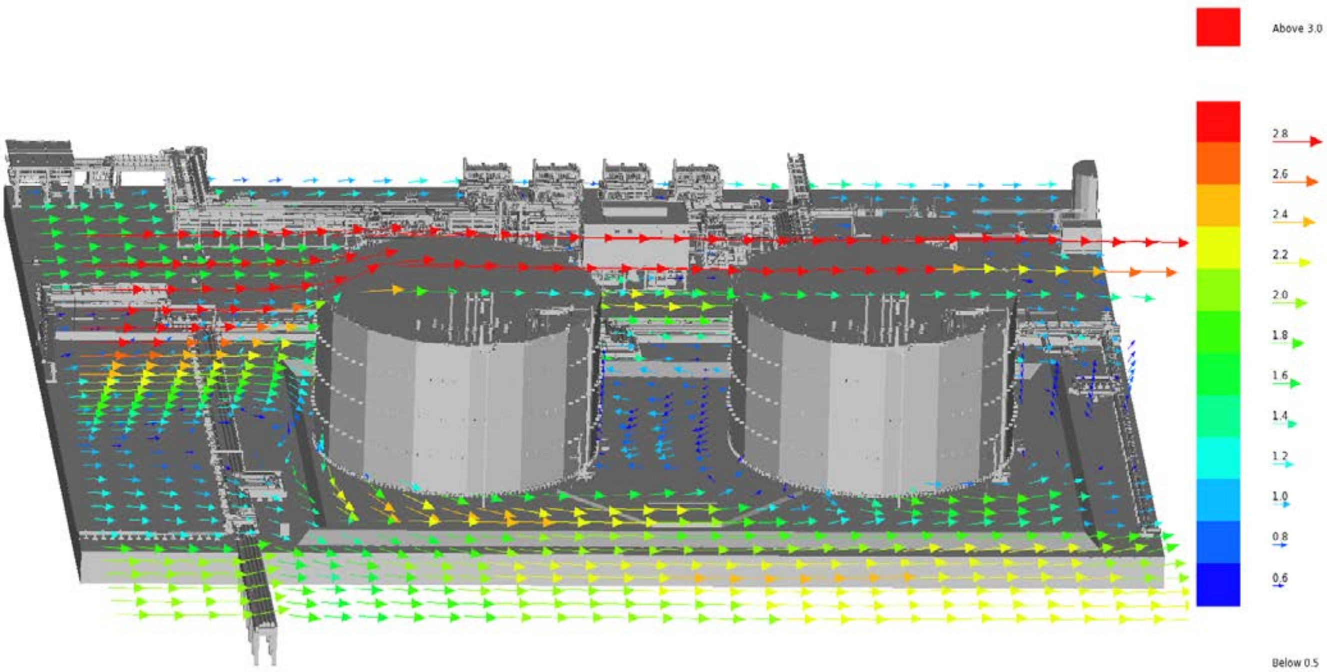


Figure 2-7 *FLACS simulation showing the complexity of a wind field moving through a process facility [1]. Wind velocities in m/s is shown in the legend to the right. FLACS simulation*

3 Gas dispersion modelling

According to [12] there are four well known approaches to dispersion modeling. These are the Gaussian approach, statistical methods, similarity models, or top hat box and slab models. A fifth choice not defined by Mannan is the CFD approach for hazardous gas dispersion considering direct modelling of the fluid mechanics equation in a domain subdivided into small control volumes.

The different approaches varies in complexity, ranging from the models mentioned above which are considered to be simple, to the fully complex three dimensional CFD models. Examples of CFD models are FLUENT, Kamelon FireEX (KFX) and Fire Dynamics Simulator (FDS).

The choice of simple models that exist in the marked today is also numerous. Degadis, Hegadis, Trace and PHAST are some of the most popular tools to mention a few.

3.1 Integral / Empirical / Simplified modelling

The Integral models consist of mathematical equations that solve the conservation of mass, momentum and the scalar quantities. The models are often validated and tuned against large scale experiments like MUST, Prairie Grass or other relevant trials.

The Figure 3-1 below gives some visual results given by simple models. Unlike the CFD analyst, the integral modeler will extrapolate the simulated gas jet leakage in every direction to account for all of the possible leakage scenarios within the estimated discharge.

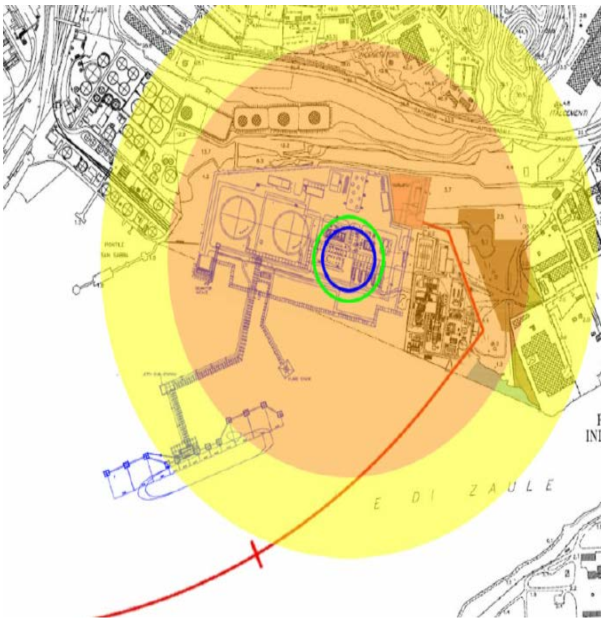


Figure 3-1 *Illustration of integral modeling simulations results, [23].*

3.2 The DNV PHAST software (or more general simplified/empirical/integral tools for dispersion modeling)

PHAST (Process Hazard Analysis Software Tool) is an integral model developed by DNV to model and access consequences of hazardous events. PHAST was initially developed by Cook and Woodward early in the 1990s. The model is a simple approach for consequence assessment and results is given within minutes for a typical scenario. This is the strength of PHAST compared to other risk assessment tools, which may require more time to give input and run lengthy simulations.

Today the model called Unified dispersion model (UDM) implemented within the DNV PHAST tool consists the following different models for dispersion modeling [24];

- Jet dispersion
- Droplet evaporation and rainout, touchdown
- Pool spread and vaporization
- Heavy gas dispersion
- Passive dispersion

The UDM uses a set of differential equations which is integrated to give the key variables as a function of distance or time [24].

Without too much details, the basic process used by PHAST to compute gas dispersion is to account for …. (along wind and concentration centerline + cross-wind distribution)

The Figure 3-2 shows how PHAST represents the results given by the simulations. In the left plot below the red circle represents the extent of the UFL concentration at downwind distance, yellow represent the LFL and the blue the LFL_2 concentration extent.

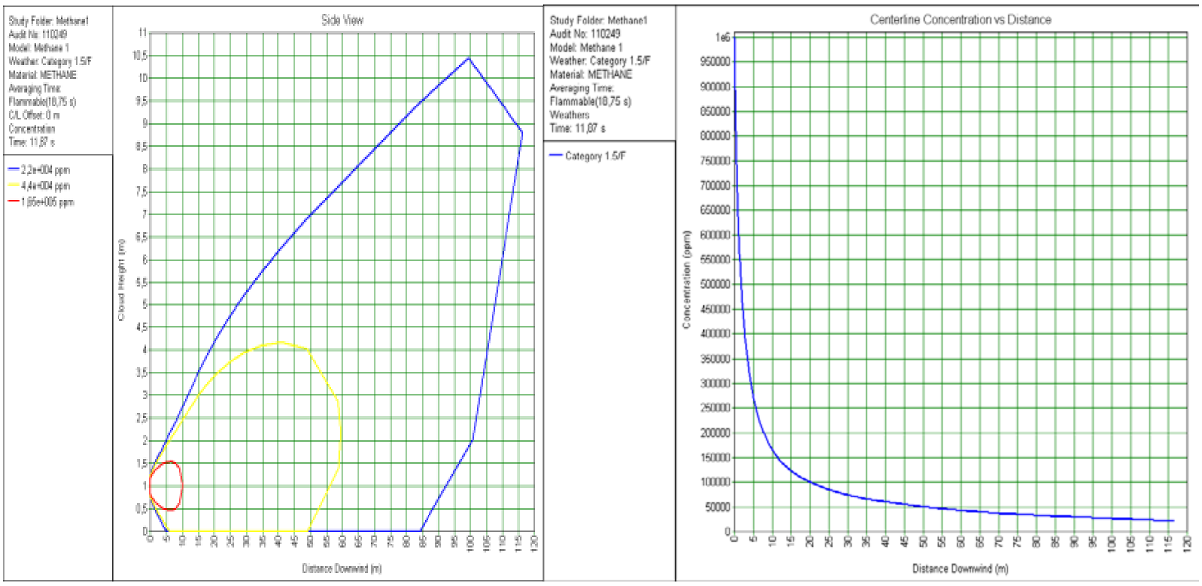


Figure 3-2 *Representation of results in PHAST. Side view and concentration decay plots.*

3.2.1 Validation of PHAST

PHAST has been validated against experimental results as per documented in [21]. Among some exisitng field experiments, the following are listed within the PHAST validation framework:

- Prairie Grass
- Burro
- Desert Tortoise
- Goldfish
- EEC
- KIT FOX

The Kit Fox experiment was in this report simulated in both FLACS and PHAST (see chapter 6).

3.2.2 Sensitivity parameters in PHAST UDM

In order for PHAST to have a way of dealing with increasingly congested environments, user-adjustable parameters within the model can be changed to try to account for geometrical effects. For the work represented in this report the ground roughness values and the horizontal impingement choice will be changed to try to account for the increased congested environments simulated in FLACS.

There are also other ways to manipulate the results given by the PHAST model. A parametric sensitivity analysis of PHAST`s atmospheric dispersion model was performed by Pandya, Gabas and Marsden [11]. This analysis studied 6o minute of continuous releases for Nitric oxide, Ammonia and Chlorine. The materials were chosen examined based on their different physical characteristics and also considering different storage conditions. The article gives a description of how the model responds to changing of the $\alpha 1$ and $\alpha 2$ values in the model among several other variables. These $\alpha 1$ and $\alpha 2$ values are for the effect of jet and cross wind entrainment. Normally the values are set to 0.17 and 0.35 in the model. According to [11] both the $\alpha 1$ and $\alpha 2$ values will have a strong influence on entrainment of air on the releases and by that greatly affecting the concentration lengths given by the simulations.

3.3 CFD modelling

This section is based on the textbook “Combustion” by Warnatz, Maas et al [2], unless differently stated.

Computational fluid dynamics, usually written by its abbreviated form as CFD, is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by given boundary conditions. The simulation domain is divided into a defined number of cells. In each of these cells the equations that govern fluid flow must be solved for each sequential time step. The resolution of this domain is then based on the number of cells.

The turbulence models are classified according to which governing equations they apply. Within these categories the number of transport equations is different. Each of these turbulence models is outlined briefly below.

DNS, Direct numerical simulations resolves even the smallest turbulent eddies at the Kolmogorov scale. This requires excessive amount of computational force and these types of simulations are only used for the very simple problems. DNS is today merely used for research purposes [2].

The Reynolds averaged Navier-Stokes (RANS) equations interpret fluid flow as average property and a fluctuating property.

Large eddy simulations (LES) is simulations based upon resolution of the largest eddies in the flow. FDS, Fire dynamics simulator is a typical LES model. FLACS is within the RANS category.

3.4 The FLACS code

FLACS is an explosion software code developed by Chr. Michelsen Institute, Chr. Michelsen Research and currently GexCon from the beginning of the 1980s. The purpose of the simulation tool was to simulate gas dispersion and gas explosions related to the oil and gas industry. Today the code also incorporates ability to simulate explosions and industrial pool or jet fires. The models solve compressible conservation equations on a 3-D Cartesian grid using finite volume method [19].The model takes into account the interaction between the gas flow and complex geometries as structures, equipment and pipework.

FLACS code is today widely accepted as an industry standard due to extensive validation of dispersion and the closely related ventilation studies. FLACS has also done very well in CFD blind benchmark studies evaluating the model against other CFD models [22].

The FLACS code suit is constituted of a geometry preprocessor, a numerical solver and a result post processor described in the following sections.

3.4.1 CASD Computer aided scenario design

Most of the commercial CDF codes have a user friendly interface. CASD is the pre-processor in FLACS. This is where you build your geometry and define and prepare the input data, or job data that defines the simulation scenario of interest. Figure 3-3 show the interface of CASD.

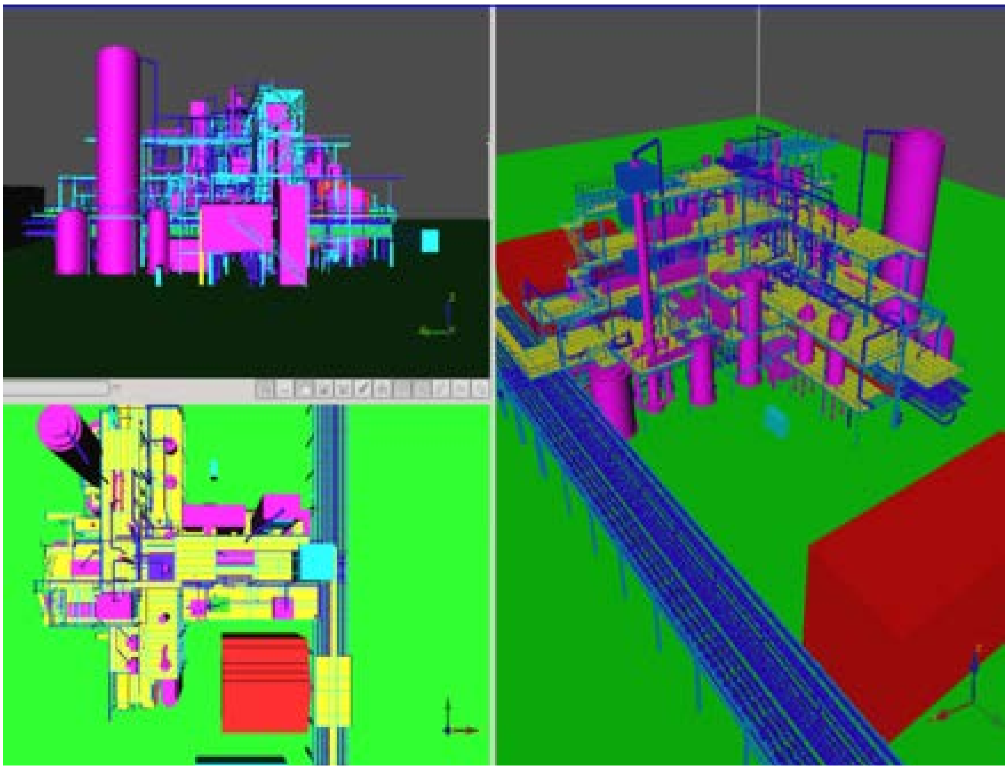


Figure 3-3 *Showing CASD and describes functionality in the user interface.*

3.4.2 FLOWVIS

Flowis is the post-processor in FLACS. It is a program for visualizing results from computer-aided simulations of gas dispersion, gas explosion and multi-phase flows. It is possible to visualize the results in both two and three-dimensional plots.

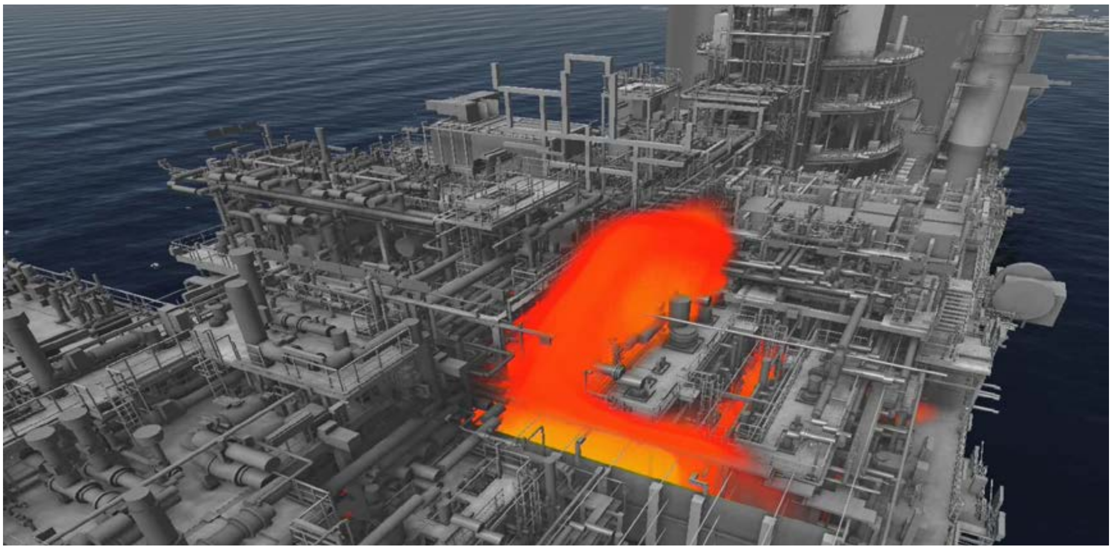


Figure 3-4 *Flowvis plot. A representation of an ignited gas release in an offshore installation, [23].*

3.5 Range of validity / Limitation within the PHAST and FLACS models

Due to inherent differences between CFD and integral models, some limitations need to be addressed to better understand the usage of these models and to interpret results.

PHAST UDM as an integral model has some limitations that need to be known to the user of the model. Wind speeds below 1 m/s is not possible to model in PHAST and the wind direction can only be modeled in the direction downwind of the release site, meaning that the wind can only be simulated behind the jet release. An implication of this is that the modeler does not have the ability to simulate the flow wind coming against the leakage direction as shown in Figure 3-5.

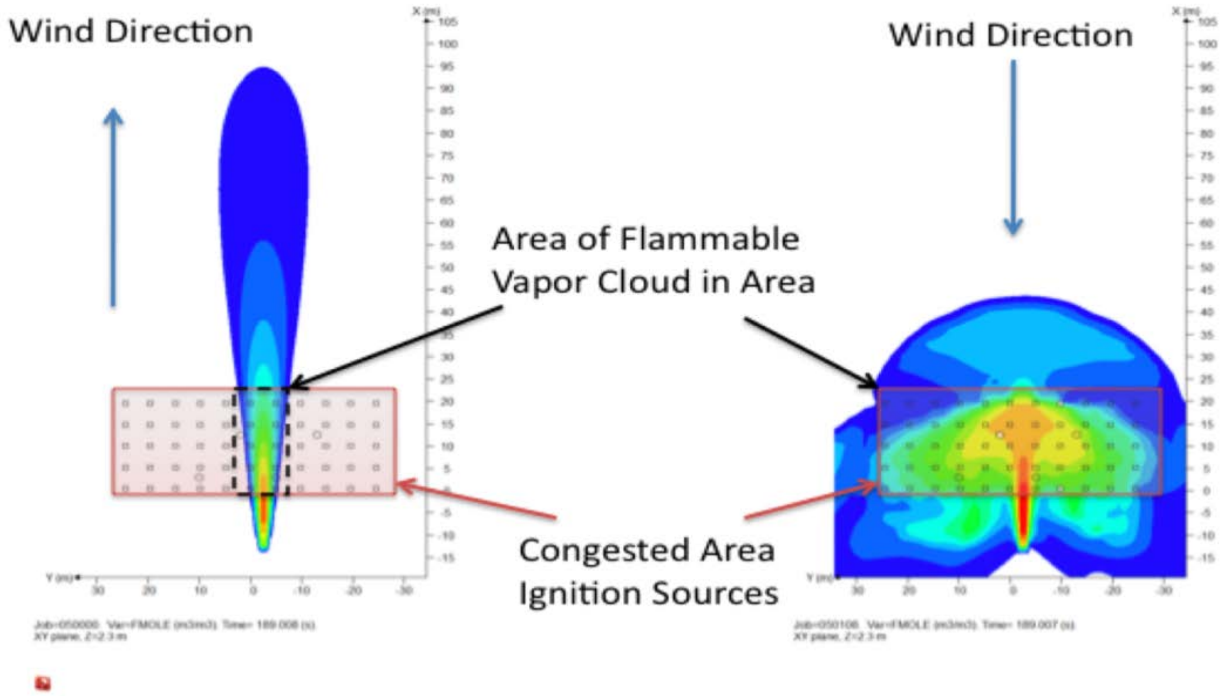


Figure 3-5 *CFD modeling of different wind directions in congested environment. Wind coming against the leak in the right example [1]. The left picture gives results in CFD that is to be expected in an integral model like PHAST. No interaction between the plume and the geometry is seen. Right figure shows a jet influenced by both the wind and the geometry.*

The area of flammable mass given by a CFD and an integral model may give large deviations as seen by when different complex wind conditions are assessed within the same congested area. The plume given by the CFD approach also has a higher explosion probability due to its expose to more ignition sources than the integral approach shown to the left [1].

The FLACS model limitations;

- Limited material database.
- Duration of setting up simulations and the need for extra computational time compared to a simple model.
- The need for a skills user is also more important in a CFD code compared to simple models.

The PHAST model limitations;

- Wind velocity range. Not able to model flow with wind conditions below 1.0 m/s.
- Wind direction related to leak orientation (Wind has to be collinear to the release axis).
- Not able to implement geometry or topography in 2D.

When it comes to the PHAST model one has to overcome the limitations to provide a conservative and reasonable consequence assessment for flammable dispersion.

All these limitations will be addressed further in this report. The aim of the thesis is too see to what extent what can reasonably / smartly overrule the limitations to provide a conservative and reasonable consequence assessment for flammable dispersion in a reasonable range of working time.

4 General methodology to perform the comparison work

4.1 Comparison methodology for free field releases

The first objective was to define a method that should be used for the comparison. Two different methodologies were decided upon for the first simulations. Each of them will be outlined below. The simulation was performed in the user perspective giving as similar input to the models as possible – starting at the input from the discharge modelling (it is worth mentioning that these inputs are the ones that are usually available to the user from flow chart or PFDs: composition of stream, thermodynamic state, orifice size).

This is here performed on the basis of how a safety engineer would perceive and solve the problem at hand.

Two different approaches were used for in this work and both of these methodologies will be outlined. Conclusions and observations are provided for each of them.

For methane and propane the following leak rates were used for the simulations given in table 4.1. Overview of wind speeds and stability classes for each of the mass flow rate run is given in table 4.2.

Table 4-1 Leak rates for methane and propane releases used throughout this report.

Leakage rate methane (Kg/s)	Leakage rate propane (Kg/s)
0,59	**0,70**
3,93	**1,95**
9,48	**7,80**

As described in the previous chapters FLACS and PHAST represent two widely different approaches for describing hazardous events such as hazardous gas dispersion and vapor cloud explosion. The basic groundwork in this report is to show were FLACS and PHAST give similar result and where they give results that deviate. The first guesswork related to this is that in the open field the results from the models will be relatively similar, as stated by several articles [1, 6, 14]. This was done to show how the models behave under circumstances where the simulations are not affected greatly by any form of congestion.

Table 4-2 *Overview wind speed and stability class used for each of the mass flow rates.*

Run	Wind speed (m/s(	Stability Class
1	**1**	**F**
2	**1,5**	**F**
3	**3**	**F**
4	**3**	**B**
5	**5**	**D**
6	**5**	**B**
7	**10**	**D**

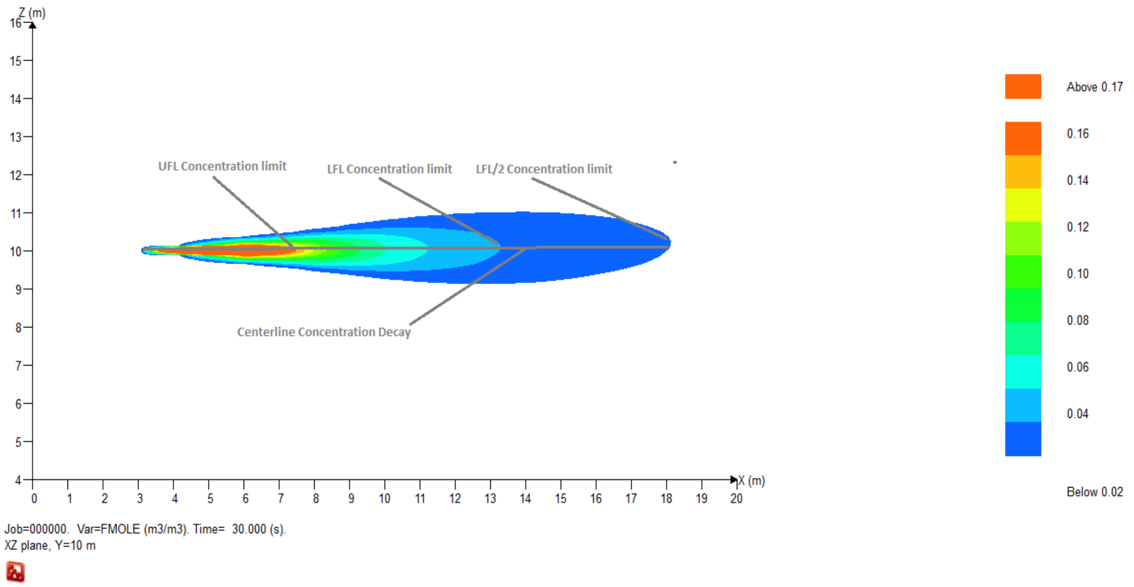


Figure 4-1 *Free methane jet release. Defined limits of concentration decay used throughout this report.*

For simplicity throughout the report the methods used are called method1 and method2. These methods are explained below will be used throughout this report for the comparison purposes.

4.1.1 Method1 Practical user perspective

This methodology involves giving equal input based on initial storage conditions, meaning starting from the discharge calculation input. This implies giving PHAST and FLACS the following similar input as a start. Here is how this was done;

In PHAST, the Vessel-pipe source functionality was used and the values were chosen to represent a pipe segment containing pressurized gas.

In FLACS the leak wizard was chosen and was given the same input as given in Vessel-Pipe source in PHAST. The models were given the same input indicated below;

- Equal ambient temperature and pressure
- Equal segment temperature and pressure conditions
- Equal orifice diameter

Some similar parameters influencing the dispersion modelling are also provided, within the range of validity of both the tools.

- Equal wind conditions and stability classes for the various simulations
- Equal Ground roughness (10 cm chosen for all simulations of non-impinging jets)

In other words, the setup of the simulation is done with similar input provided on the basis of the storage / stagnation conditions for both the tools.

For simplicity this method is referred to as method1 throughout this report.

The discharge modelling and the subsequent dispersion modelling are performed in a linked chain of routine with no guarantee that the intermediary calculations performed by each of the discharge calculation routines are providing identical results.

4.1.2 Method2 Focus on the dispersion model

The discharge calculations were first run in FLACS using the Jet utility program. Output given from the FLACS / Jet utility-calculations was used as input for the PHAST dispersion simulations.

The jet utility program was preferred for the discharge calculation utility from the PHAST package. Indeed, gas releases are considered in this document and chock equations are used in the jet utility calculations process. In the PHAST utility, the conservation and state equations are computed to assess the final state of the expanded jet (the start of the dispersion process) but criteria's of velocity capping (500 m/s) and final state characterization are used which is less accurate than within the jet utility approach.

For the dispersion calculations, the user defined source, was used in PHAST.

In this case, the dispersion modelling is based on the same input, regardless of the differences between the discharge calculations for similar storage conditions.

This method thus focuses more on the dispersion models themselves. However, it is worth noting that it isn't the common (and simplest) way of setting up a case from a practical user perspective.

Note also that this approach preferring the FLACS discharge modelling is justified by the consideration of pure gas releases. It is obvious that the most accurate discharge modelling drives this approach and that PHAST can be promoted in other specific cases.

The input that was set equal in the two models was the following;

- Equal mass flow rate
- Equal expanded temperature
- Equal discharge velocity
- Equal wind conditions and stability classes for the various simulations
- Equal ground toughness (10 cm chosen for all simulations for non-impinging jets)

For simplicity this method is hereby mentioned as the method2 in PHAST throughout this report.

4.1.3 Influence of ground interaction

Initially methane jets were simulated in both FLACS and PHAST for free field Jets releases 10 meters above ground level. The input given to both FLACS and PHAST was in accordance with the methodology defined in 4.1. These initial simulations were done in order to see what differences that exist between the models without any influence of the ground. The results are shown in chapter 0.

For similar mass flow rates the wind speed and stability class was changed for each run. All of the other properties of the simulations were kept similar. Both the gas jets of methane and propane are in this context assumed to behave as a pure gas. Duration of the jet releases was set to give a steady state plumes with unchanging concentration limits within the timeframe of the release.

The sole purpose of these initial simulations was to discover potential differences in near and far field effects between FLACS and PHAST for variable mass flow rate, wind conditions and stability classes for methane and propane releases for unobstructed flows, and also to see what effect changing the properties would have on the flammable extent of the dispersion plumes.

5 Free Field Releases

5.1 Comparison for elevated free jets

At an elevation of 10 meters above ground the jet itself isn't strongly influenced by ground effects, through frictional forces or flow modifications. This should therefore give a good starting point for the comparison between FLACS and PHAST, since this corresponds to an idealized free jet in open field.

At 10 meters above ground level the wind velocity is constant and not very affected by the boundary layer close to the surface. FLACS and PHAST handle this boundary layer different and elevating the jet to 10 meters avoids this effect.

Figure 5-1 illustrates the concentration decay of a free jet in FLACS together wind a description of the external wind field.

For the startup of the comparison a series of comparison were made for these jets to show how well the models compared, results are shown in Figure 5-2 for three wind conditions.

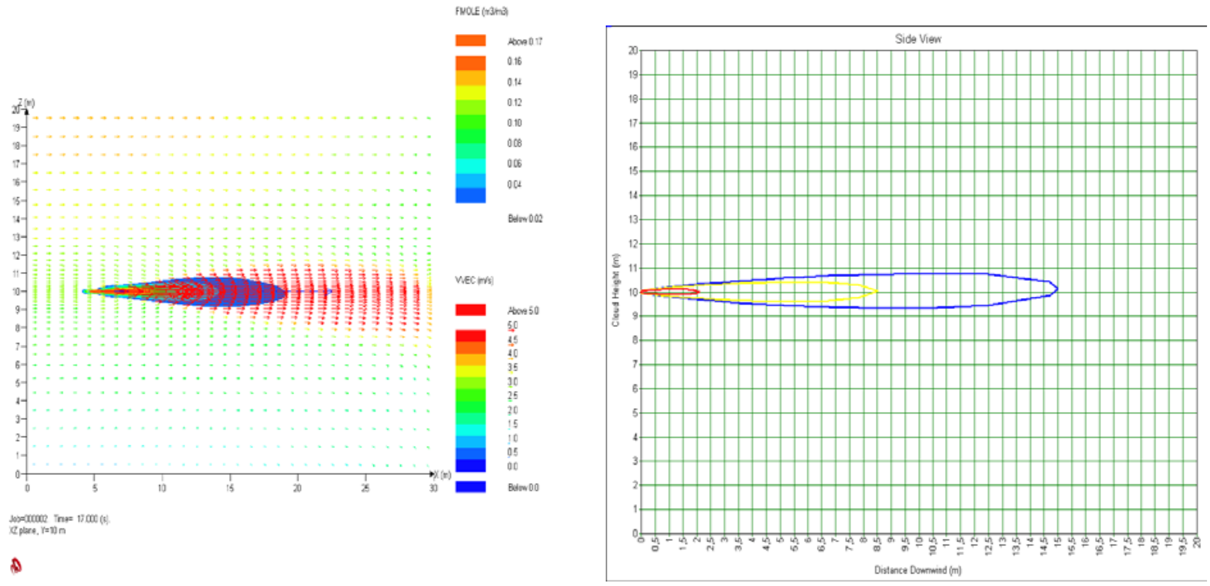


Figure 5-1 *Left figure shows a FLACS jet with wind conditions of 3 m/s stability F. Right figure show the comparable PHAST jet.*

Figure 5-2 show trends for the three initial cases for various wind speeds and stability classes. The plot describes the ratio of PHAST / FLACS concentration values for UFL, LFL and LFL_2 at the given downwind distances. The value 1 indicates a perfect match between the models for the specified concentration limit.

P1/F gives the values for PHAST method 1 divided by the FLACS value. P2/F gives PHAST method2 divided by the FLACS value.

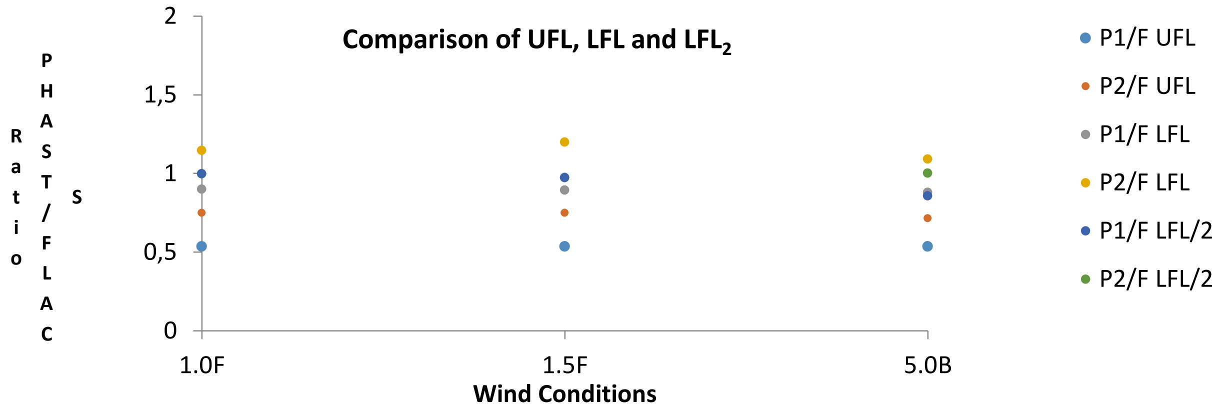


Figure 5-2 *Initial comparison of FLACS and PHAST for downwind concentration decay for three different wind conditions. UFL, LFL and LFL_2 values are compared for jet releases at wind conditions 1.0, 1.5 and 5.0 m/s wind. F and B are in this context two different classes of stability. To generate each comparison the ratio of distance in meter along the centerline where the cloud reached 2.2 Vol% (LFL_2), 4.4 Vol%(LFL) and 16.5 Vol% (UFL) was used for the comparison.*

The following conclusion can be drawn for the first comparison of FLACS and PHAST.

Table 5.1 shows that Method2 gives the most comparable results with the FLACS model. For LFL and LFL_2 the values are within a deviation of 15 % compared to FLACS. Method1 also gives very comparable values for LFL and LFL_2, within 10 %. However, the UFL values deviate by roughly 46 % for method1. The models are more comparable for concentration values closer to LFL_2 and LFL than the initial release values of UFL within the jet. The UFL values deviate more for both method1 and 2. This indicates that PHAST and PHAST have a different way of dealing concentration close to the leakage source for pressurized releases.

Table 5-1 *Percentage deviation between FLACS and PHAST for ideal free jets when comparing the downwind concentration.*

Concentration values	Deviation Between FLACS and PHAST for Method 1	Deviation Between FLACS and PHAST for Method 2
$ULF_{average}$	46.43%	25%
$LFL_{average}$	10%	14.6%
$LFL_{2\ average}$	5.7%	1%

5.2 Free field ground releases

5.2.1 Method

Free field methane and propane releases were simulated in both FLACS and PHAST for various mass flow rates and wind conditions described in Table 4-1 and Table 4-2. The jets were released 1.5 to 2 meters above the ground level.

For methane a total of 21 simulations were performed in FLACS, and 42 calculations in PHAST adding up to 63 simulations for the comparison. For the propane scenarios the same amount of simulations were performed, adding up to a total of 126 simulations.

In FLACS the centerline concentration was extracted using a command line defining the concentration along the centerline at the leak elevation. In PHAST concentration was taken from the dispersion report, commentary report and the graphs given for each of the simulations. This was also the method used for the propane releases.

This was done to find the concentration decay along this centerline up to the LFL_2 value. Lower downwind concentration was not compared. The data was then plotted to compare the concentration decay of the plume`s given in FLACS and PHAST. The comparison is shown below in Figure 5-3 and Figure 5-4 for the different mass flow rates with wind speed of 5.0 with stability class D for methane. Similar plots were made for each of the seven wind directions and stability classes with different mass flow rates. Only the 5.0 m/s wind speed with stabililty class D is represented here for the three different mass flow rates was reviewed.

The comparison is also summarized in a complete comparison plot that compares the values given for UFL, LFL and LFL_2 for the different mass flow rates and wind scenarios.

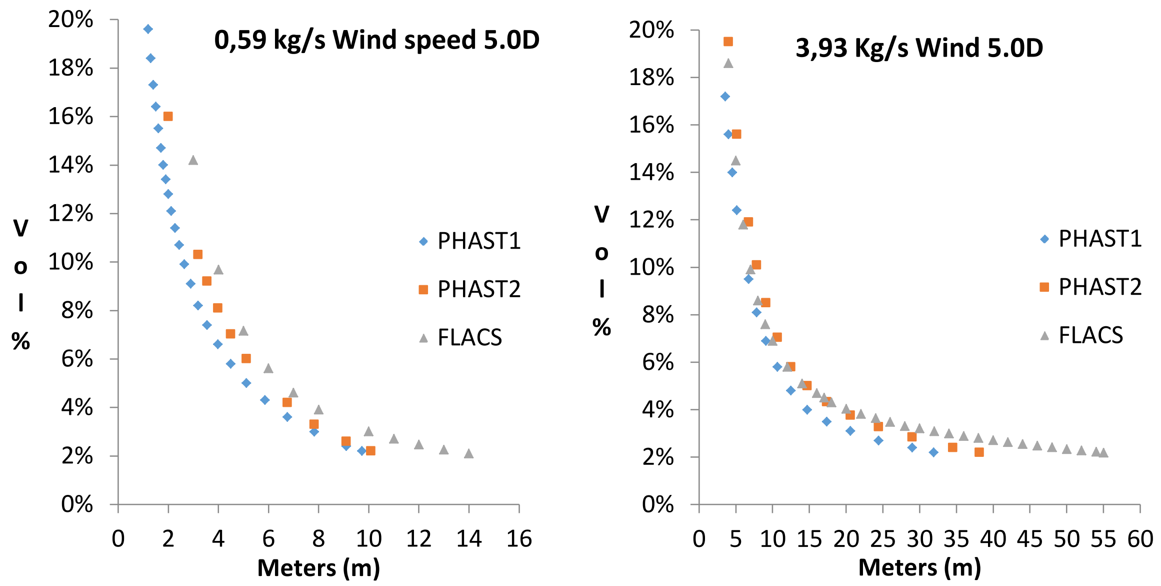


Figure 5-3 *Comparison plots of centerline concentration decay as a function of downwind distance up to LFL_2 criteria. Left plot show 0.59 kg/s at wind speed 5.0D. Right plots show 3.93 kg/s of 5.0D. FLACS results extracted along centerline through plume at 1,5-2 meters. PHAST centerline profile extracted from the dispersion report.*

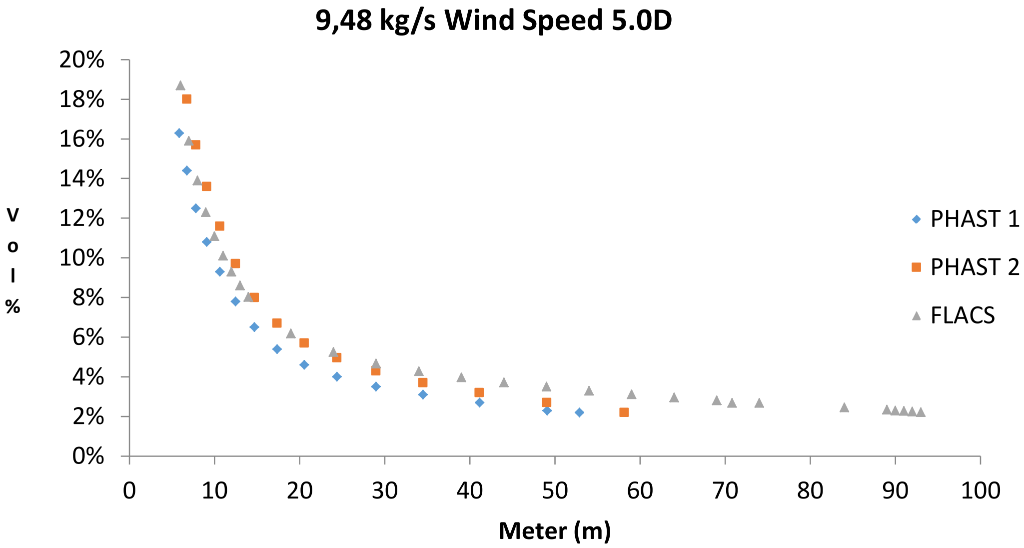


Figure 5-4 *Comparison plots of centerline concentration decay as a function of downwind distance up to LFL_2. 9.48 kg/s scenario at wind speed 5 m/s at stability class D. FLACS results extracted along centerline through plume at 1,5-2 meters. PHAST centerline profile extracted from the dispersion report.*

5.2.2 Methane results

5.2.2.1 Small releases 0.59 kg/s 1.5 meters above ground level

The simulations shown below gives all of the various wind conditions run for the small 0.59 kg/s mass flow rate run in FLACS. The plots are extracted at steady state where concentration limits are unchanging in time.

Figure 5-7 gives the full comparison for the FLACS/PHAST ratio of UFL, LFL and LFL_2 values at the downwind distances at the different wind conditions.

The simulations run at the low wind speeds 1.0F and 1.5F in FLACS showed a touchdown phase in the LFL_2 regime due to low wind speeds at the ground level. This was not seen in PHAST for the comparison simulations for method1 or method2. For all the simulations run at higher wind speed touchdown was not seen for the simulations in FLACS or PHAST.

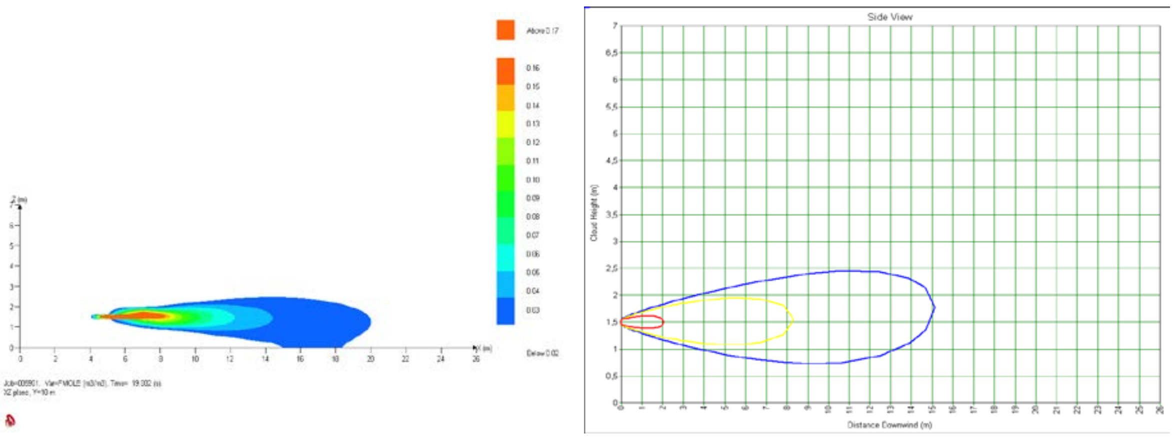


Figure 5-5 *Showing 0.59 kg/s methane jet with touchdown shown in FLACS. No touchdown seen in the comparison jet in PHAST.*

The distance from the release to the UFL limit was approximately 2.5 to 2.8m for the different simulations for the FLACS model. This limit was reached at shorter distances by the PHAST model for both method1 and method2. Method1 giving a distance between 1.42 to 1.55 meters, and method2 somewhat closer to the FLACS model with a distance ranging from 1.8 to 2.1 meters. This is in agreement with the results seen for elevated free jet releases without the ground interaction.

Table 5-2 *Overview of wind conditions in FLACS simulations shown below.*

Sim nr	**Wind condition and stability class**
005900	***1.0F***
005901	***1.5F***
005902	***3.0F***
005903	***3.0B***
005904	***5.0D***
005905	***5.0B***

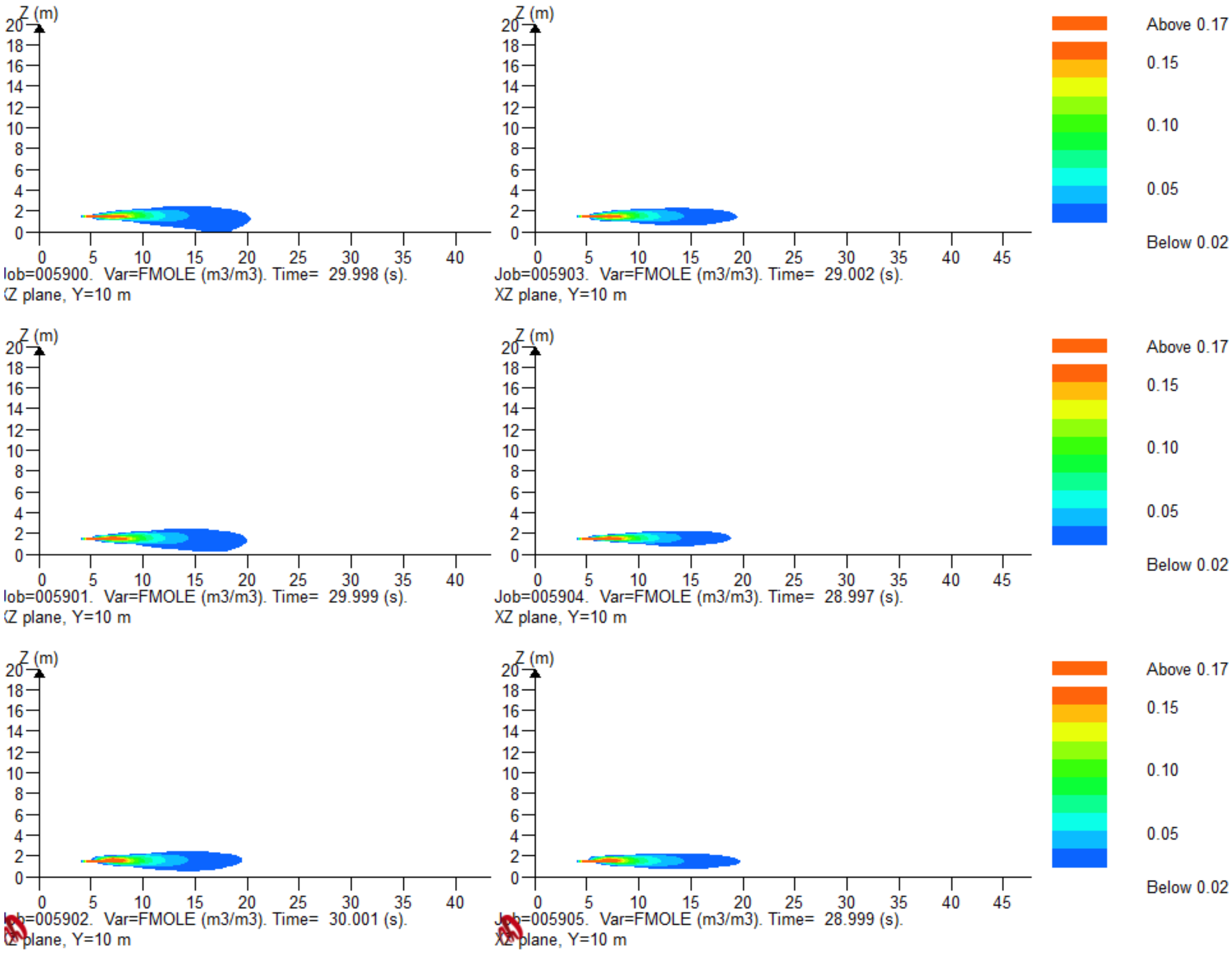


Figure 5-6 *Simulations run in FLACS for 0.59 kg/s for the different wind conditions. Simulation wind conditions given in* **Table** 5-2.

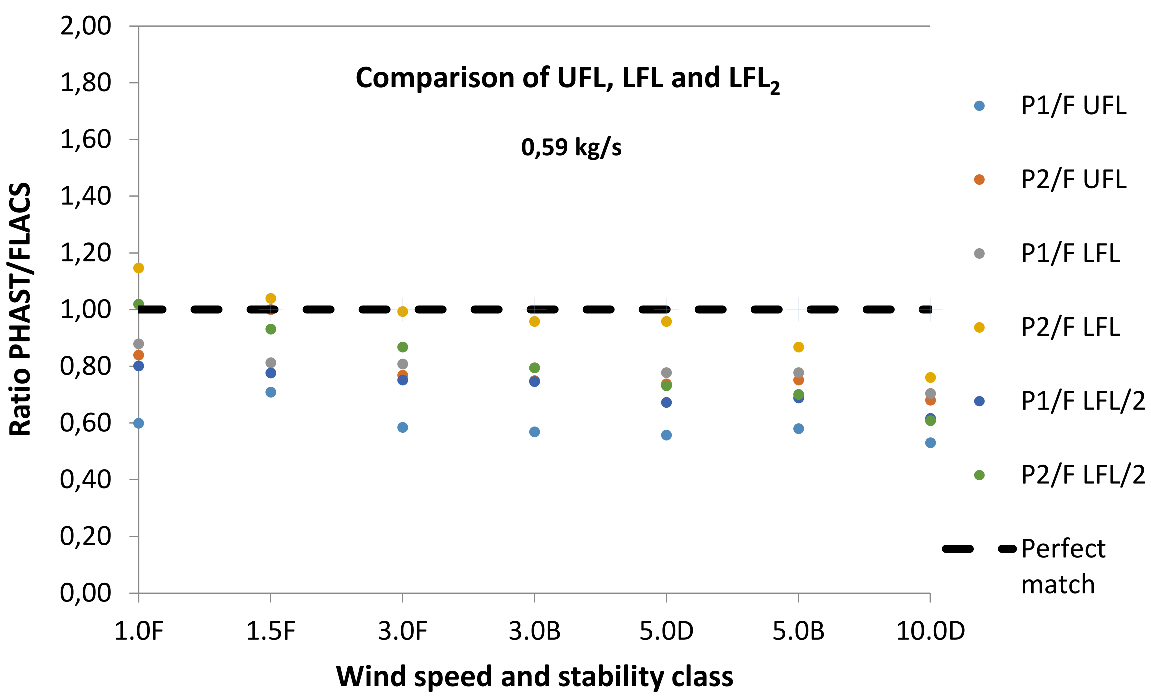


Figure 5-7 *Comparison of FLACS and PHAST for downwind concentration decay for three different wind conditions. UFL, LFL and LFL$_2$ values are compared for jet releases at wind conditions 1.0, 1.5 and 5.0 m/s wind. F, D and B are in this context two different classes of stability. To generate each comparison the ratio of distance in meter along the centerline where the cloud reached 2.2 Vol% (LFL$_2$), 4.4 Vol%(LFL) and 16.5 Vol% (UFL) was used for the comparison.*

The PHAST1 values represent PHAST method1 and PHAST2 values represent the method 2. A perfect match between the models will again give a value of one.
The P2 values are much closer to the FLACS value than the P1 values, indicating that method2 are more comparable with the FLACS model for these small releases.

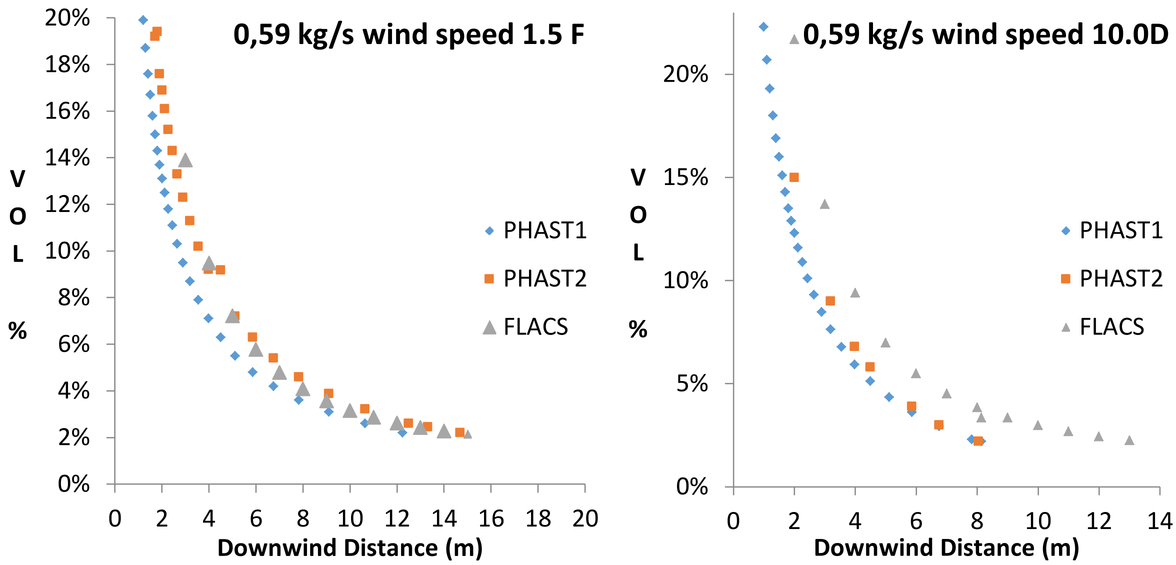


Figure 5-8 Left figure is a *comparison plot for wind speed 1.5 with stability F. Right figure is a comparison plot for wind speed 10.0 with stability D. Larger deviation between PHAST and FLACS is seen for higher external wind speeds.*

Higher wind speed causes the models to deviate at a larger degree than low wind speed used for the comparison. The trend shown in these figures also indicates equal handling of the concentration decay by the models when results are illustrated by the centerline approach.

5.2.2.2 Medium releases 3.93 kg/s 1.5 meters above ground

For the medium release of 3.93 kg/s of methane the results show some of the same trend as the small releases with method2 again being more comparable than method1 for the centerline concentration decay. The results show overall good agreement and show the same trends with increasing external wind speed. The plots below show impact of different external wind speeds in the jet phase.

Table 5-3 *Overview of FLACS simulations shown below.*

Sim nr	*Wind condition (m/s) and stability class*
260301	**1.5F**
260302	**3.0F**
260303	**3.0B**
260304	**5.0D**
260305	**5.0B**
260306	**10.0D**

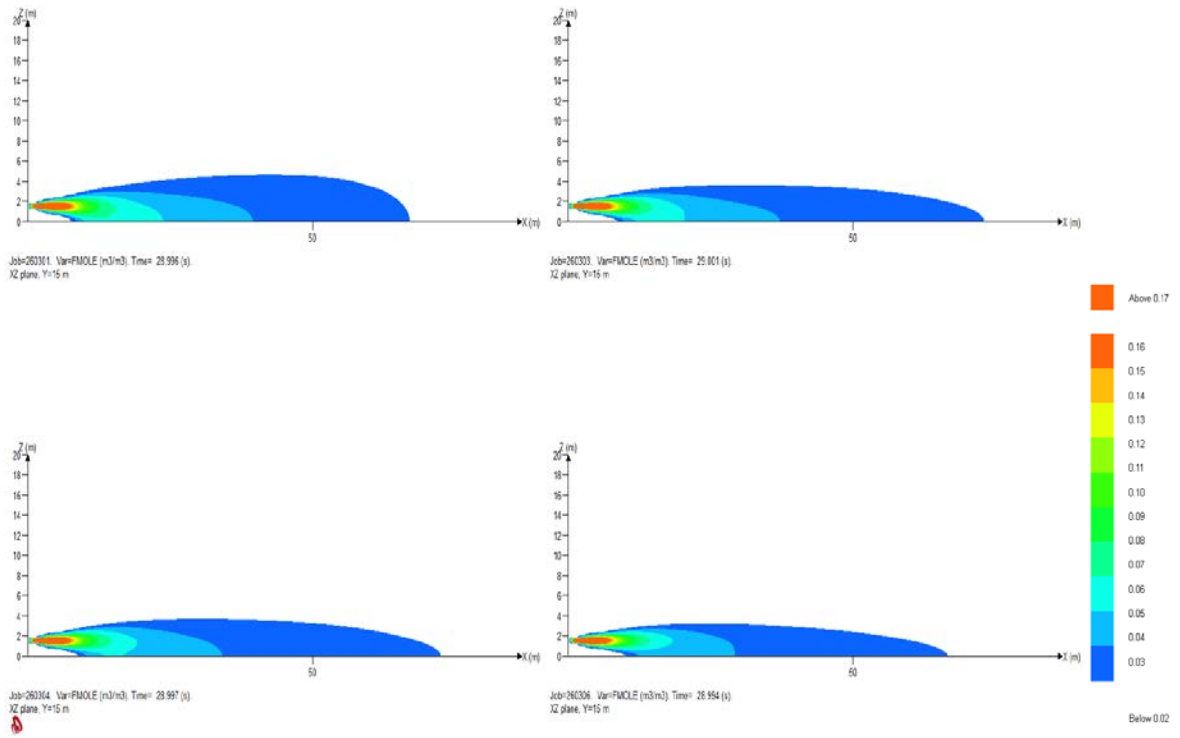


Figure 5-9 *Simulations run in FLACS for medium size leak (3.93 kg/s) for four different wind conditions. Discharge velocity of 251.27 m/s. Concentration values decay up to 2.2 Vol%. Concentration legend to the right.*

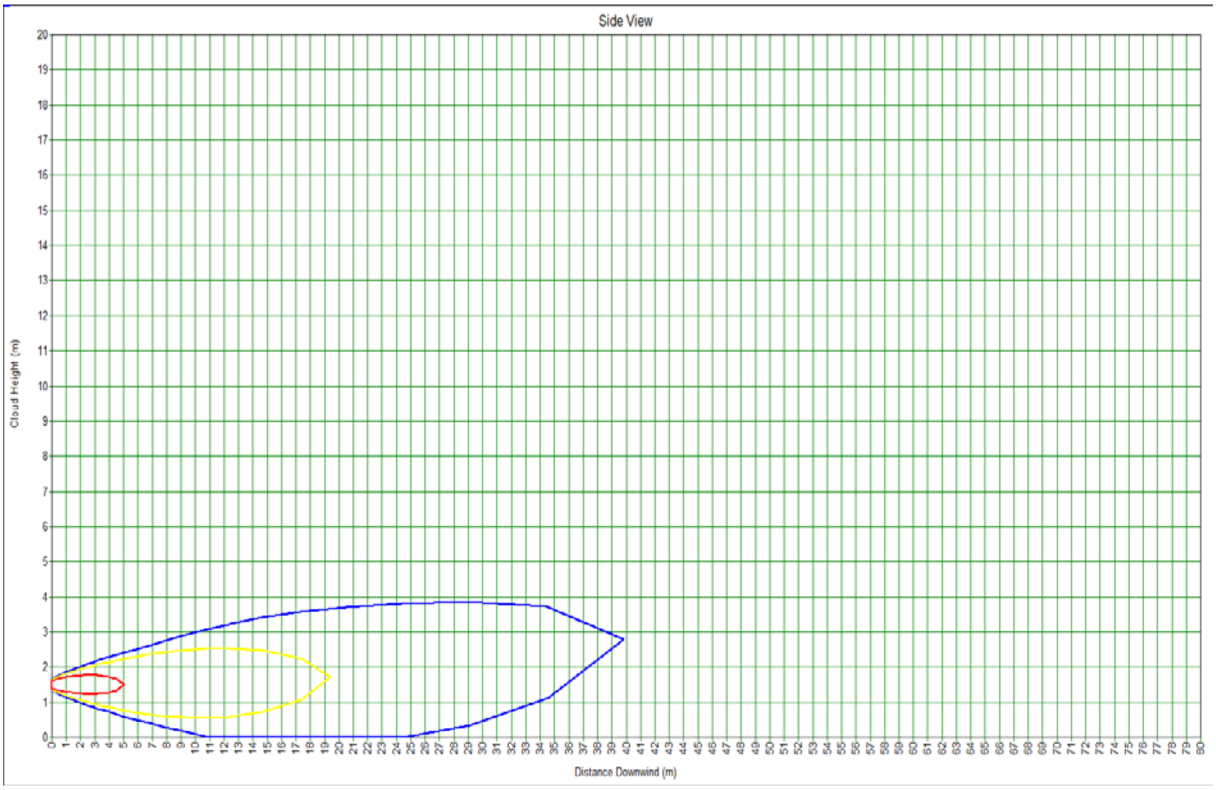


Figure 5-10 *PHAST method2 jet release of medium sized (3.93 kg/s) of wind conditions of 3.0 m/s stability B. (UFL is indicated by the red color, yellow represents the LFL concentration extent, and blue represent the LFL_2 range. FLACS comparison plot is 260303 shown in Figure 5-9.*

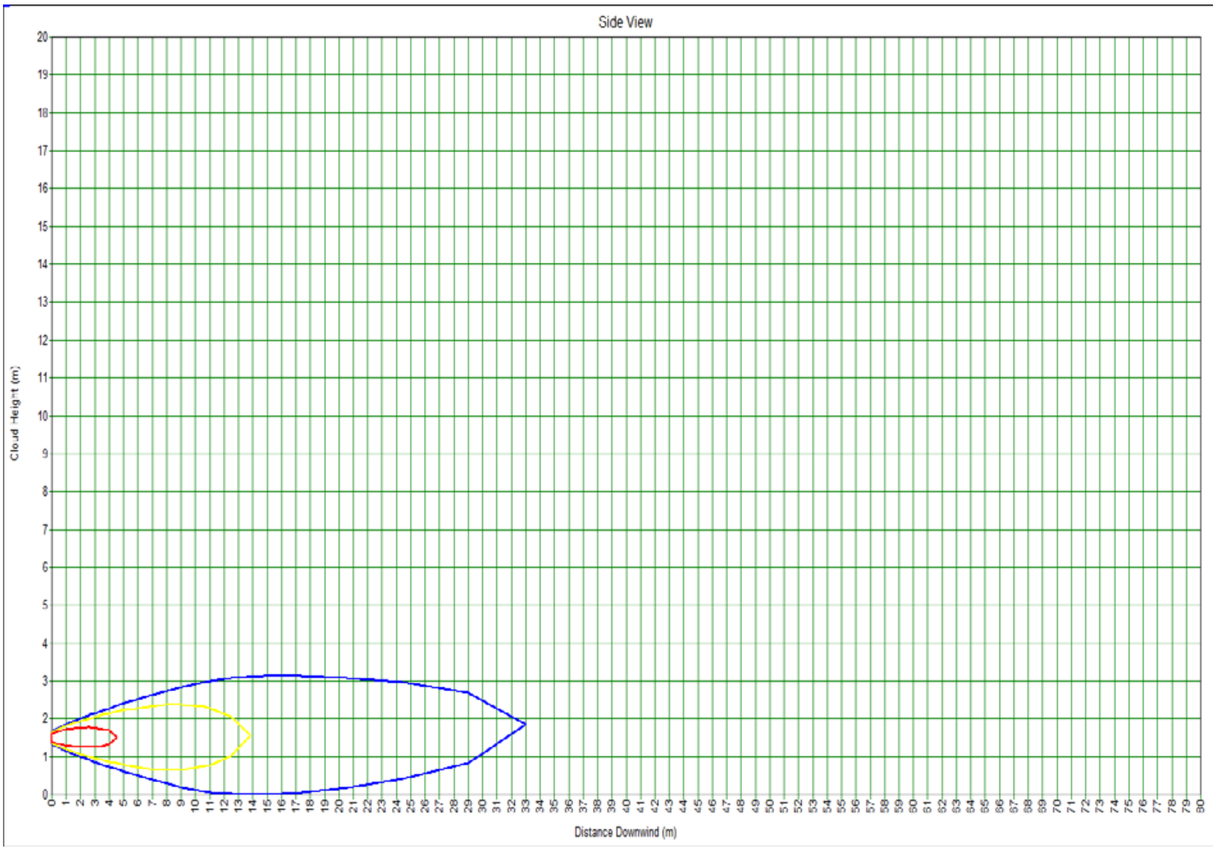


Figure 5-11 *Side view plot; PHAST method2 10.0D jet release of medium sized release (3.93 kg/s). (The UFL value is shown by the red color, yellow represents the LFL concentration extent and blue represent LFL_2. FLACS comparison plot is 260306 shown in Figure 5-9.*

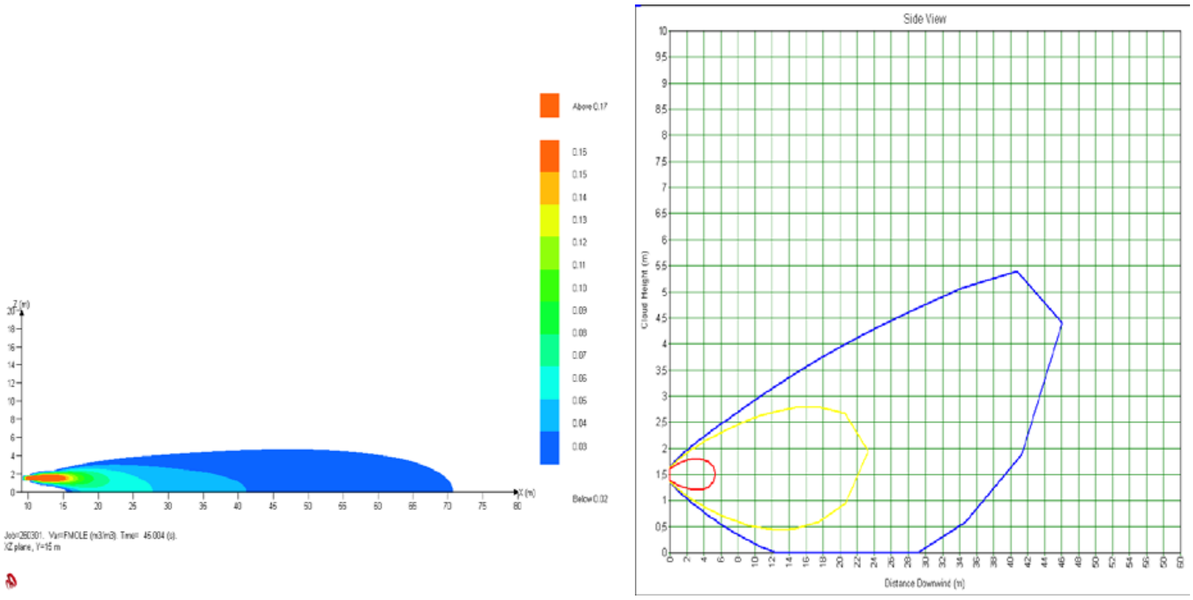


Figure 5-12 *Side view plots of Jet release of 3.93 kg/s methane jet with 1.5 m/s wind F stability. Comparison jet in PHAST shown in figure to the right. Similar discharge properties (method2).*

Figure 5-13 *Comparison jet in PHAST Method1 jet in PHAST with wind conditions of 1.5 m/s with stability class F.*

Seen from Figure 5-12 and Figure 5-13, the methane releases show some differences in the behavior or the gas plumes. The FLACS release is not as buoyant as the PHAST when using method2 release. The FLACS releases also have a tendency for touchdown in the LFL range while PHAST having touchdown in lower concentration, within the LFL_2 range. PHAST method2 jet also enters the passive regime at higher concentrations than FLACS and has more buoyant plumes than the FLACS model.

Seen from the plot below the most comparable concentration values are seen in between FLACS and PHAST for the P2/F LFL. The P2/F UFL value in this regime is also in good agreement between the models.

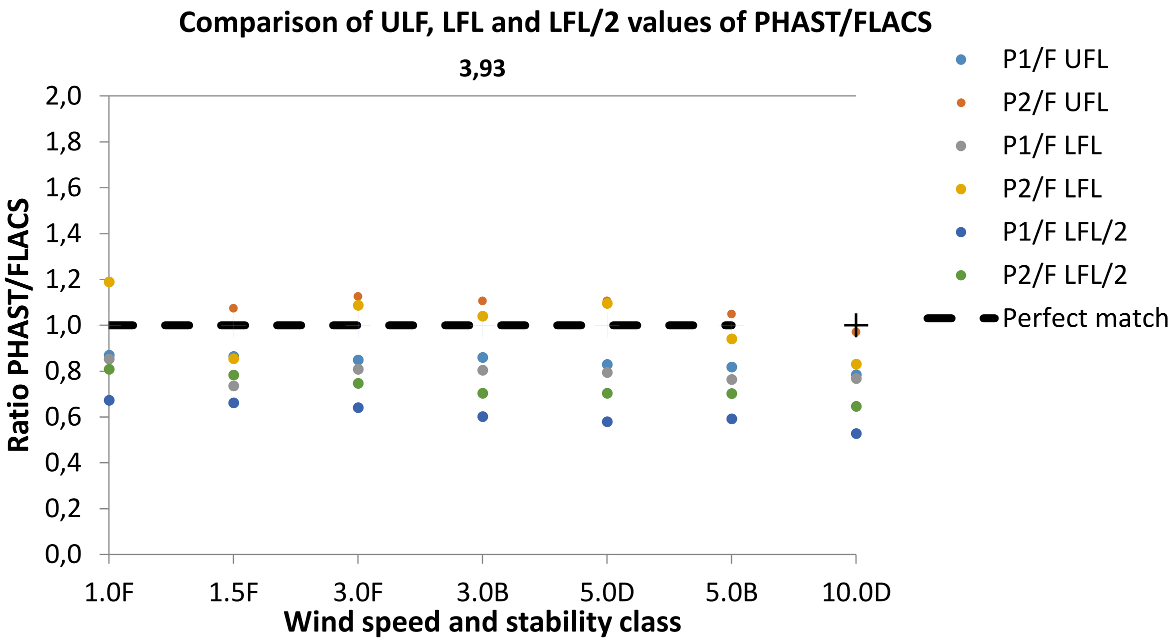


Figure 5-14 *3.93 kg/s comparison of PHAST/FLACS for UFL, LFL and LFL_2 values for the different wind conditions. To generate each comparison the ratio of distance in meter along the centerline where the cloud reached 2.2 Vol% (LFL_2), 4.4 Vol%(LFL) and 16.5 Vol% (UFL) was used for the comparison.*

5.2.2.3 Large release 9.48kg/s, 2 meters above ground

The same release setup was used for the large jets of 9.48 kg/s. The Figure 5-15 below show the concentration down to LFL critiera. LFL_2 is not shown in this figure.

Table 5-4 Overview of wind conditions for the large methane simulations in FLACS shown below.

Sim nr	***Wind condition (m/s) and stability class***
094800	***1.0F***
094801	***1.5F***
094802	***3.0F***
094803	***3.0B***
094805	***5.0B***

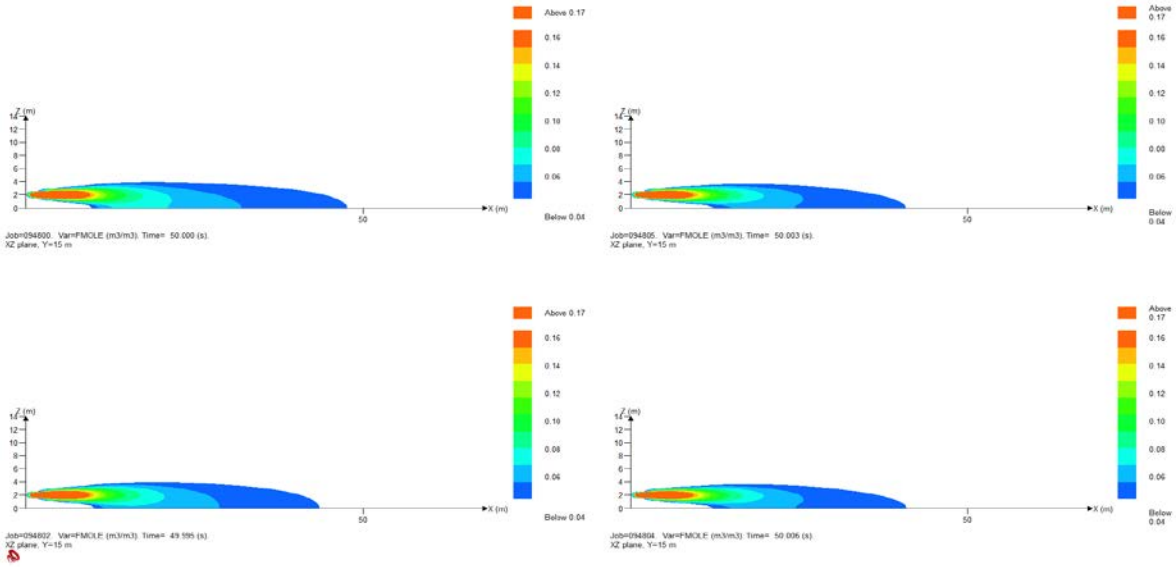


Figure 5-15 *Large release of 9.48 kg/s, discharge velocity of 251.07 m/s. Concentration up to LFL 4.4 Vol%.*

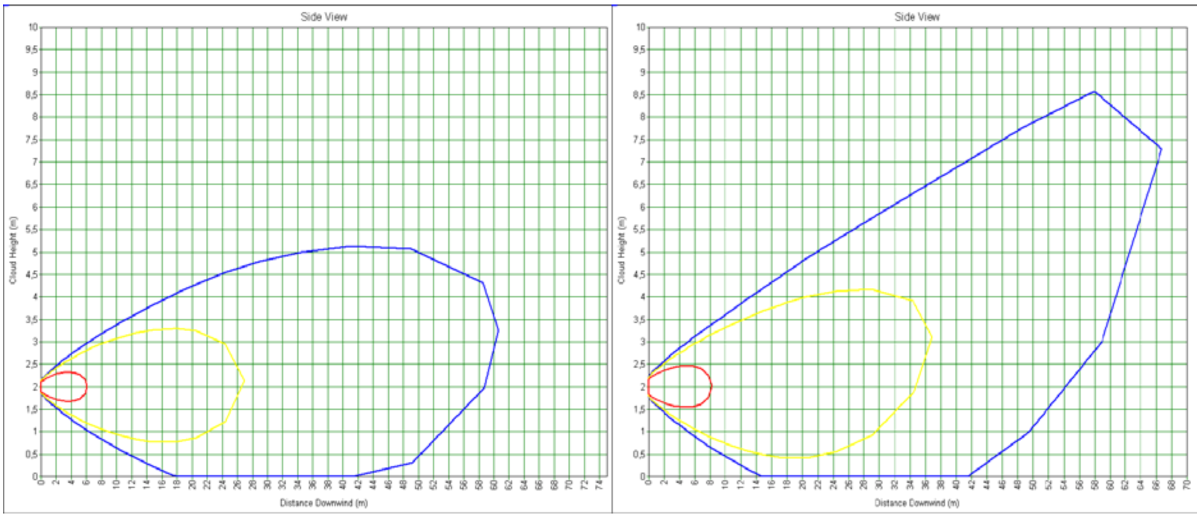


Figure 5-16 *Comparison of method1 and 2 for 9.48 kg/s. Right figure is method1 and left figure show the more buoyant method2. Wind speed of 1.5 m/s stability F.*

Figure 5-16 show the differences between method1 and method2. The method2 jet is more buoyant that the release shown for the method1 jet for the same wind conditions.

The concentration spread downwind for PHAST method2 is also longer despite the more buoyant character.

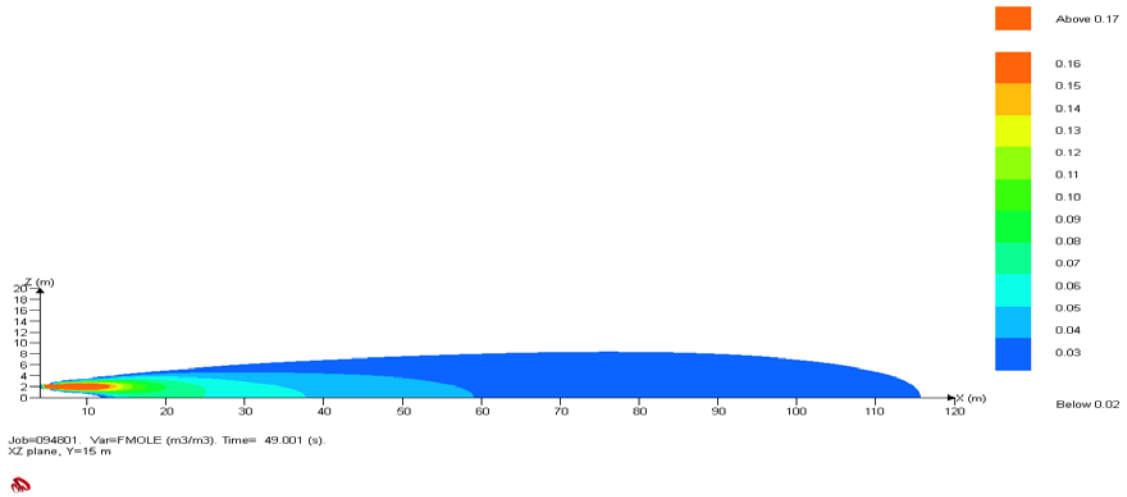


Figure 5-17 *FLACS jet comparison plot showing LFL_2 domain.*

The FLACS jets show that the touchdown regime is developed within the LFL concentration. The PHAST simulations do not show this trend with touchdown only in the lower concentrations, within the LFL_2 regime. The FLACS jets are also larger in terms of the widths than PHAST indicating that the FLACS jets are larger in terms of both width and length than the jets modeled in PHAST.

For the comparison the UFL values in PHAST for method2 gave higher concentration values than the FLACS simulations, as shown in Figure 5-18. This trend was also shown for 3.93 kg/s simulations indicating that PHAST has higher concentration closer to the leak than FLACS for mass flow rates within the range examined. For all the different mass flow rates run the models were most comparable for the LFL distances of concentration for the method2.

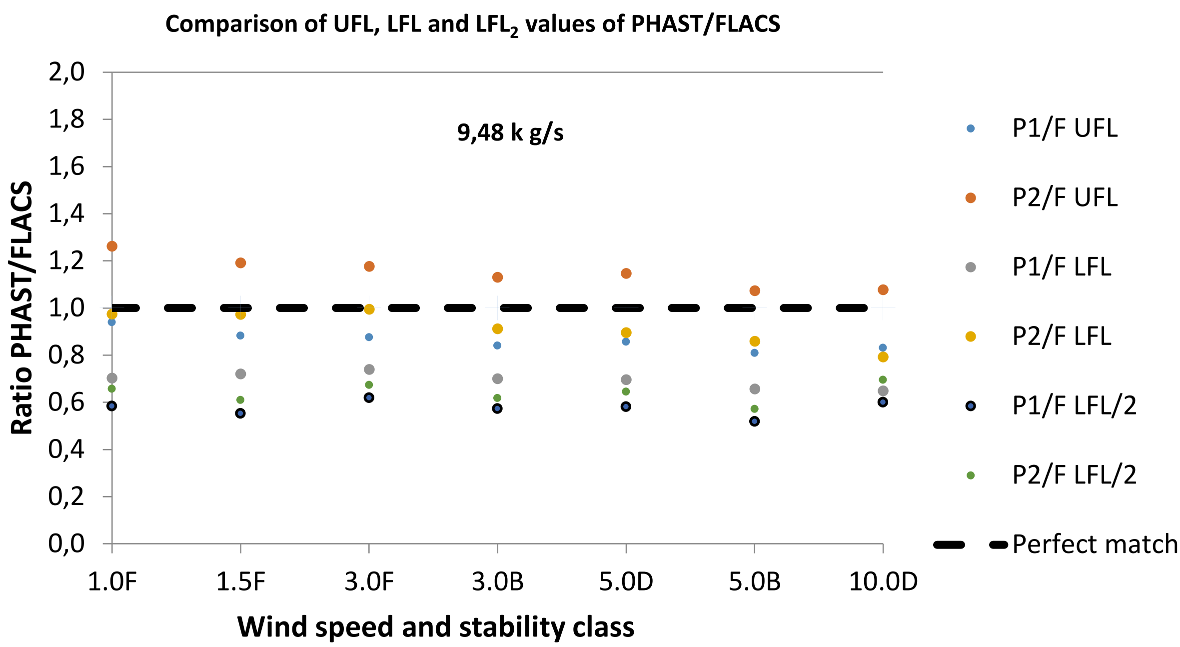


Figure 5-18 *9.48 kg/s Comparison of PHAST/FLACS for UFL, LFL and LFL_2 values for the different wind conditions. To generate each comparison the ratio of distance in meter along the centerline where the cloud reached 2.2 Vol% (LFL_2), 4.4 Vol%(LFL) and 16.5 Vol% (UFL) was used for the comparison.*

5.2.3 Propane results

The same methodology as used for the methane simulations was used for propane. Propane was released 1-2 meters above ground level and the concentration profile along the centerline was tracked. Three mass flow rates were run as described above. Propane has an explosive range of 2 to 9.5 Vol% mixed with air [13] and the graphs show this range approximately up to 10%.

Figure 5-19 and Figure 5-20 below show the flammable range for 0.702, 1.95 and 7.8 kg/s releases performed with 3.0 m/s wind speed and F stability.

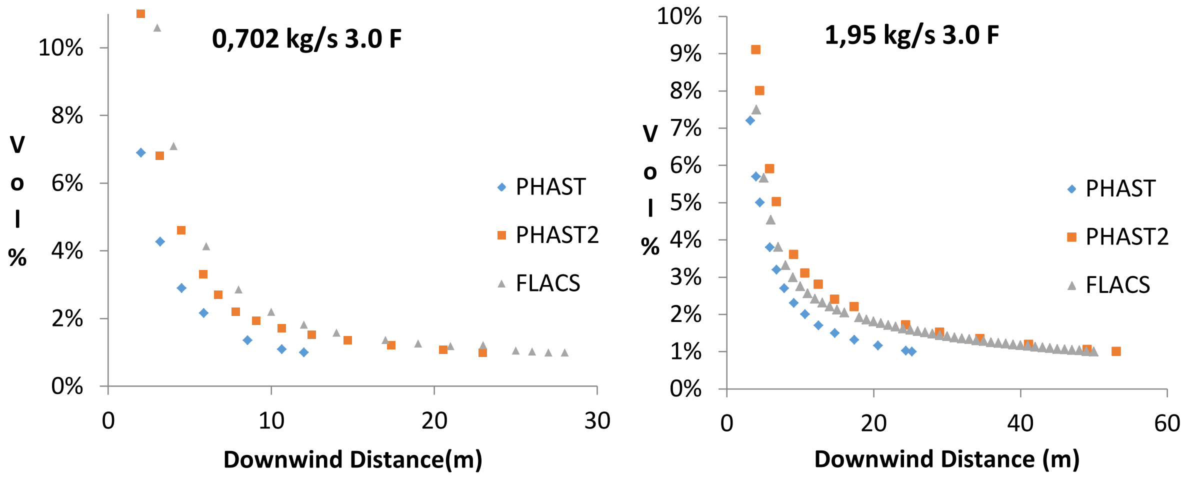


Figure 5-19 *Centerline concentration up to LFL_2 of 0.702 kg/s with discharge velocity of 155.67 m/s and 1.95 kg/s with discharge velocity of 138.15 m/s. Wind speed 3.0 m/s stability F.*

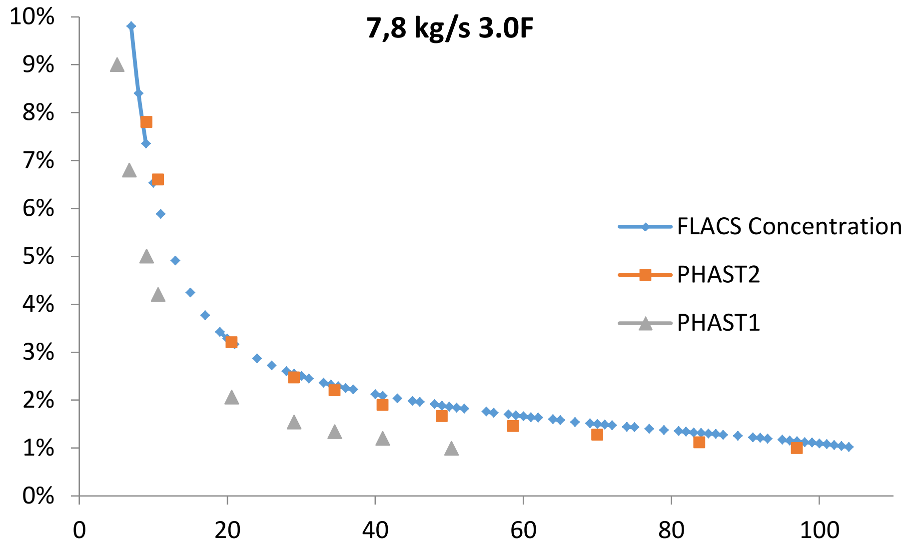


Figure 5-20 *Centerline concentration of 7.8 kg/s up to LFL_2 with discharge velocity of 138.2 m/s. Wind conditions of 3.0 m/s with F stability.*

5.2.3.1 Small releases 0.702kg/s

For the small releases of 0.702 kg/s the FLACS model gives the longest UFL, LFL and LFL_2 value for downwind concentration. PHAST reaches the UFL values at lower lengths downstream of the leak than FLACS. The deviations become larger as the wind speeds increase and just as for the methane releases.

Table 5-5 *Overview of wind conditions for Propane simulations in FLACS shown below.*

Sim nr	***Wind condition (m/s) and stability class***
300200	*1.0F*
300201	*1.5F*
300202	*3.0F*
300203	*3.0B*
300205	*5.0B*
300206	*10.0D*

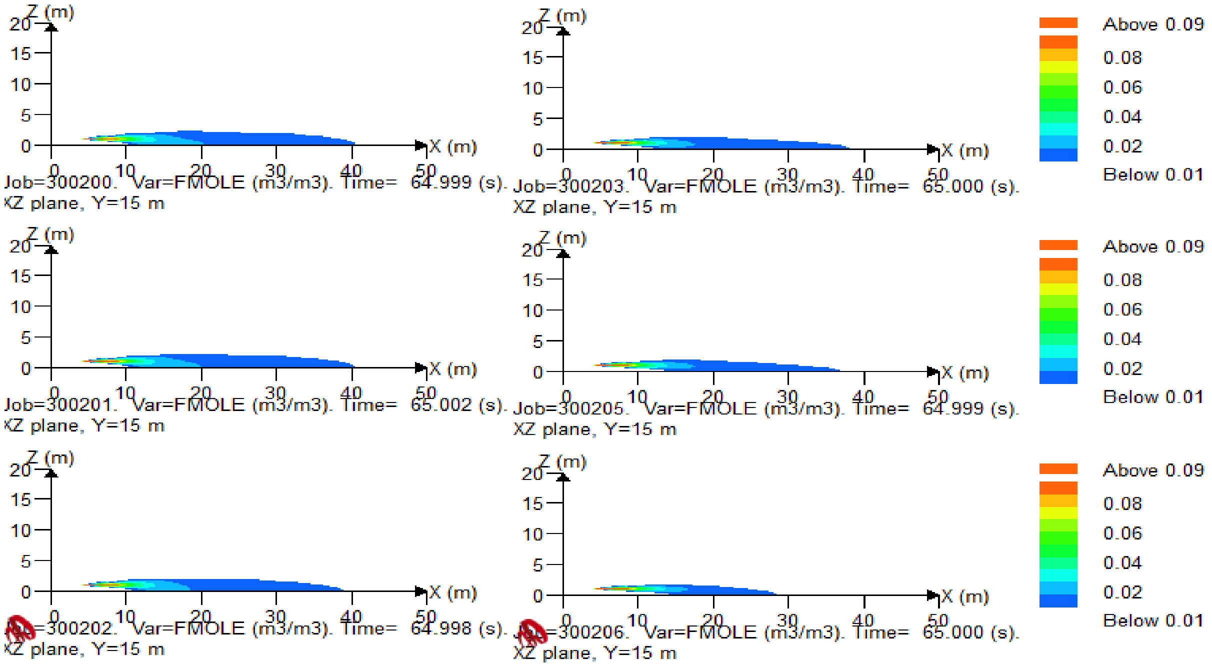


Figure 5-21 *Propane releases small jet at steady state. Various wind conditions up to LFL_2 Distances at 65 seconds.*

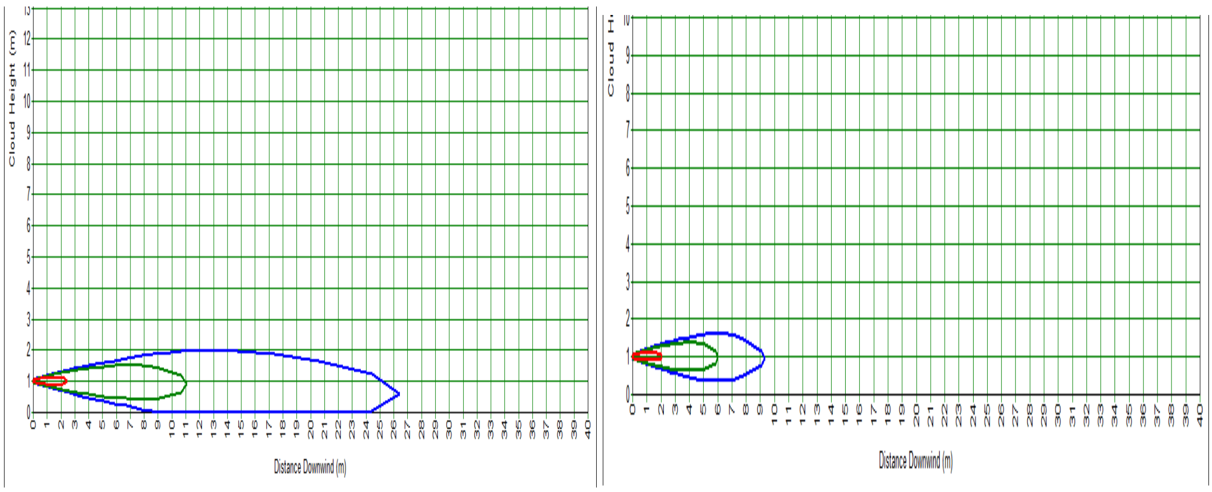


Figure 5-22 *Left figure is a representation of a propane jet with concentration up to LFL_2 using method2. Wind speed 1.0 m/s stability 2. Right figure is a representation of the same propane jet with concentration up to LFL_2 using method2. Wind speed of 10.0 stability D.*

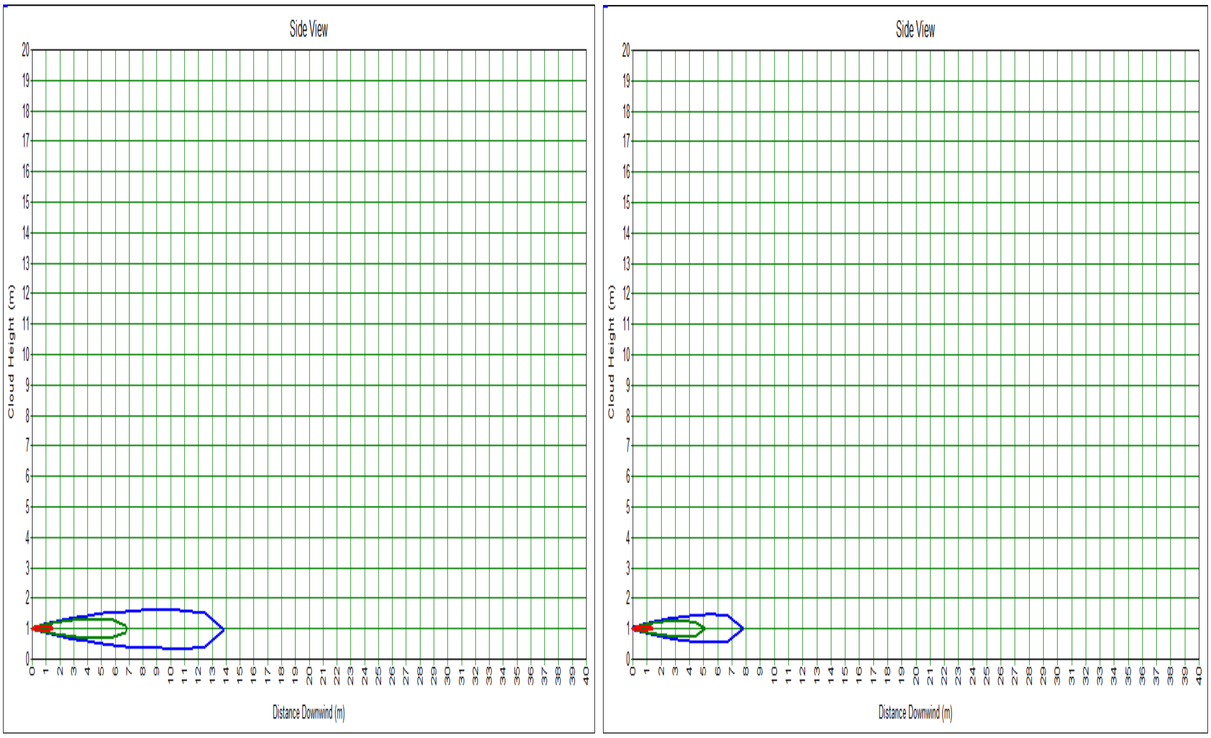


Figure 5-23 *Left figure is a representation of a propane jet with concentration up to LFL_2 using method1. Wind speed 1.0 m/s stability 2. Right figure is a representation of a propane jet with concentration up to LFL_2 using method1. Wind speed of 10.0 stability D.*

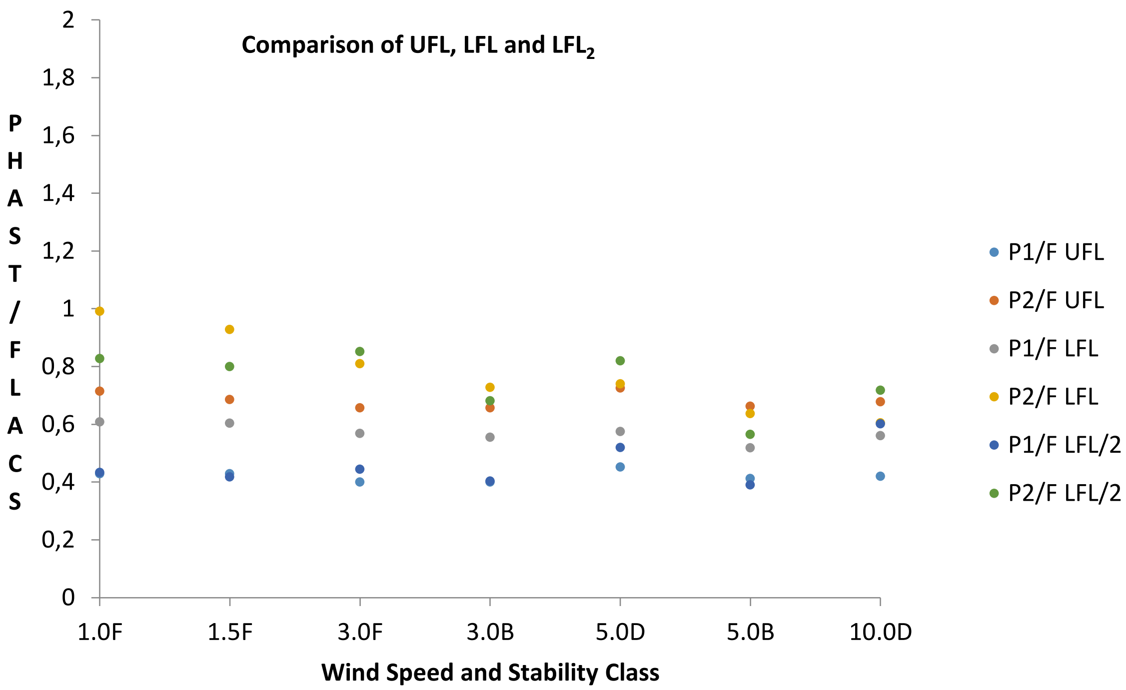


Figure 5-24 *0.702 kg/s Comparison of PHAST/FLACS for UFL, LFL and LFL_2values for the different wind conditions. Discharge velocity of 155.97 m/s*

5.2.3.2 Medium releases 1.95kg/s

The mass flow rate of 1.95 kg/s was simulated in the same manner as the 0.702 and 7.8 kg/s scenarios.

Figure 5-25 below gives a good visual illustration of the differences between method1 and method2 for the 1.95kg/s mass flow rates. The method1 jet is approximately half the size of the method2 jet.

Table 5-6 *Overview of wind conditions for Propane simulations in FLACS*

Sim nr	***Wind condition (m/s) and stability class***
290200	***1.0F***
290201	***1.5F***
290202	***3.0F***
290203	***3.0B***
290205	***5.0B***
290206	***10.0D***

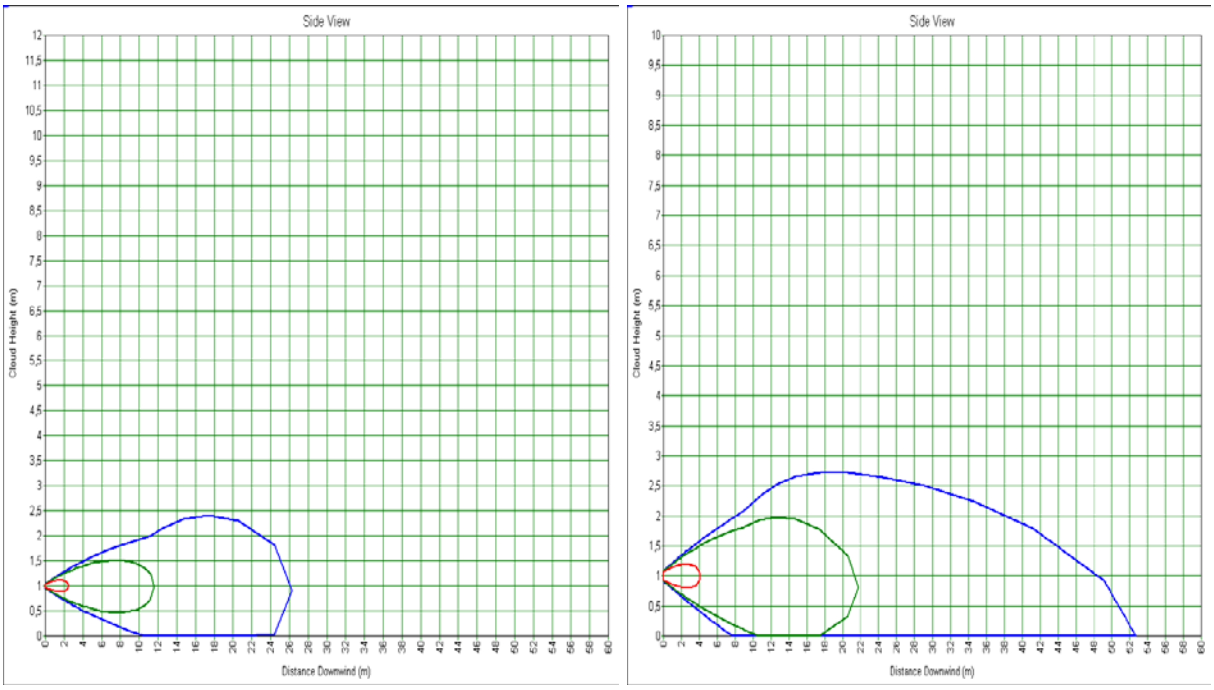


Figure 5-25 *Comparison of PHAST method1 and method2; Left figure is a representation of PHAST method1 concentration up to LFL2. Wind speed 1.0 m/s and stability class F. Right figure is a representation of PHAST method2 concentration up to LFL2. Wind speed if 1.0 m/s with stability class F.*

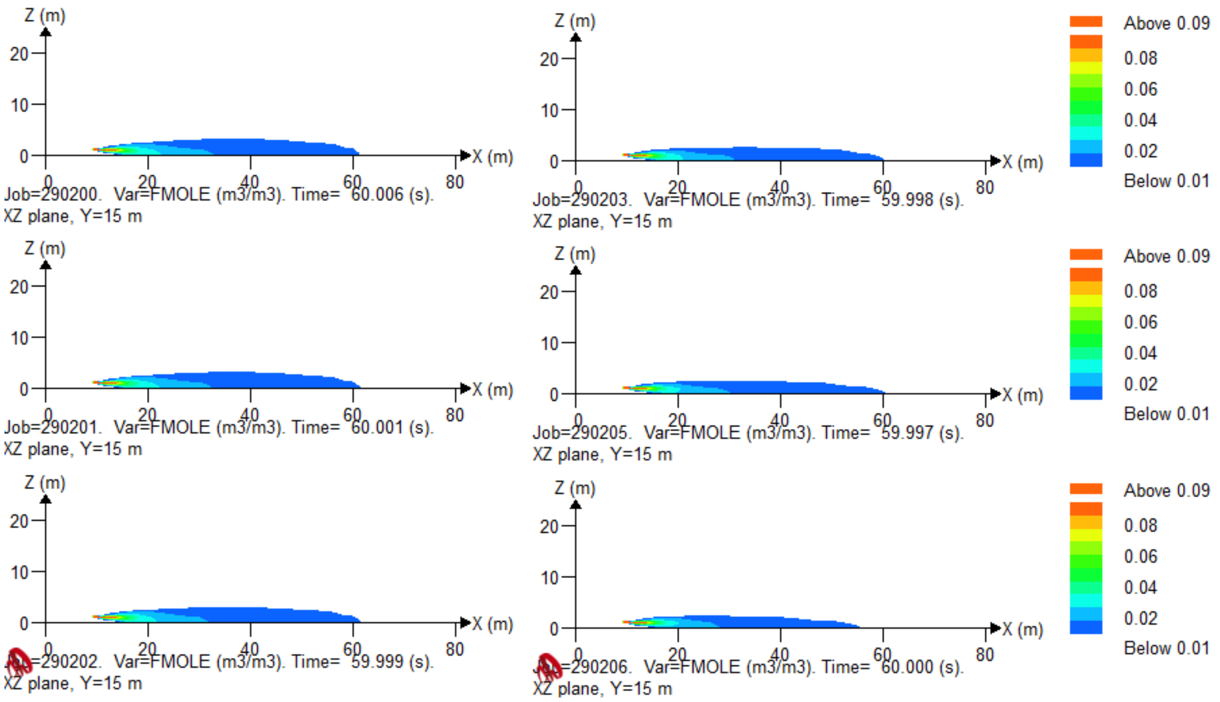


Figure 5-26 *Propane releases medium jet. Various wind conditions up LFL_2 Distances at steady state at 60 seconds. Discharge velocity of 138.15 m/s.*

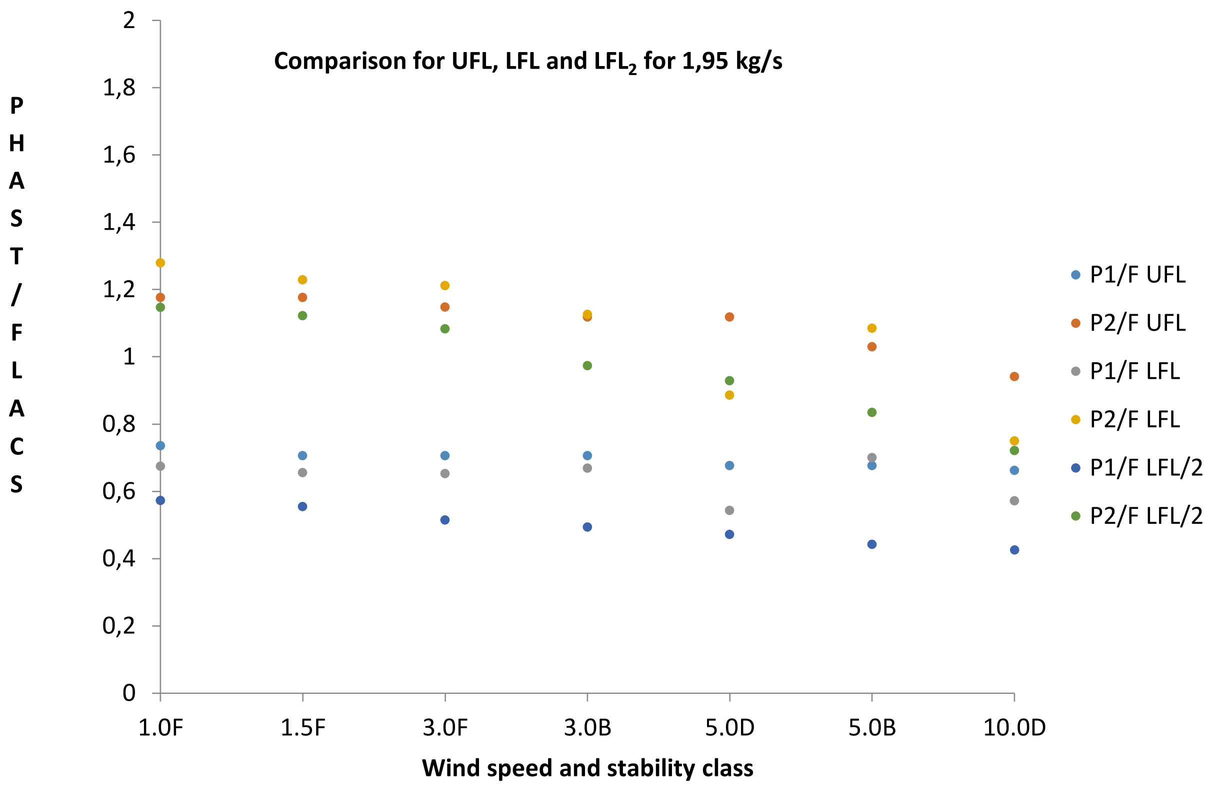


Figure 5-27 *1,95 kg/s Comparison of PHAST/FLACS for UFL, LFL and LFL_2 values for the different wind conditions. Discharge velocity of 138.15 m/s.*

Once again we see a closer relationship between PHAST method2 and the FLACS results compared to method1 in PHAST. The results for UFL for method2 are within an average range of 12 % deviation from the FLACS results for the various wind conditions used for the simulations. The LFL values deviate stronger, with an average percentage deviation between the models of 18.5% for the different wind conditions. For the LFL_2 values the average range of deviation was around 12.5 %.

5.2.3.3 Large releases 7.8kg/s

The FLACS plots below show the jet up to a concentration of 2.2 Vol%, LFL.

Table 5-7 *Overview of wind conditions for Propane simulations in FLACS shown below.*

Sim nr	***Wind condition (m/s) and stability class***
300001	***1.0F***
300002	***1.5F***
300003	***3.0F***
300005	***3.0B***

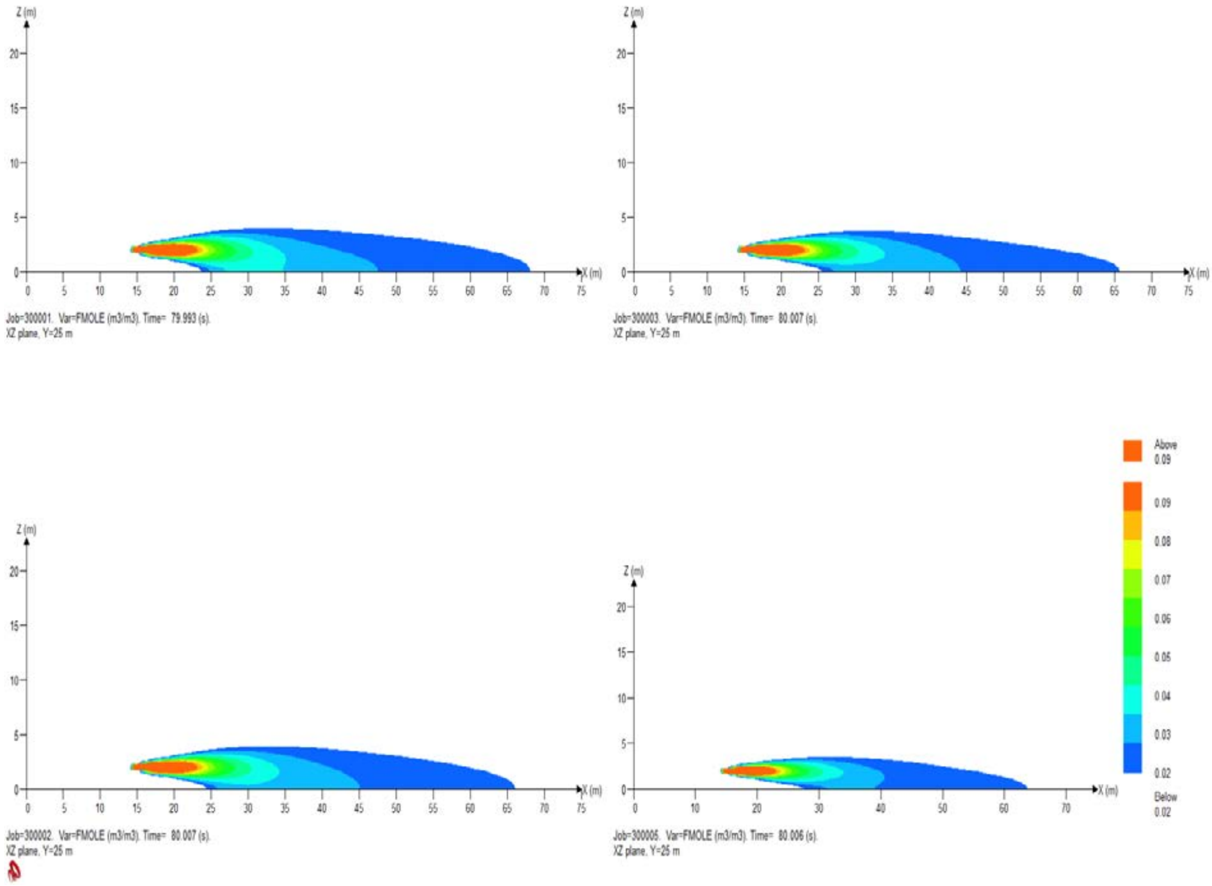


Figure 5-28 *Large releases 7.8 kg/s, FLACS simulations for various wind conditions up to LFL concentration values (2 vol%).*

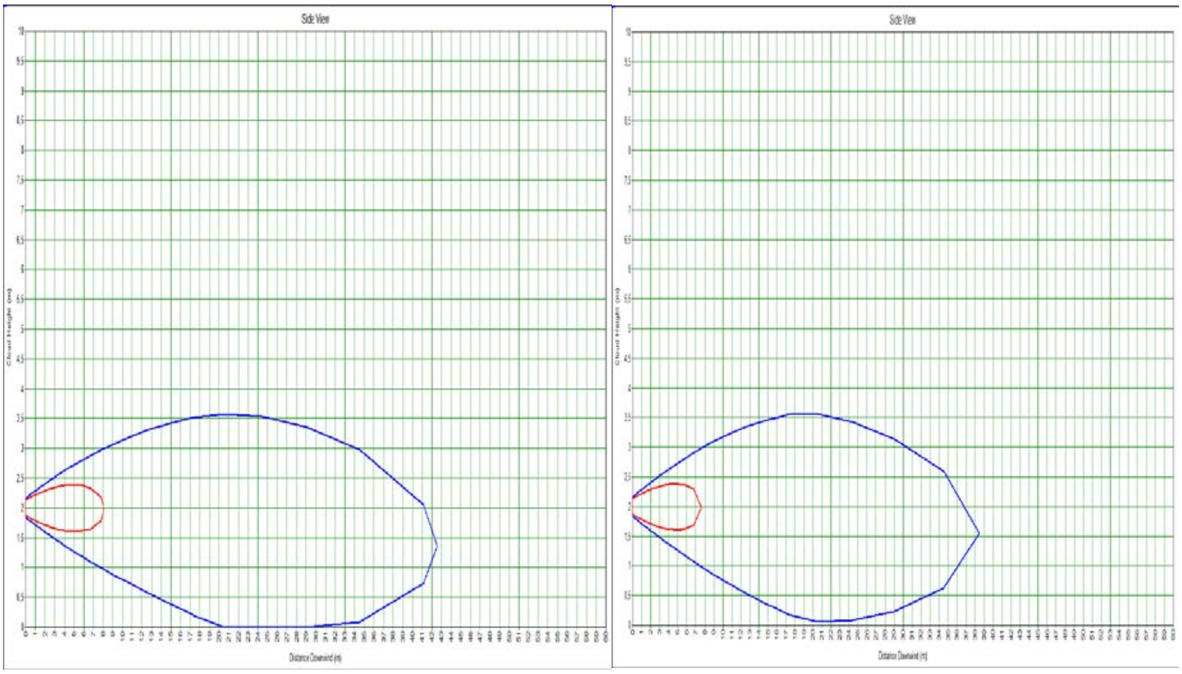


Figure 5-29 *Comparison plot of Method2 wind speed of 1.0 m/s stabillity class F in left figure. Wind speed of 3.0 m/s stabililty class F to the right. Concentration up to LFL 2 VOL %.indicated by blue. Red indicates UFL value (9.5 Vol%).*

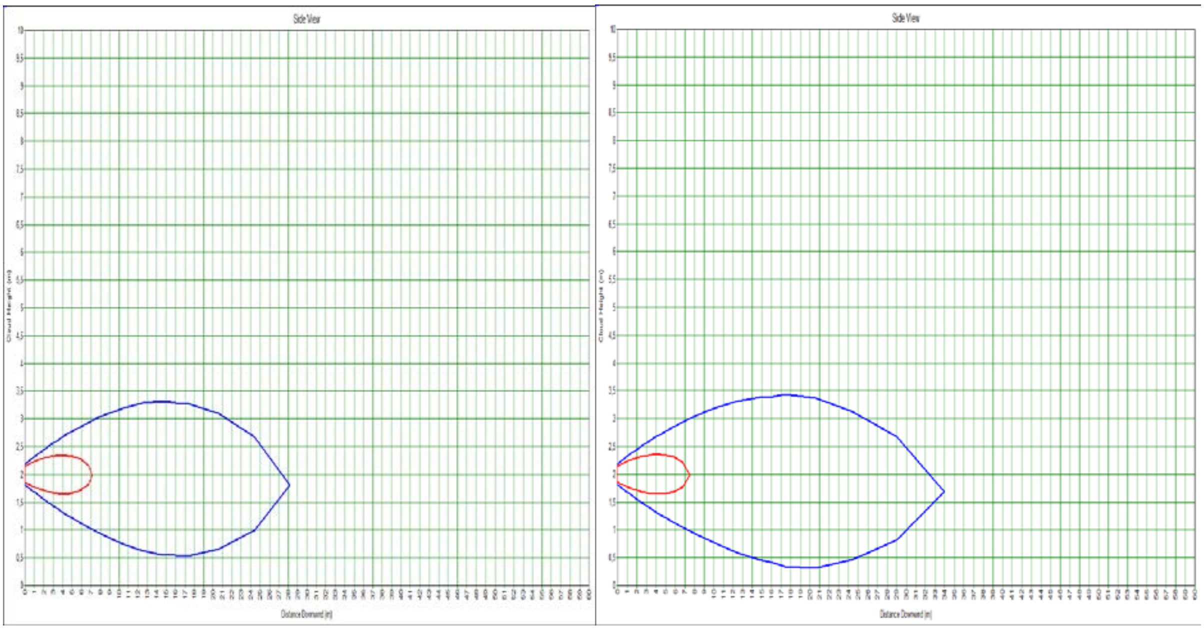


Figure 5-30 *Comparison plot of Method2 wind speed of 5.0 m/s stabillity class B in left figure. Wind speed of 3.0 m/s stabililty class B to the right. Concentration up to LFL 2 VOL %.indicated by blue. Red indicates UFL value (9.5 Vol%).*

5.3 Flammable mass Comparison methane Free Jets

A comparison was done to compare the flammable mass for the free jet simulations of ATEX-like scenario and the large leakage scenario. Both method 1 and 2 was used in PHAST for these simulations and the results was compared against the FLACS results for the various cases. The trend shown was that at higher wind speeds the lower the flammable mass was seen. The pushing force of the wind will enhance the entrainment of air of thereby dilute the concentration of the gas plume. The flammable mass comparison plot for free jet ATEX and large release scenario is shown below. Again method2 gives the most comparable results with FLACS. For the large mass flow rates the results are very comparable.

For the higher wind speeds of 5.0D, 5.0B and 10.0D PHAST would not give a flammable mass for the simulations with method1. The flammable mass values were found in the late explosion report in PHAST. In FLACS the flammable mass was extracted from the fuel file.

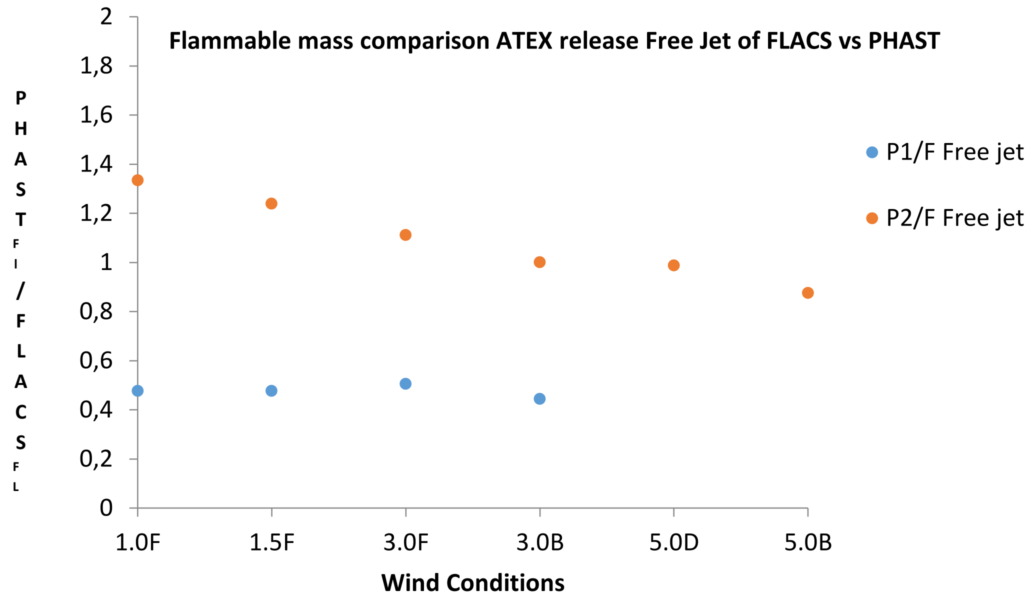


Figure 5-31 *Flammable mass comparison for Free Jets 1.5m above ground for various wind conditions. Value of flammable mass ratio in kg used to generate plot. No information regarding flammable mass was given in PHAST for Method1 wind conditions of 5.0D and 5.0B*

5.4 Grid Sensitivity methane/propane Jets

All the FLACS simulations for the small, medium and large Methane jet was run with 1m*1m*1m grid and grid cells close to the leakage source were refined in accordance with the grid guideline within the model.

A sensitivity analysis was performed using 2*0.5*0.5 m grid. No significant differences in terms of concentration decay and flammable mass was seen compared to the grid chosen for the comparison.

For the propane simulations the grid used for the comparisons of the three different mass flow rates was a 1m*1m*1m grid. Grid sensitivity was performed also for the propane releases using different grid. For the 0.702 kg/s case a 2m*0.5*0.5 grid was chosen. No significant differences in terms of concentration decay and flammable mass was seen compared to the grid chosen for the comparison.

5.5 General conclusion methane/propane free jet releases with ground interaction

As a general conclusion the results given by PHAST user defined source, is more comparable with the FLACS model than the Vessel/Source model in PHAST, for centerline profile concentration decay of free jets. This indicates that when the discharge modeling in FLACS and PHAST are similar the results gained through a comparison show good agreement between the model for open field jet releases. Input derived from FLACS jet utility are implemented in the PHAST user defined discharge, so that only the dispersion model in the source of deviation of the two models. A review of the comparison plots documents this for the UFL, LFL and LFL_2 values for methane and propane.

The deviation between the models was largest in the LFL_2 concentration. A close relationship is seen for the downwind concentration of LFL values for user defined discharge in PHAST and the FLACS values. The LFL values shown in PHAST are within a deviation of 20% of the FLACS results for almost all the simulations run, indicating good agreement between the models. For method2 the UFL values for medium and large mass flow rate the values in PHAST gave higher downwind concentrations than the FLACS model using the centerline concentration approach, otherwise the FLACS model gave the highest concentrations downwind for all other cases.

The simulations run FLACS model show that this model is more conservative in terms of the concentration lengths of the flammable domain for almost all the mass flow rates run in the part. The FLACS jets are larger in terms of both width and length of flammable domain, and also up to the concentration limits of the LFL_2 criteria, 2.2 Vol%.

Touchdown phase was shown in FLACS for the ATEX (0.59kg/s) case at low wind speeds of 1.0 and 1.5F. This was not shown in the PHAST model or FLACS for the higher wind speed simulations.
For the large mass flow rate simulations the PHAST jet enters the passive phase at higher concentrations than FLACS thereby resulting in more buoyant jets and lower concentration limits compared to the FLACS results for the methane jets. This indicates a difference in how the model treats interaction with the ground and entrainment of air due to initial turbulence.

In terms of risk assessment the deviation between method2 and FLACS are not large enough to make consequence assessments based on these results significant different. There is however some differences that should be known to the modeler using both the models, when simulating jets in free fields.

6 Field Trials

6.1 Introduction

The point of reproducing these trial tests was:

- Comparing two modelling tools is only relative. Comparison with experiments remains mandatory. This comparison may serve as a bridge between congestion environments (CFD validity range) towards open free field terrain (integral modelling validity range).
- The selected trials are used both in the validation documentation of the two tools.
- The selected trials contain both near and far field data. In addition, a small level of congestion will be considered compared to the scale of the dispersing cloud – what serves the current subject of the thesis.

6.2 Description of KIT FOX experiments

The 52 Kit Fox CO_2 gas release trials in 1995 was conducted on a large terrain called the Frenchman Flat where obstacles was put up to resemble or demonstrate a process facility in 1/10 of the scale of a normal process facility. Observation of the concentration of CO_2 downwind from the release site was monitored at 25, 50, 100 and 225 meters.

Both FLACS and PHAST models have earlier been validated against the Kit Fox experiment and the experiment has played a part in developing of the two models. DNV describes the validation of PHAST 6.0 and PHAST 5.20 against the Kit Fox experiment in their own validation document [25].

The field trials were in this report used to show how the results given by FLACS 10.0 and PHAST version 6.7 compare in terms concentration decay and how the models compare against the experimental results.

To patterns of obstacles were used for the experiment, the Equivalence roughness pattern (ERP) and the Unified roughness array (URA). The obstacles were made to study the effects of increased ground roughness at an industrial process facility [5]. This case study examines only the URA continuous trial 0604. For this purpose the ERP obstacles were removed in the geometry.

The URA is covering an area of about 120m crosswind by 314 m downwind. The obstacles had an area of 20cm height and 80cm width. According to [25] this would add up to a ground roughness of 0.01 or 0.02m. Figure 6-1 below show the plot plan of the obstacles that were used at the test site. figure

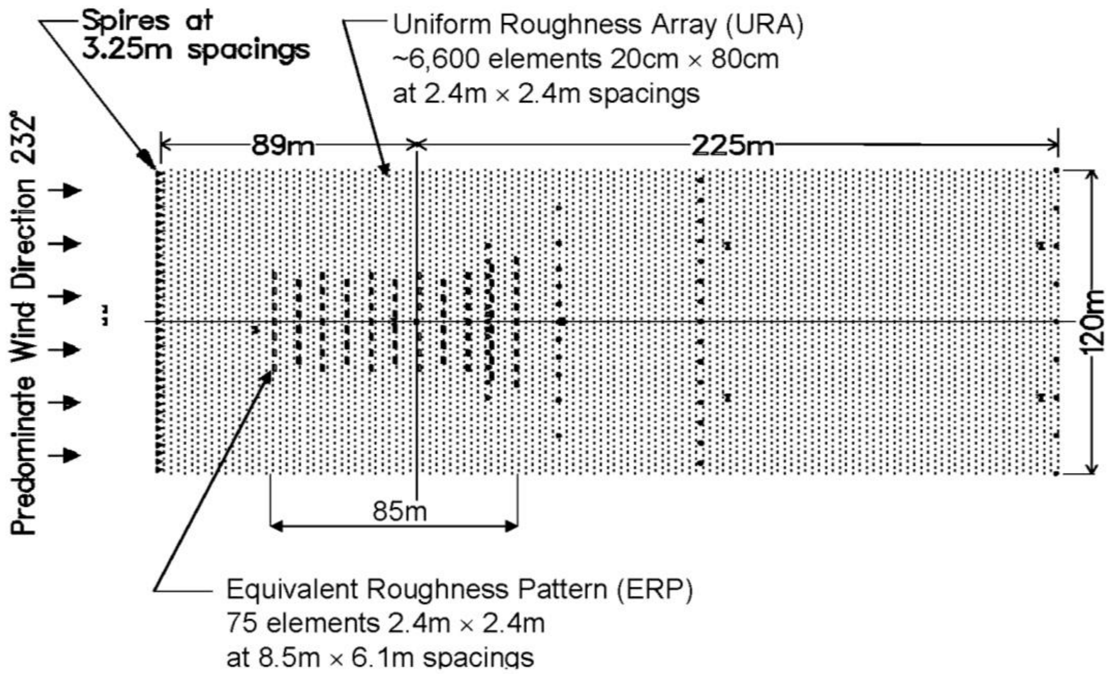


Figure 6-1 *Kit Fox experiments release site. Plot plan showing the location the obstacles [20].*

6.3 Comparison between PHAST and FLACS for the field trials

The trial URA 0604 have been simulated in both FLACS and PHAST for this report. Unlike the cases earlier run is this report (jet releases), the Kit Fox experiment was simulated in FLACS as a diffuse release. Relevant input Information, (mass flow rate, wind conditions, temperature ….), was extracted from the Kit Fox validation document [25]. Wind conditions was simulated with 4.09 m/s stability class D. In PHAST the value of ground roughness 0.01m was used for these experiments.

The trial URA 0604 have been simulated in both FLACS and PHAST for this report. Unlike the earlier run cases from this report (jet releases), the Kit Fox experiment was simulated in FLACS as a diffuse release. Wind condition is simulated with 4.09 m/s, stability class D. In PHAST the value of ground roughness 0.01m was used for these experiments.

6.4 Results Kit Fox and experimental comparison against FLACS and PHAST

The figure below shows the results for the URA 0604 continuous simulations performed. The PHAST results are presented first for 1000, 2000, 5000 and 10 000 ppm iso-contours.
Secondly the FLACS results are presented in Figure 6-4 (concentration fluctuation at the monitor points at distance 25, 50, 100 and 225 meters downwind).

PHAST results is reasonable good agreement with the experimental results for 25 and 50 meters, within 20 % deviation of under prediction. The model under predicts downwind at 100 and 225 meter distances, with given concentration values around 50% of the experimental value. This is the results when using ground roughness of 0,01 as explained in the Kit Fox validation document.

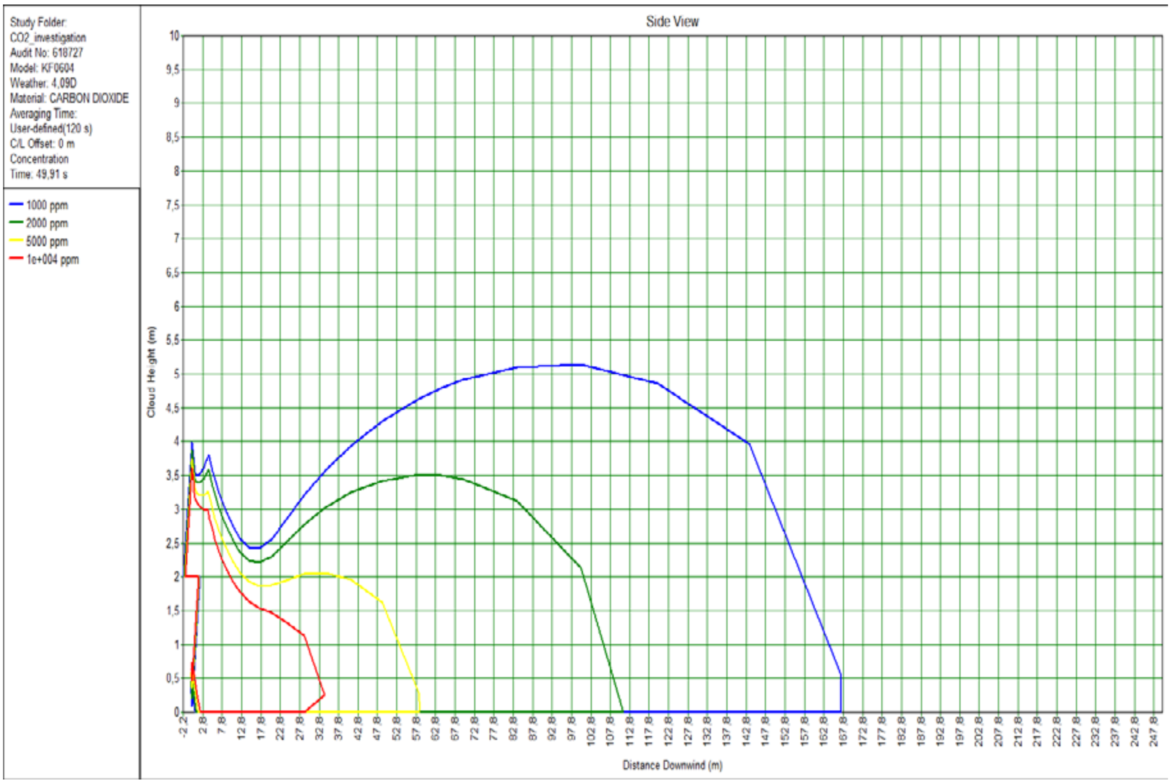


Figure 6-2 *Kit Fox 0604 Side view plot of simulation.*

Figure 6-3 *Kit Fox 0604 Cloud width of PHAST simulation, footprint*

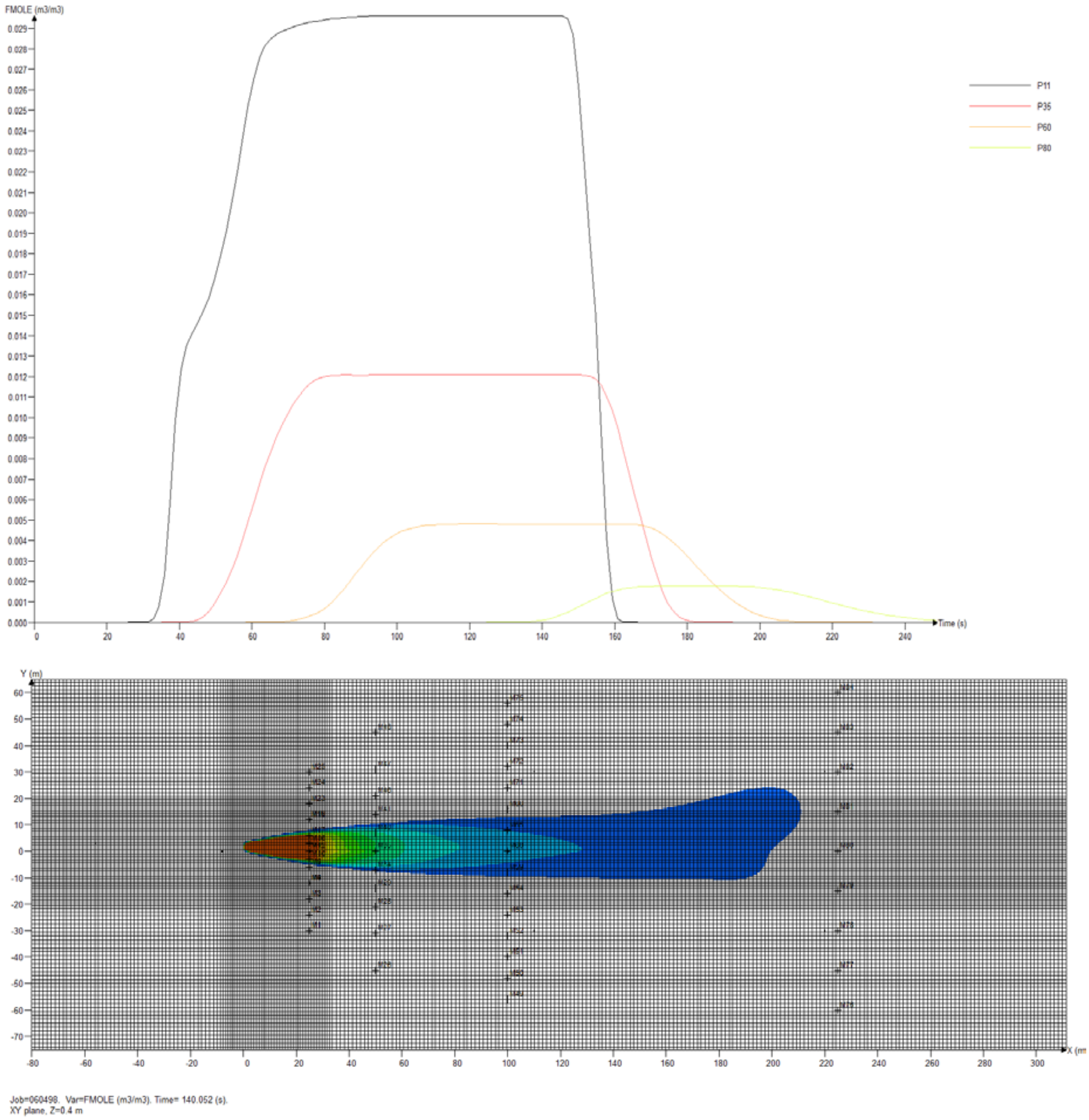


Figure 6-4 *Kit Fox 0604 FLACS simulation showing the results in flowvis and a plot showing the concentration fluctuation at monitor points at distance 25, 100 and 225 meter downwind the release. MP 11 is the concentration fluctuation at the monitor point 25 meters downwind.MP35 is at 50 meters, MP 60 give the concentration at 100m and MP 80 gives the concentration at 225 meters downwind the release. The lower figure also show the grid refinement at the leak source.*

Results from the FLACS simulations show overall a good agreement between the models and the experimental data. FLACS values were extracted from monitor points at 25, 100 and 225 distance. PHAST values were extracted from the PHAST dispersion report. The experimental values extracted from the PHAST validation document at 25, 50, 100 and 225 downwind distance.

FLACS over predicts the near field with around 30% for the concentrations at 25 and 50 meters downstream compared to the experimental value. The downwind predicts are excellent with 13% deviation at 100 and 12% deviation at 225 downwind distance.

The global comparison of the two tools against the experimental results is documented in the following figures.

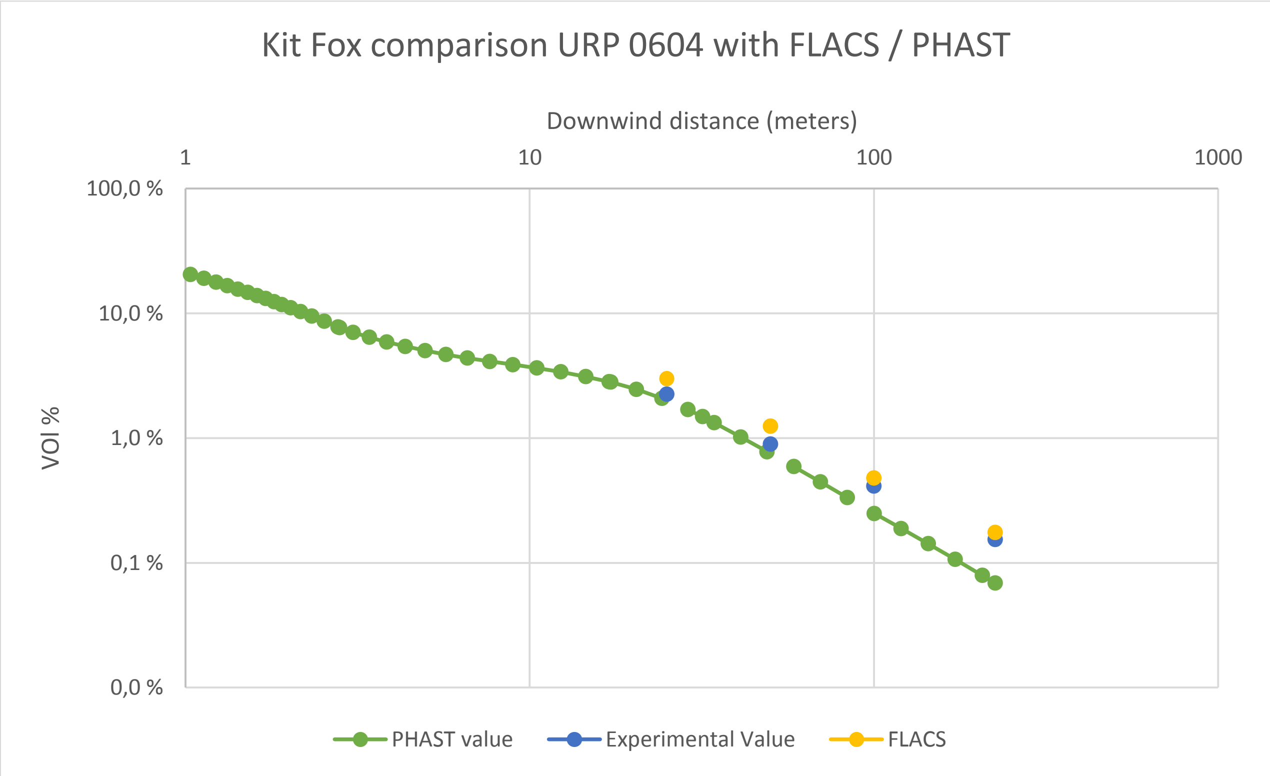


Figure 6-5 *Kit Fox trial URP 0604. Comparison of simulations with experimental values.*

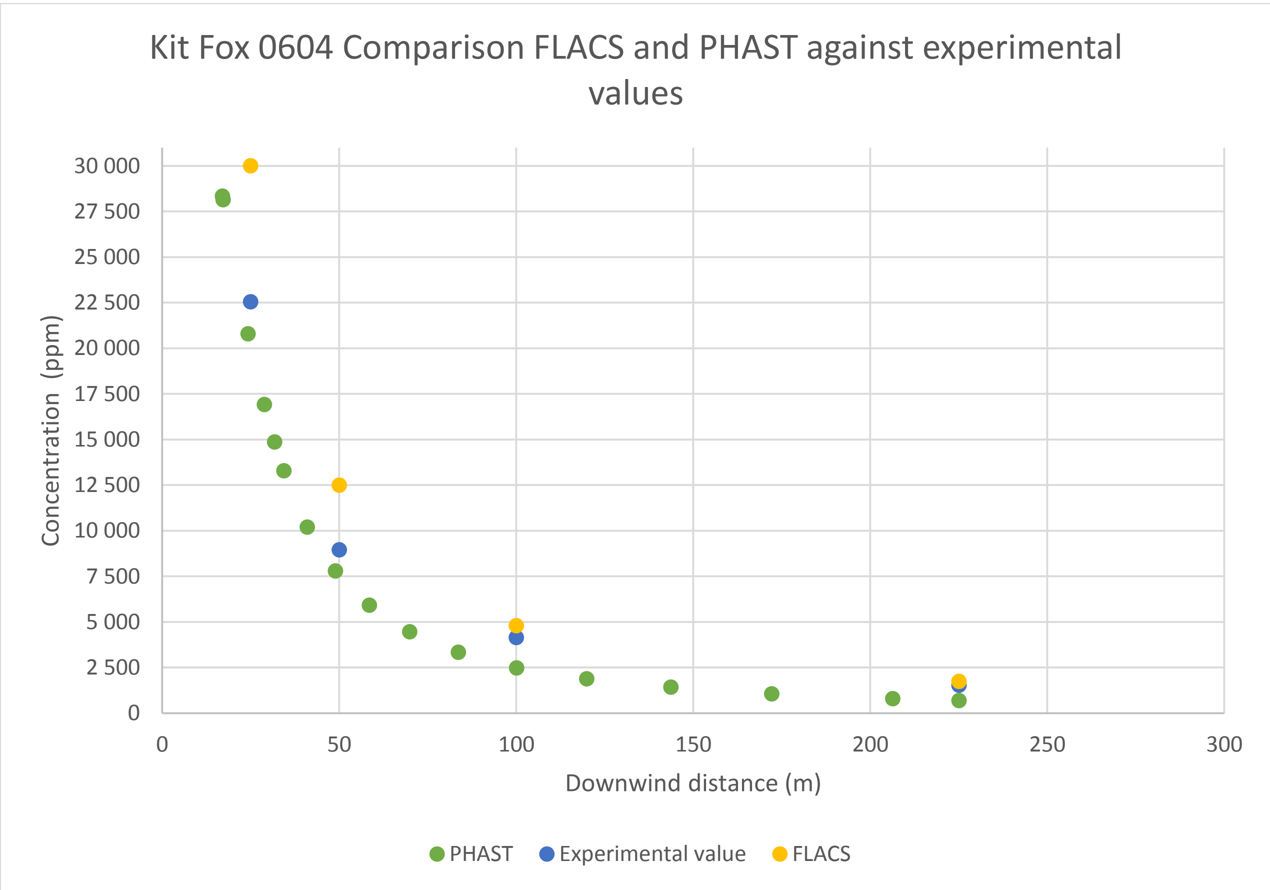


Figure 6-6 *Kit Fox trial URP 0604. Comparison of simulations for FLACS and PHAST with experimental values.*

In the near field the PHAST model compared very well against the experimental results. This was the case even though the obstacles were placed close to the leak source. This indicates that the PHAST model can represent this form of congestion for the Kit Fox experiment by using the defined ground roughness scale within in the model.

The total Kit Fox experiments consisted of 52 different trials with various wind conditions. Only URA 0604 continuous was simulated as part of this work, and is therefore not representative for the Kit Fox experiment as a whole. For validation purposes 30% deviation is considered as a limit in terms of overall agreement. With this figure in mind the comparison results are approximately around this figure for near field in FLACS, and very good for far field effects, still on the conservative side. PHAST is just within the criteria for near field effects, for far field this limit was exceeded.

7 Jet dispersion into congested area / Pipework

7.1 Introduction: justification for the comparison of the models under influence of geometrical effects.

There is today no inherent methodology or instructions for a comparison of a three dimensional CFD software like FLACS with the two dimensional integral model PHAST. Several difficulties arise when comparing the models like the mentioned handling of wind directions that an integral model is unable to simulate or account for. Geometrical effects will also have an implication on the local wind velocities inside the geometry of interest where the dispersion is occurring and may contribute to differences / deviations between simulation tools. Buildings, terrain and geometry in general will have recirculation zones and wakes that will influence the local air movements [7].

The PHAST model is tuned and validated against large scale experiments documented in the PHAST validation report [21]. These large scale experiments do involve some form of vegetation and other topographical effects which te PHAST model has taken into account as a form of congestion and the effects on the concentration decay is taken into account for these scenarios.

The major difference is that CFD models fully can take advantage of its way to model three dimensional objects and to simulate the flow around those objects. The question still unanswered is whether it is necessary to incorporate three dimensional CFD models to simulate the flow in areas which are considered to have a relative low congestion. This could be a natural ventilated open deck on an offshore facility or a large onshore chemical plant. A question that also should be addressed is how to quantify an environment as low, medium or highly congested for a comparison purpose. A method for estimating the relative size of the geometrical influence has been used in this work (using a packing density ratio). The description of the way the geometry used in this report is generated is fully described in chapter 7.3.

Will small or large releases in confined / congested spaces behave in such a manner that the flow itself can be simulated without representation of the geometrical objects in the model, and by that not excluding the PHAST model as an option for these scenarios? If the domain of the leak and the extent of distances of the UFL, LFL, LFL_2 values, and also that the flammable mass can be equally represented by the models for the same scenario with an estimated congestion value, then both the models will be applicable for that specific case. The hazard represented by that leakage scenario will then be equal and the risk conclusion will be relatively similar.

This part of the study therefore tries to move a step further into the congested environment, and try to describe in detail how the increasingly geometrical environment will influence the flow of the jet, and to represent the flammable range of the plumes. In this section a pipework geometry will be used in FLACS and compared against the ground roughness in the PHAST model. The application horizontal impingement will also be used in the PHAST model.

For the initial part of the work with this report the main focus was to use the models within their range of accuracy (open area with no topographical effects). The next part will now try to move into scenarios where simple models may fail to represent the hazard or risk associated with a dispersion cloud. This will done by testing the models to its ability to see how the models compare to what will be defined as small, medium and highly congested areas.

Two different mass flow rates will be examined for what will be a small leakage defined as an ATEX-like leakage and one for a large leakage scenario.

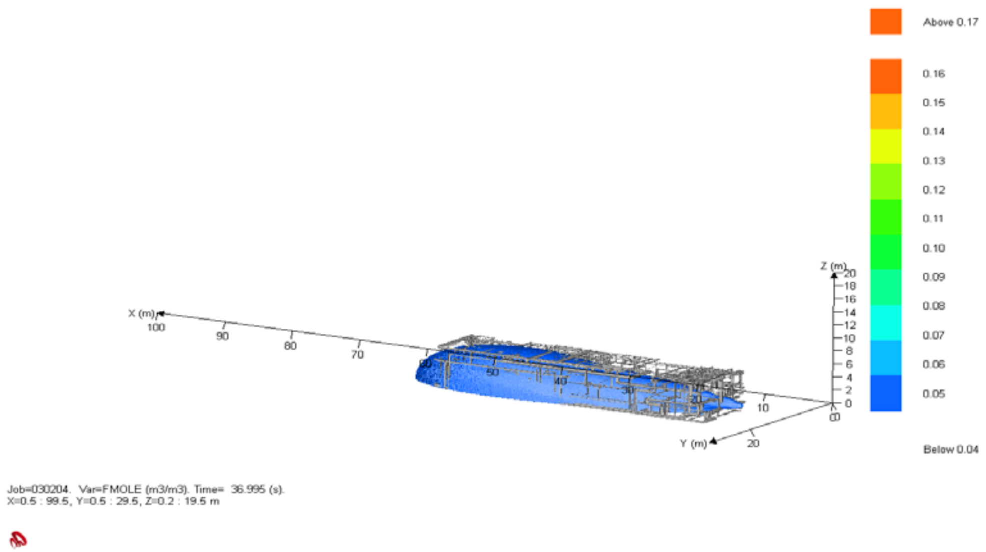


Figure 7-1 *Representation of the flammable domain of a methane release in a congested environment taken from the simulations performed at CMR GexCon.*

7.2 Flow rate sensitivity

In the perspective of the comparison, it hasn't been possible to perform as many cases as performed during the deepest academic comparison. The total number of simulations performed for this part of the work is described in 7.3.3 and 7.3.4. Some specific input have to be fixed to both reduce the amount of simulation work and still guarantee the accuracy of the comparison conclusions.

At an offshore plant hazardous gas leaks will take place in different magnitudes depending on the leakage orifice size, initial storage conditions and containment volume.
Two different mass flow rate regimes of the leakages were selected and are examined in this part. These mass rates are selected to be representative of the flammable gas hazards present in a real facility. One "relatively small" (0.59kg/s) and one medium leak flow rate (9.48kg/s) are selected.

1. The first leakage chosen will be a leakage defined as an ATEX release in this study. An ATEX-like release will typically be a small leakage from a valve or flange, with low mass flow rates (0-1 kg/s).
2. The second release will be of relative high mass flow rate compared to this ATEX-like case.

In order to ease comparison between the cases, the flow rates chosen in this part of the study is the same mass flow rates as used in the initial free jet study will be used, namely the 0.59 kg/s for the ATEX-like case and the 9.48 kg/s for the large leakage scenario.

For the free field jet the comparison of FLACS and PHAST was based on the centerline approach. This approach was valid for the free field jets due to the low buoyancy of the high velocity methane up to LFL_2 concentration downwind, and also for propane jets up to the concentration values of the LFL_2 range. For the FLACS simulations the centerline will not be used for since the geometry will make the concentration decay calculations erroneous. In PHAST it is still possible to extract the concentration from centerline decay in the dispersion report for various ground roughness while also using the horizontal impingement. This will be done to see how changed these parameters will affect the dispersion.

The flow pattern will be limited by the geometry and by that reducing the velocity of the jet and allowing for more buoyancy in the plume. The footprints and side view plots of the leaks will be used for the comparison purposes to show the effect of geometry.

7.3 Comparison method

7.3.1 Explanation of geometry build-up

The experience gained from the previous runs of simulations without geometry was used in this section. To begin with, the volume that would encapsulate the flammable range of the dispersed clouds without geometry was identified considering the selected mass flow rates; this volume was used to specify the region of space where random piping was added up to represent congestion.

For example, in the case of the ATEX-like scenario, the jet was assumed to disperse into a parallelepiped volume of (9x8x4) meters, adding up to a total volume of $288 m^3$, shown in Figure 7-2. For the large leakage scenario the volume of pipework was made within $2400 m^3$. This volume was chosen based on the plume size of the free jets expected to encapsulate the geometry. The X-Y and Z directions were chosen based on the extent of the plume to the LFL.

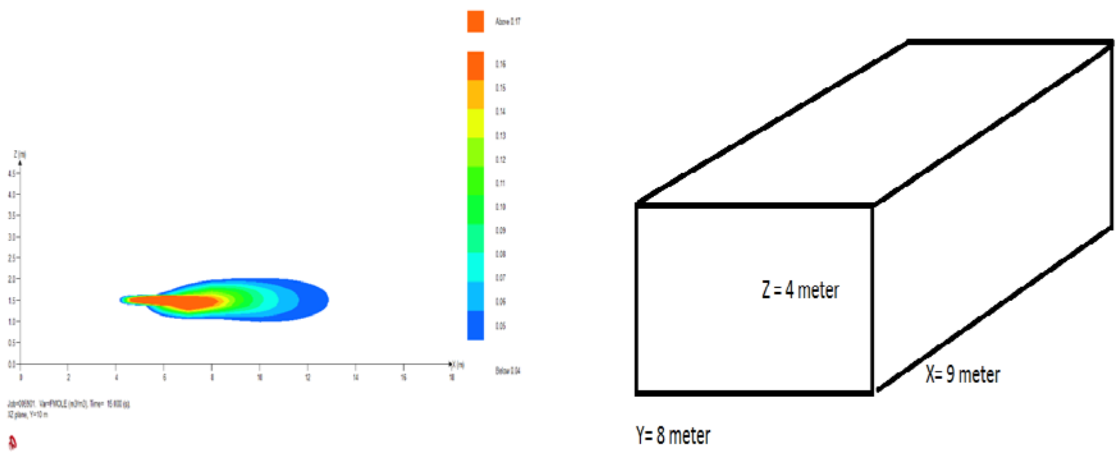


Figure 7-2 *Flammable domain of the methane jet run used for geometry set up.*

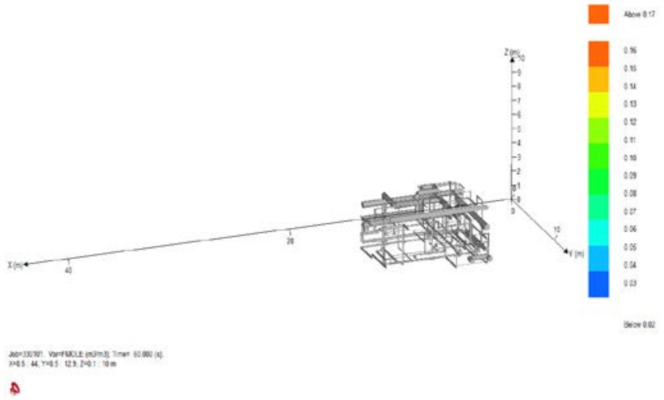


Figure 7-3 *Small geometry used for ATEX-like leakage. Pipework generated on the basis of the free jet size.*

Within this volume the pipes were generated with a pipework generation script from GexCon.

Basically, based on experience and on the run of a large significant amount of Explosion Risk Analysis within several platforms in the North Sea (UK and Norwegian sectors) and in the entire world, GexCon has summed up the geometrical characteristics representing a so-called “low congested”, “medium congestion” or “highly congested” areas in a facility, through an empirical geometric factor called the packing density. Packing density is expressed as the length of pipe present in a given region volume, in m/m3.

The differentiation of this parameter can obviously be module specific, but also region of the world specific. Note also that this parameter can be completed with additional geometrical criteria; meanwhile, the current study will consider packing density alone.

In the practical perspective, it is worth noting that the packing density parameter is very useful when performing safety studies for new built projects. Indeed, the safety studies are often to be performed in an early stage of the project where only the largest process lines, skids and structures are available. Smaller pipework description – less than 6” for example – often comes at a later stage. Development of topsides design by engineering contractors is an iterative approach associating layout, safety and structural disciplines. In addition, the safety studies are often rerun at the different stages of a project (early phase, FEED, Detail). When performing explosion simulations, it is therefore mandatory to account for the missing description within its work and adding up anticipated congestion up to a degree that fits with the packing density of as built facilities is one way of doing it.

See Figure 7-4 below based on a platform case study to have better understanding.

(1) Major equip only
(2) Equip, No pipe, Struct>40”
(3) Equip No pipe Struct >= 20”
(4) Equip +Pipe & Struct >= 10”
(5) Equip +Pipe >=8” Struct >= 5”
(6) Equip +Pipe >=6” Struct >= 5”
(7) Equip +Pipe >=4” Struct >= 5”
(8) Equip +Pipe >=3” All struct.
(9) Equip +Pipe >=2” All struct.
(10) Equip +Pipe >=1” All struct.
(11) All

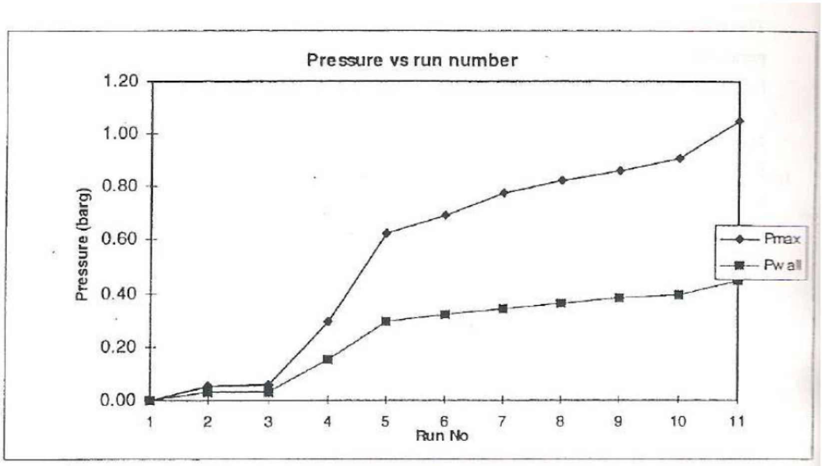


Figure 7-4 *Explosion overpressure as a function of different congestion stages in project developments, [**Error! Reference source not found.**].*

The congestion value would then be dependent on the degree of pipes filling a specific volume. The pipes were then added up in all three Cartesian directions to give to congestion value.

In the meantime, it is obvious that the diameter of these randomly placed pipes may affect the results (especially for explosion simulations). Thus, commonly, a representative distribution of pipe size is used with more small pipes than large ones.

GexCon provided its input on this field to help building the pipe distribution. In the particular case of this study, the pipe generation process assumed the following congestion values to account for small, medium and the large congested environments;

• Small congestion: mean packing density over the considered volume 0.70 $\frac{m}{m^3}$.

• Medium congestion: mean packing density over the considered volume 1.00 $\frac{m}{m^3}$.

• Large congestion: mean packing density over the considered volume 1.40 $\frac{m}{m^3}$.

Figure 7-1 is showing the pipework generated by FLACS for the large leakage scenario to represent a high degree of congestion. A total of six different pipework geometries were made for the simulations, three for the ATEX-like scenario (0.59 kg/s) and three for the larger leakage rate scenario (9.48kg/s).

The purpose of simulating the different congested environments was to somehow try to link the information regarding congestion in the FLACS model with parameters in the PHAST model. By this it is meant that the pipework geometry or any form of congestion in FLACS can be taken into account in PHAST by changing ground roughness alone or together with the horizontal impingement choice in the model and then attempt to tune PHAST into giving comparable results with the FLACS model.

Pipework distribution for the ATEX-leak for pipework of a volume of 288m^3 is shown below in Figure 7-5 and Figure 7-6. The same distribution for the large leak scenario is also shown Figure 7-7 and

Figure 7-8. The large leakage scenario Pipework generation based on 40x10x6=2400m^3.

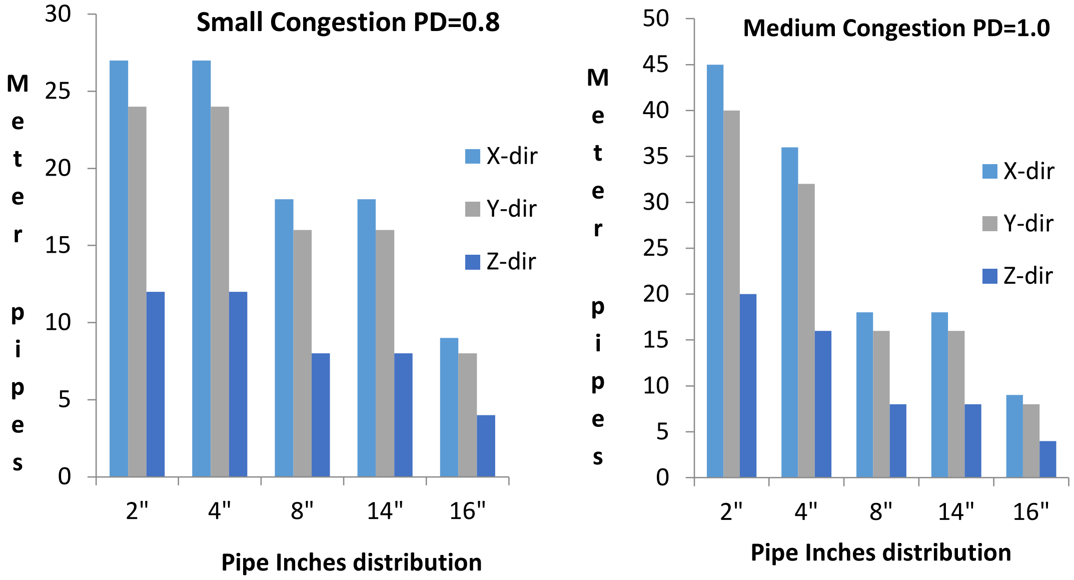


Figure 7-5 *Pipe distribution of packing density for small and medium (0.8 and 1.0 m/m^3) pipework based on 288 m^3.*

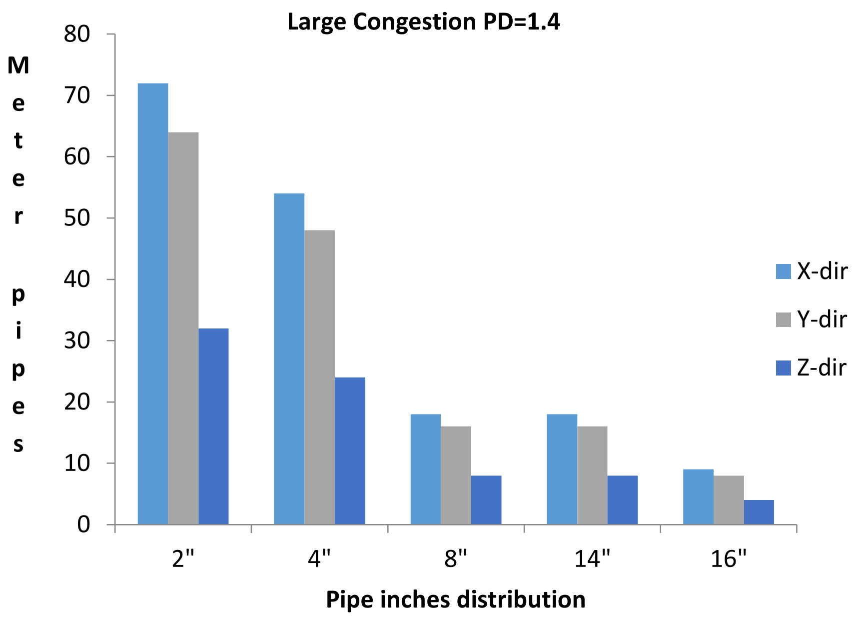


Figure 7-6 *Pipe distribution of packing density of 1.4 m/m^3 for pipework based on 288 m^3.*

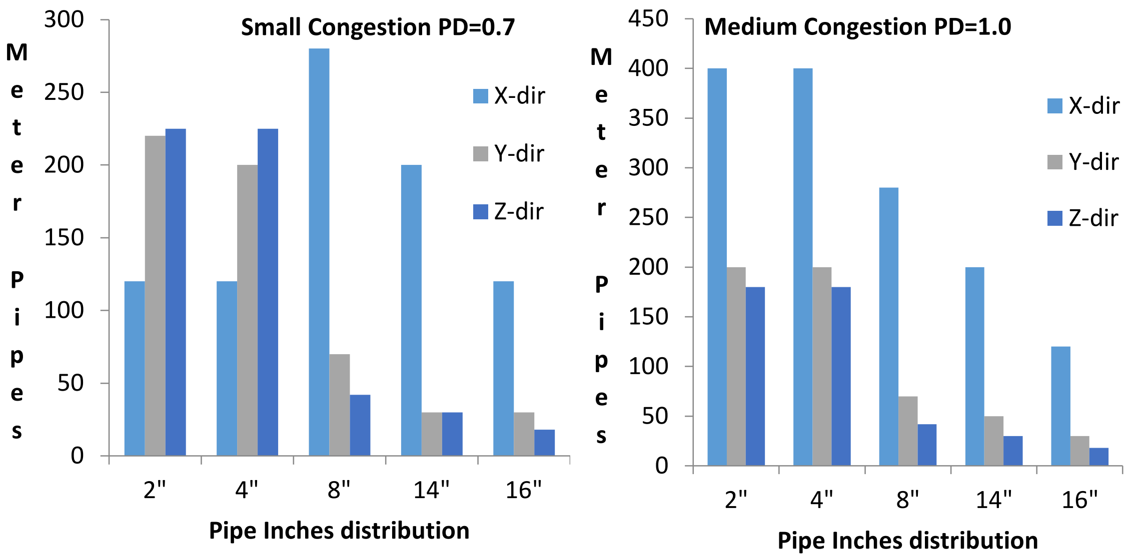


Figure 7-7 *Pipe distribution of packing density of 0.7 and 1.0 m/m^3 for pipework based on 2400 m^3.*

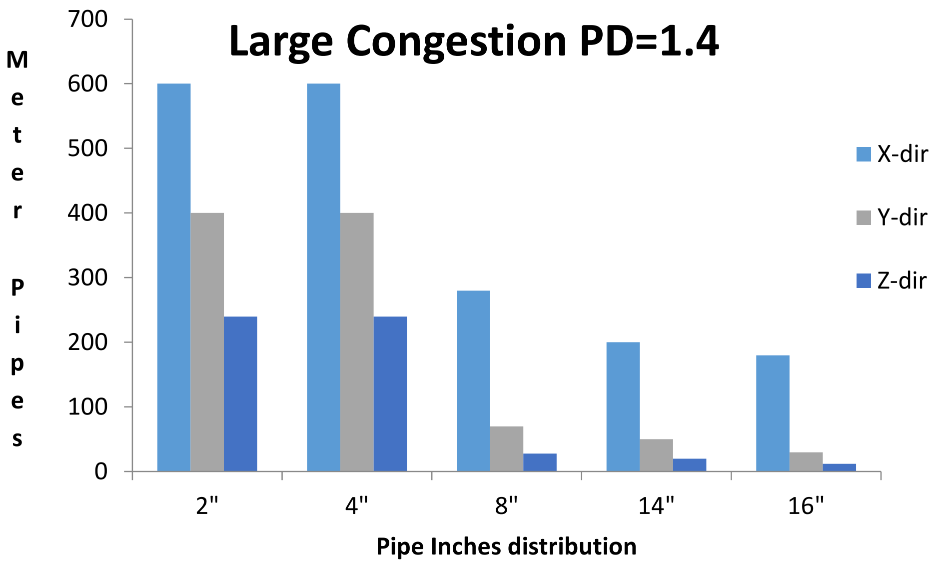


Figure 7-8 *Pipe distribution of packing density of 1.4 m/m^3 for pipework based on 2400 m^3.*

7.3.2 Impinged velocity factor Sensitivity in PHAST

Due to the differences between FLACS and PHAST, the same sensitivities are not possible to implement in the simulations. For PHAST the sensitivity will be changing of the ground roughness from 0.2mm to 3m. The second sensitivity is to use the impingement choice in the model with the impinged velocity factor set at default value of 0.25. There is also a possibility to set different values of the impinged velocity factor to see effects on the dispersion. These values will only change the results as long as the impingement choice is used in the PHAST model.

For FLACS the sensitivity will be rotating the geometry to see if the dispersion behaves is a different manner inside the same geometry.

When using the horizontal impingement in PHAST, the loss of inertia resulting from impingement is represented by this impinged velocity factor. In PHAST it is possible to use this factor within the range of 0.001 to the value of 1. Giving it a low value will greatly reduce the velocity of the jet. Default value of the factor is 0.25 meaning that by default, PHAST considers that impingement lower the initial velocity by a factor of 4. Thus, all the subsequent parameters driven by the initial velocity are affected, that is for example, air entrainment, droplet break-up for two phase releases …. Consequently, the flammable mass values and the flammability extent will also change if subjected to a change in the impinged velocity factor.

Figure 7-9 below shows how this factor influences / modifies the jet dispersion pattern for a low 1.5F wind condition, when setting this values at the two extremes of its scale in the PHAST model, 0.01 and 1. 1.0 corresponds to a free non impinging jet.

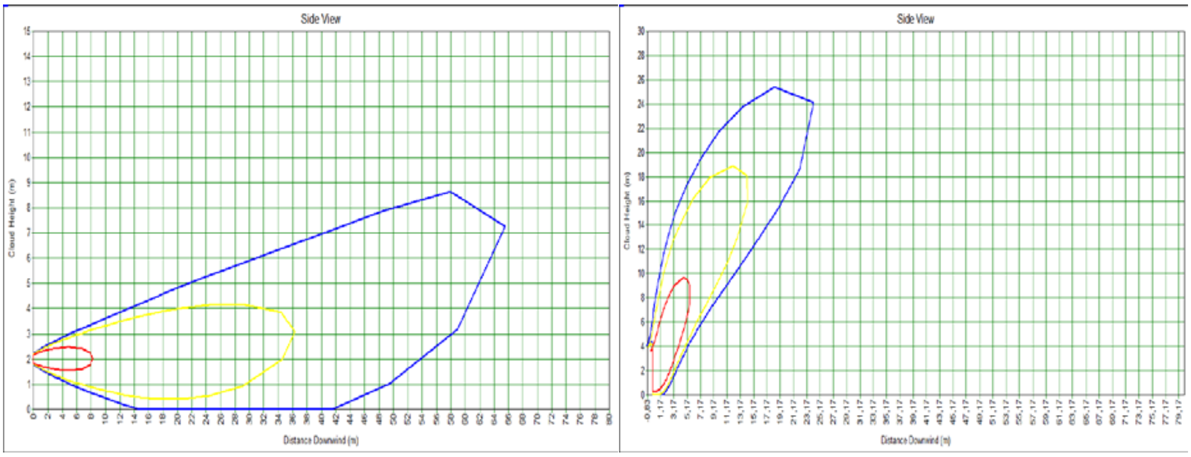


Figure 7-9 *Same jet with different impinged velocity factor. Left figure is impinged velocity factor of 1.0, right figure is impinged velocity factor of 0.01*

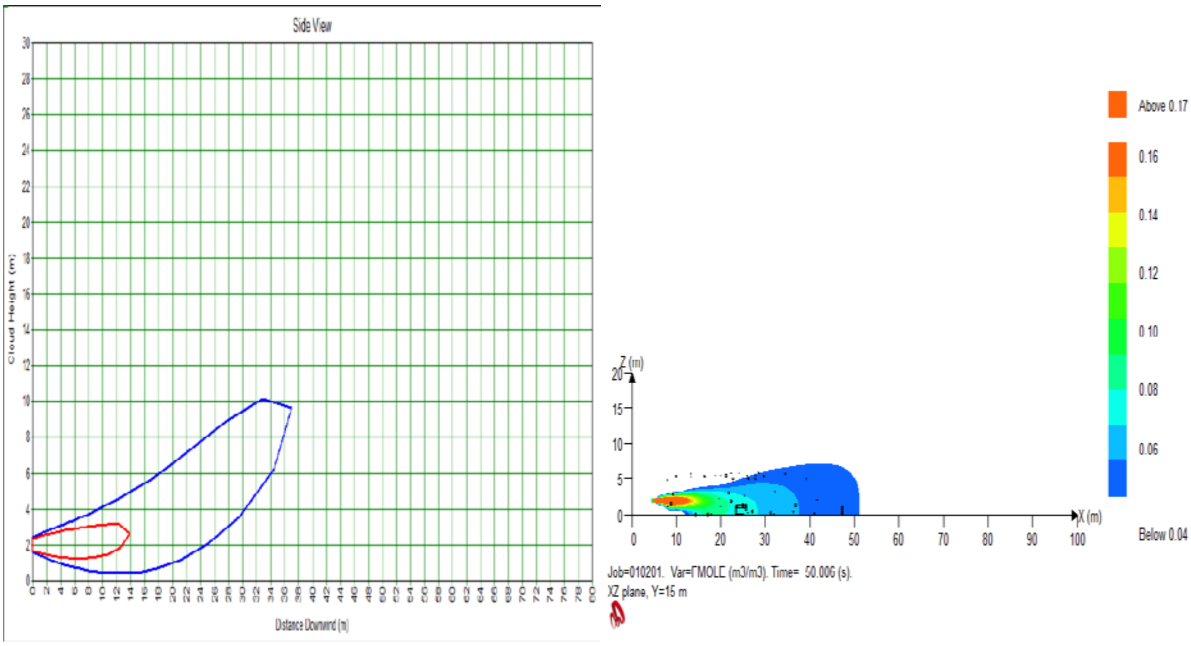


Figure 7-10 *LFL distances using method2. Wind speed of 1.5 m/s with stability F. Default 0.25 Impinged velocity factor Comparison leak in FLACS Small geometry with small congestion (packing density 0.7).*

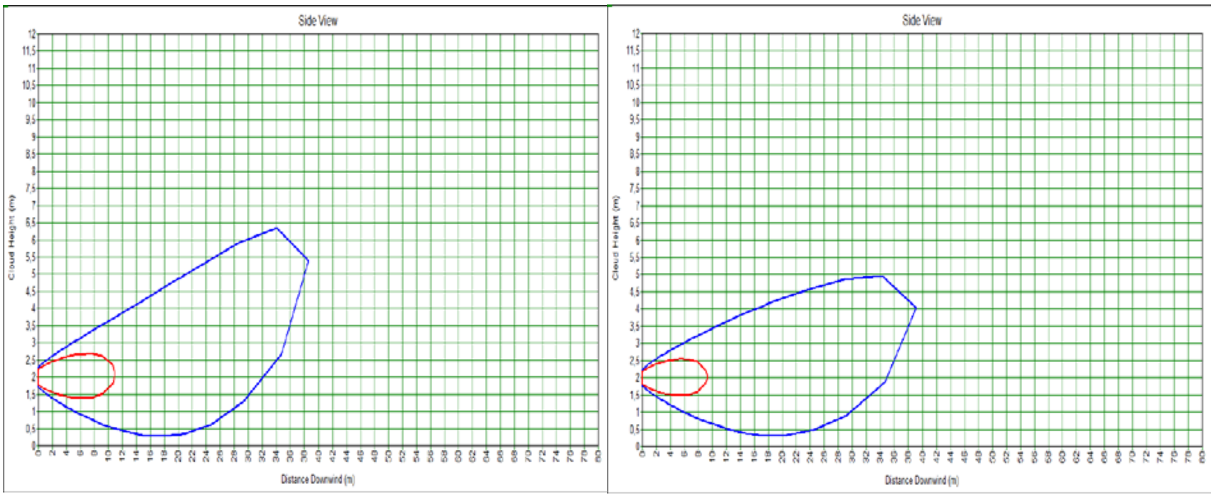


Figure 7-11 Further *description of impinged velocity factor for same jet as above in Figure 7-10; Left picture with a value of 0.5, right picture is showing a value of 0.75. Concentration up to LFL value.*

Table 7-1 *Method2 Flammable mass calculations for various impinged velocity factors for PHAST simulations. Wind speed 1.5 m/s , stability class F.*

Impinged velocity factor	Flammable mass (kg) PHAST
0,75	13,44
0,5	18,22
0,1	31,53
0,01	28,61
0,05	30,18
0,25	23,30

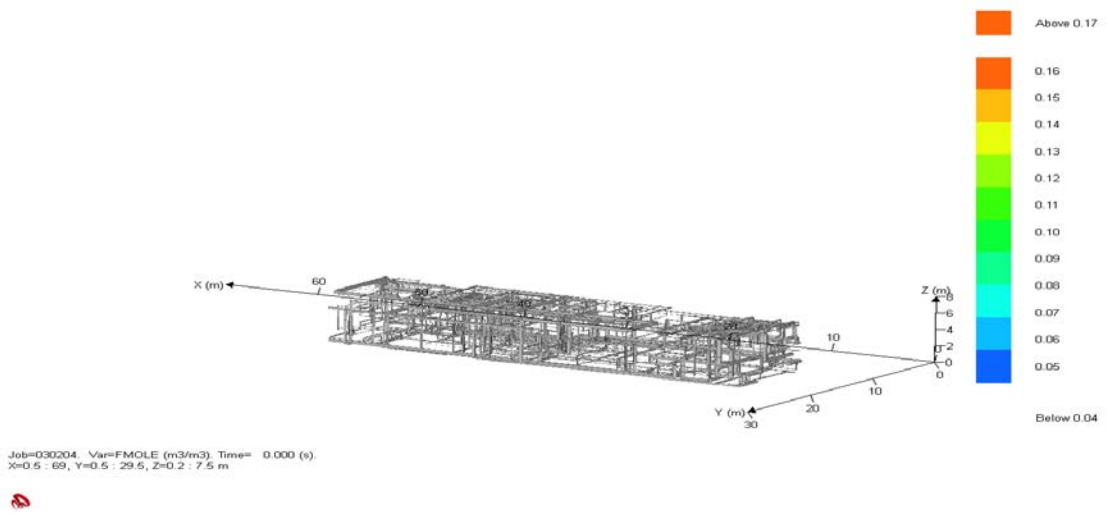


Figure 7-12 *Showing the pipework developed for the highly congested large methane leak scenario, PD=1.4 m/m^3.*

7.3.3 FLACS simulations including idealized geometry

Figure 7-13 is showing the experimental scenarios performed for the ATEX-like release scenario (0.59 kg/s) and the larger leakage rate scenario (9.48 kg/s).
Three different pipework geometries for each flow rate were made with increasing packing density values to account for different degrees of congestion.

A total of 36 simulations were performed in FLACS, the experimental setup in FLACS is shown below. Sensitivities were also run in FLACS. Sensitivities was performed by rotating the geometry to investigate if this had effects on the plume spread distances and flammable mass.

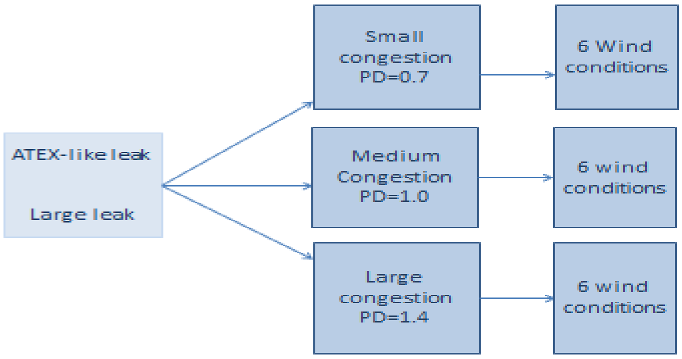


Figure 7-13 *Experimental setup of FLACS simulations for the ATEX-like case and the large release scenarios. A total of 36 simulations were performed in FLACS with the different geometries.*

The free horizontal jets that was simulated in FLACS for part one, was used as a basis for releases subjected to congestion, meaning that the same grid and scenario files in FLACS was reused for these simulations. This allowed a significant extension of the work (at least of output to process for comparison) at low cost.

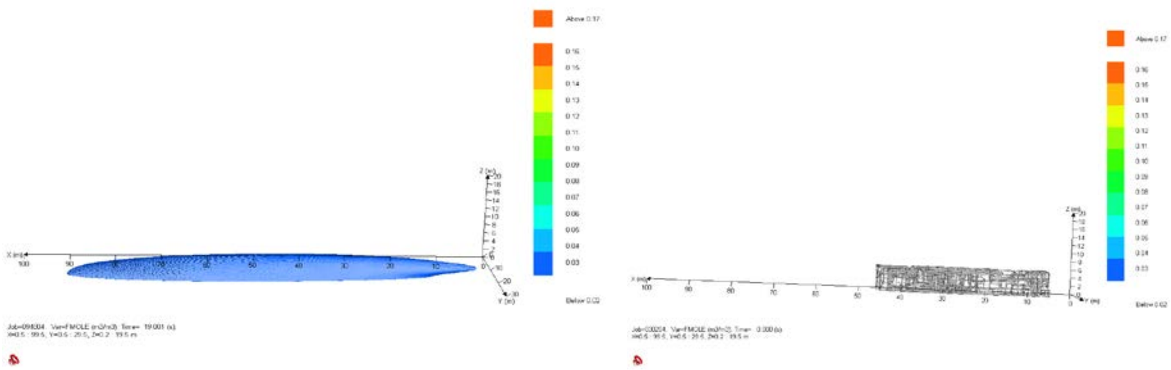


Figure 7-14 *Showing Free Field Methane Jet used to develop pipework and showing one of the geometries used.*

Figure 7-14 above shows examples of the pipework`s used for flow obstructive purposes and leak used to generate size of geometry. The leak file was made to impinge the jet into the pipework 2 meters from the pipes. This pipework was made up to resemble a process module, and to see what effect the different geometries had on the leak.

7.3.4 PHAST Simulations: trials to represent the congestion effect

Figure 7-15 below gives a visual representation of the performed PHAST simulations. The wind conditions given in table 4.2 were chosen for the simulations, using again method1 and 2. Four different ground roughness values chosen were 0.2mm, 0.5m, 1.5m and 3.0m, to cover the entire span of ground roughness values in PHAST, adding up to a total of 208 simulations in the PHAST model when simulating 7 different wind conditions.

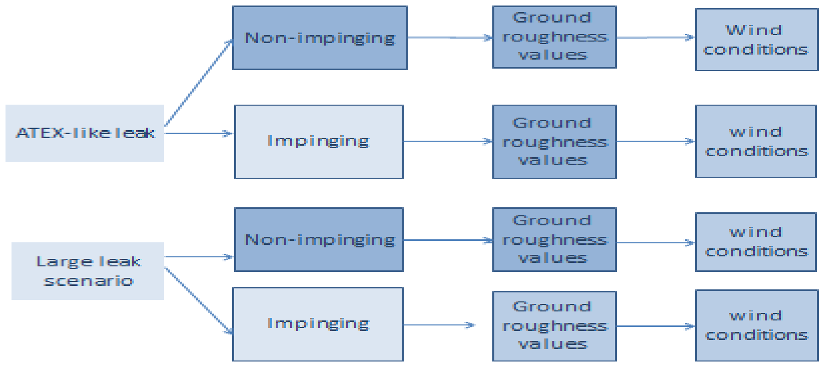


Figure 7-15 *PHAST experimental setup for ATEX-like case and large leakage scenario for the defined method1 and 2.*

The roughness length was changed to give geometrical effects. The choice horizontal impingement in the model was also used. The effect by changing roughness length and horizontal impingement on the plume given in PHAST was then compared to the FLACS simulations with varying degrees of congestion.

The wind conditions 1.5F and 5.0D was extensively investigated with changing the mentioned parameters, since this is the analyst`s most likely choice of wind conditions.

The following span of roughness lengths are defined in the PHAST model.

Table 7-2 *PHAST Definitions of ground roughness values taken from [24].*

Roughness Length	Obstacles defined as
0.2mm	Open water
5.0mm	Mud flats or snow
30mm	Open flat terrain
100mm	Low crops
250mm	High Crops
500mm	Parkland
1000mm	Regular large obstacles coverage
3000mm	City center

7.4 RESULTS; Limited ATEX-like mass flow rate scenario 0.59kg/s

Below the results for the ATEX-like scenario is shown. All the results for the three different geometries are represented and FLACS results are presented first, PHAST results is then shown. The wind scenarios of 1.5F and 5.0D have been extensively investigated since this is the most likely reviewed scenarios by a safety analysis

7.4.1 FLACS; Low congestion pipework

The simulation run for the small geometry (Packing density=0.8) for the ATEX-like scenario is shown in the figures below. The side view plots show the different simulations done in PHAST on the same premises as the FLACS simulation.

Table 7-3 *Overview of wind conditions for simulations in FLACS shown in figure below for small geometry.*

Sim nr	*Wind condition (m/s) and stability class*
330101	*1.5F*
330102	*3.0F*
330103	*3.0B*
330104	*5.0D*
330105	*5.0B*
330106	*10.0D*

The snapshots are taken at steady state where the concentration limits are steady state. This form the basis of how the comparison will be performed for small, medium and large geometry. The concentration range shown is up to LFL_2. The concentration range shown is up to LFL_2 (2.2 Vol%).

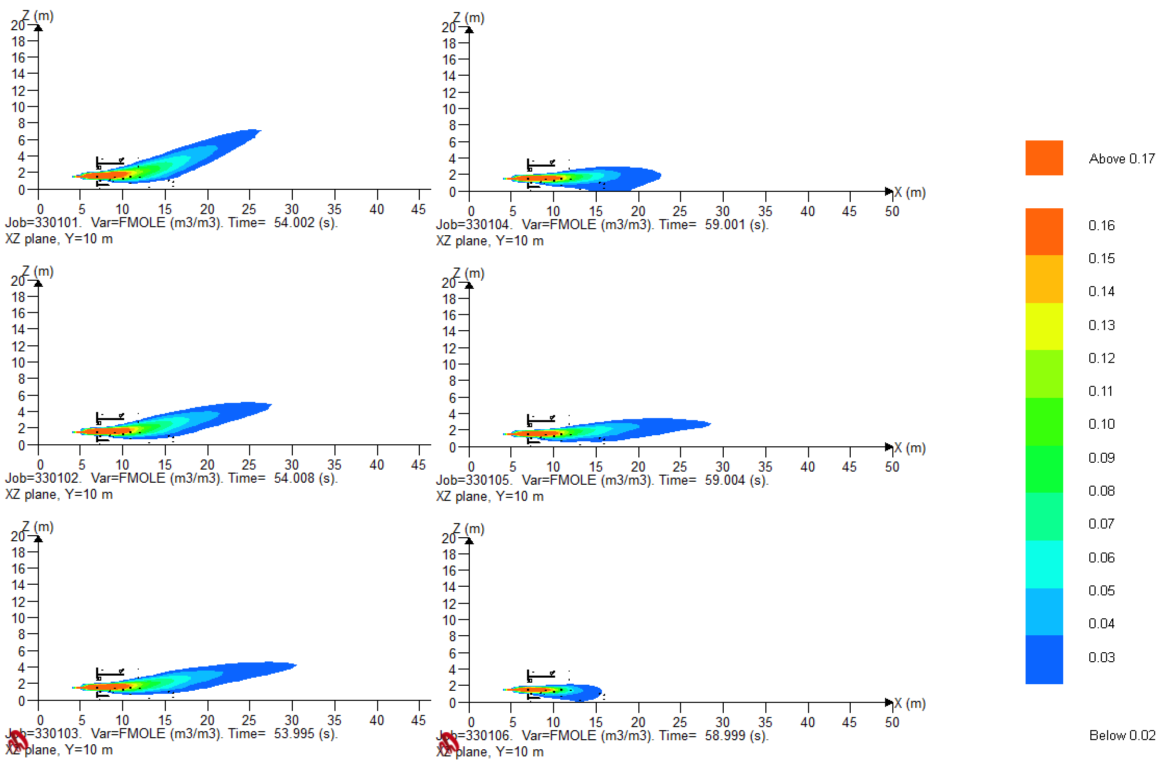


Figure 7-16 *Overview simulations for Small geometry in FLACS for six different wind conditions through the same pipwork. Concentration legend to the right, showing the range from 2-17 Vol%.*

7.4.2 FLACS; Medium congested pipework

For the medium geometry (Packing density =1.0) the wind showed a large impact on the release. Figure x.x below show the FLACS simulations and the importance of different wind conditions for the same jet going through the same geometry.
The jets with the lowest external wind field, 1.0 and 1.5F, are more buoyant and show a different behavior than the jet facing a more forceful external wind field. A wind field of 5m/s forces the jet closer to the ground as shown for the 220004 and 220005 below.

Table 7-4 *Overview of wind conditions for simulations in FLACS shown in figure x.x below for medium geometry*

Sim nr	***Wind condition (m/s) and stability class***
220000	***1.0F***
220001	***1.5F***
220002	***3.0F***
220003	***3.0B***
220004	***5.0D***
220005	***5.0B***

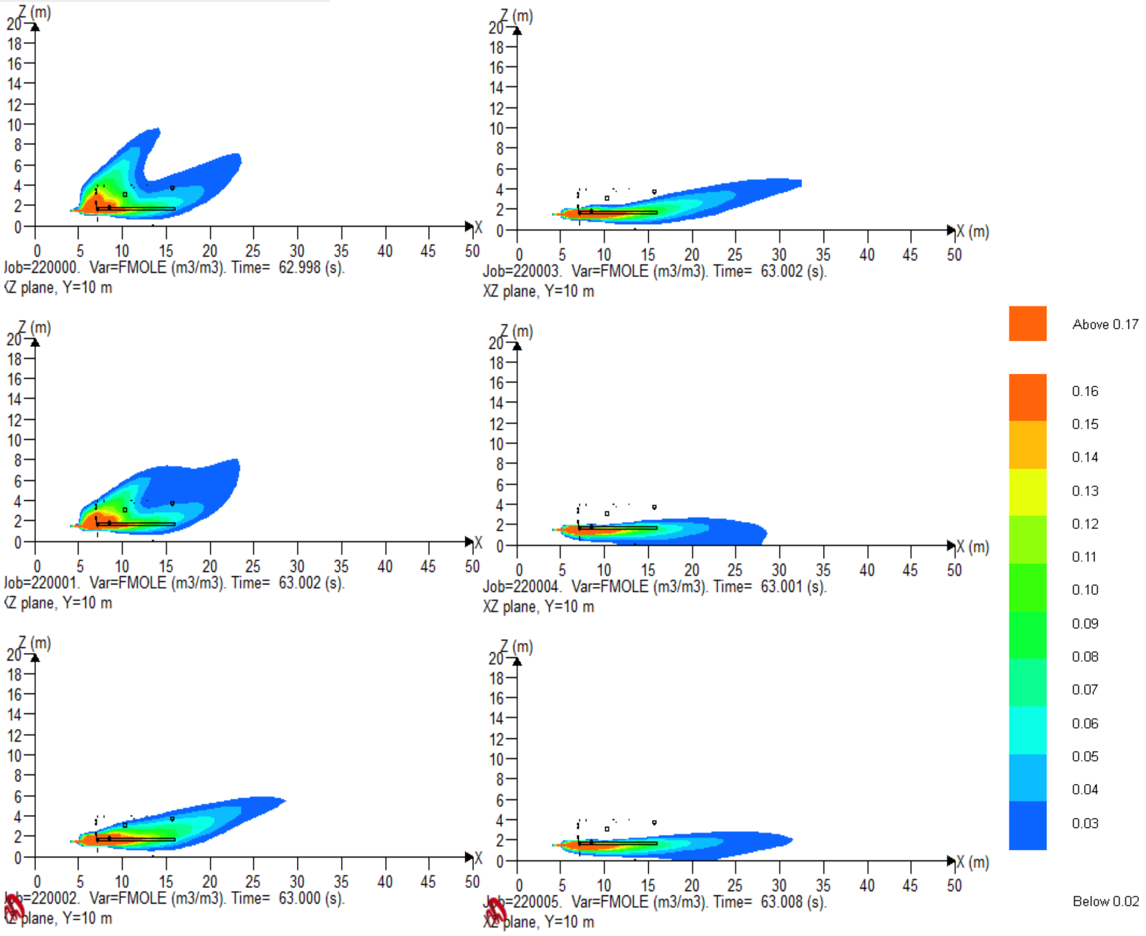


Figure 7-17 *Overview simulations for medium geometry in FLACS for six different wind conditions through the same pipwork. Concentration legend to the right, showing the range from 2-17 Vol%.*

The only change is the increased wind velocity with stability class D. The higher wind velocity of the wind field around the geometry pushes

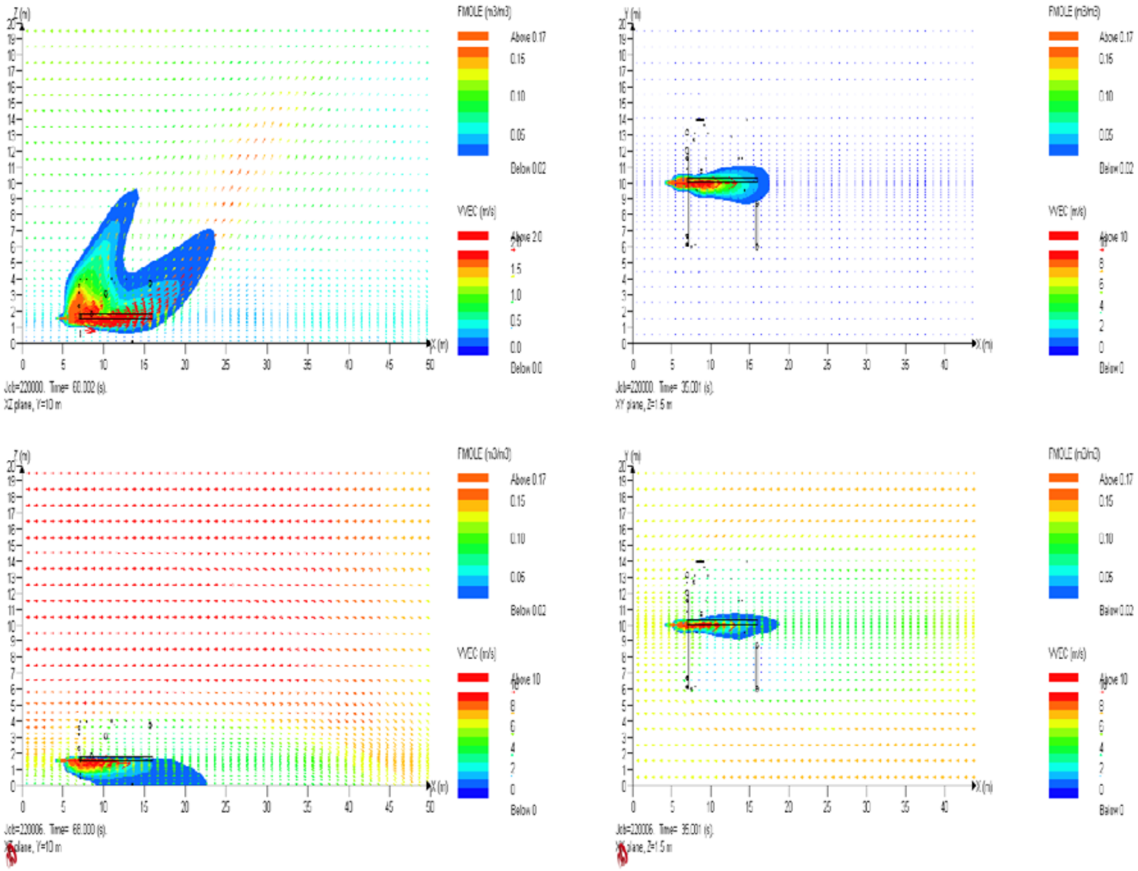


Figure 7-18 *High and low wind speed for same jet seen from above and side view plot.*

The external wind field has a large impact on the local air movements inside the geometry. The high velocity of the external wind field in job 220006 pushes the plume against the ground due to the difference in wind speeds. In the geometry above the external wind field is stable at 10m/s. The same scenario above, job 220000, the wind field does not force the plume through the geometry in a similar manner as for the 10.0D case.

7.4.3 FLACS; Highly congested pipework

The simulation`s show below for the large geometry (Packing density=1.4) in FLACS behaved fully as a free jet. The flammable mass comparison also indicates this with its low value for flammable mass that are fully comparable with a free jet in FLACS. This behavior was not expected due to the jet impinging into the largest and the most congested of the three geometries made for part3 for the ATEX-like case.

Table 7-5 Overview of wind conditions for simulations in FLACS shown in figure x.x below for medium geometry

Sim nr	*Wind condition (m/s) and stability class*
440000	*1.0F*
440001	*1.5F*
440002	*3.0F*
440003	*3.0B*
440004	*5.0D*
440005	*5.0B*
440006	*10.0D*

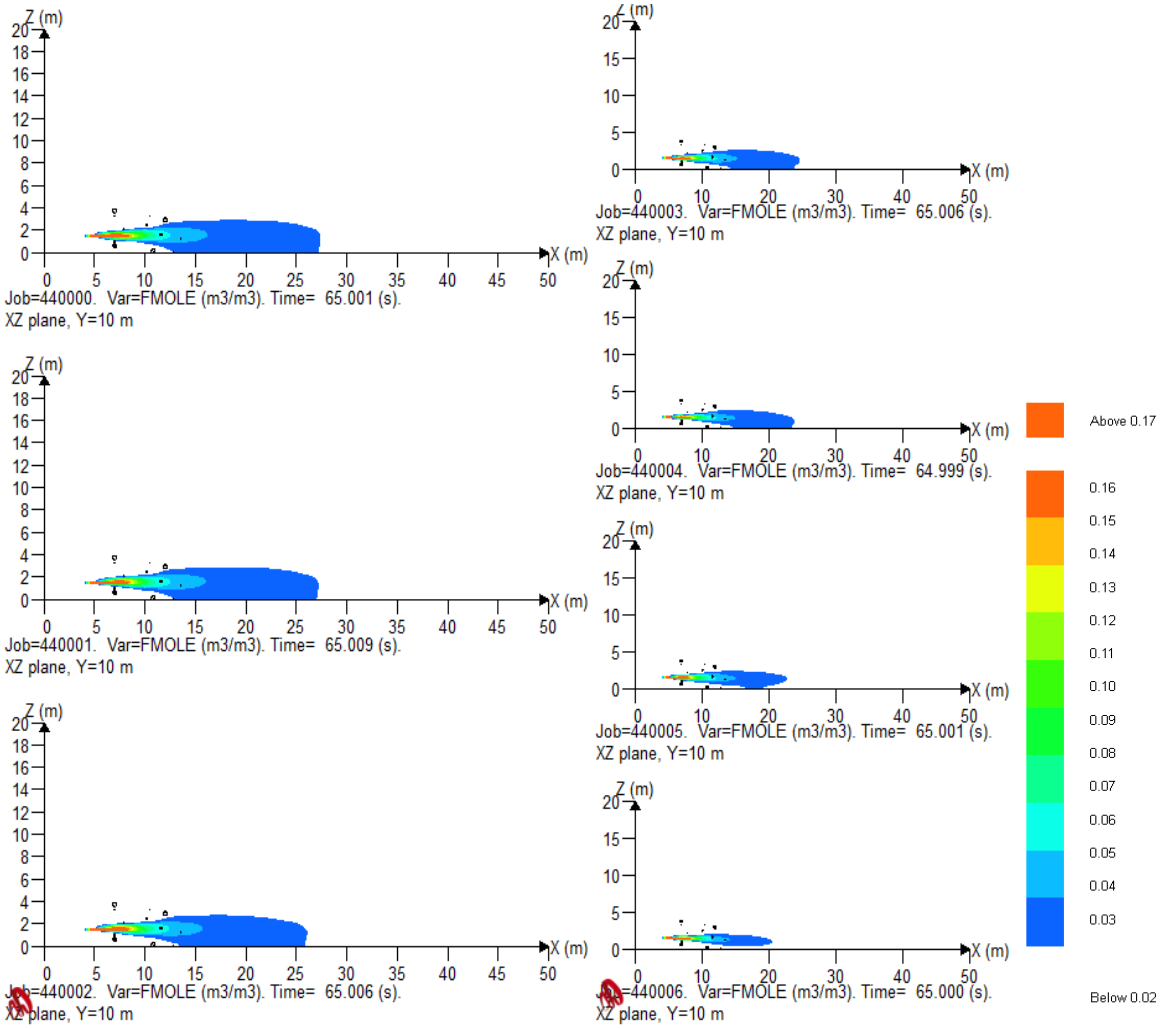


Figure 7-19 *Overview simulations for large geometry in FLACS for six different wind conditions through the same pipwork. Concentration legend to the right, showing the range from 2-17 Vol%.*

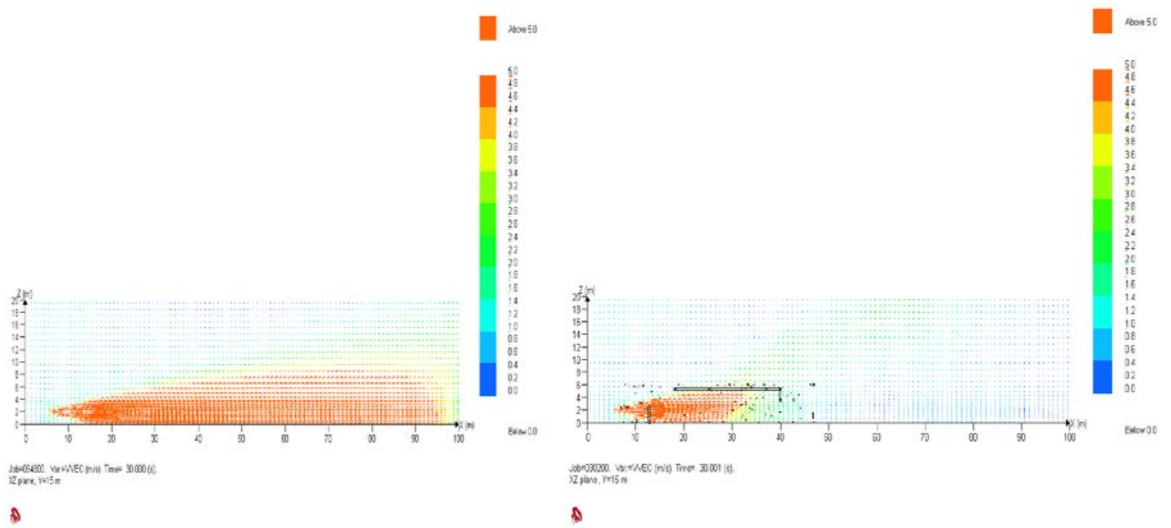


Figure 7-20 *Velocity wind field comparison Free Jet against jet impinging into geometry*

7.4.4 PHAST ATEX-like leak; attempts to account for congestion

To represent the PHAST scenarios the simulations with wind speed of 1.5F and 5.0D is shown below. Since this is the most likely wind conditions assessed. The initial simulations showed that the horizontal impinging choice is most comparable with FLACS only the simulations run with this parameter are shown below. For the PHAST scenarios a total of 56 simulations were run for the ATEX-like scenario.

The PHAST simulation`s shown below is for two different wind conditions with four different values for the ground roughness ranging from 0.2mm to 3000mm. The wind conditions 1.5F and 5.0D is outlined below.

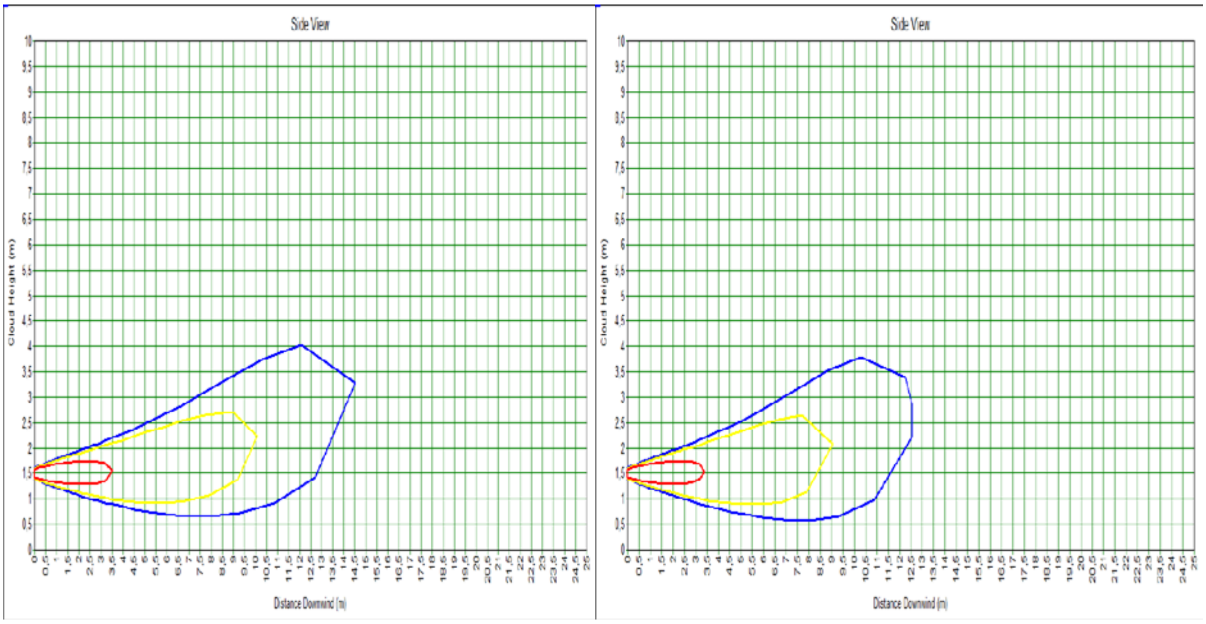


Figure 7-21 *Flammable (up to 2.2 Vol%) domain of methane release (0.59 kg/s with discharge velocity of 255.7m/s) for steady state plumes for left ground roughness of 0.5m and right 1.5m. Wind conditions are 1.5m /s of F stability.*

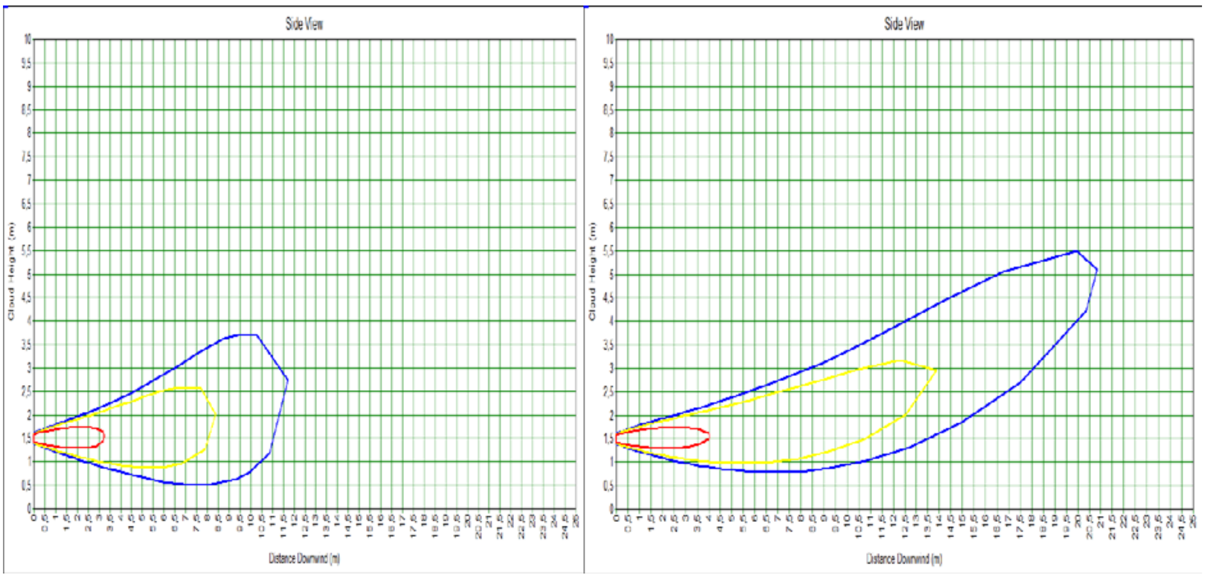


Figure 7-22 *Flammable (up to 2.2 Vol%) domain of methane ATEX-like release (0.59 kg/s with discharge velocity of 255.7m/s) for steady state plumes for left ground roughness of 3.0m and right 0.2mm. Wind conditions are 1.5m /s of F stability.*

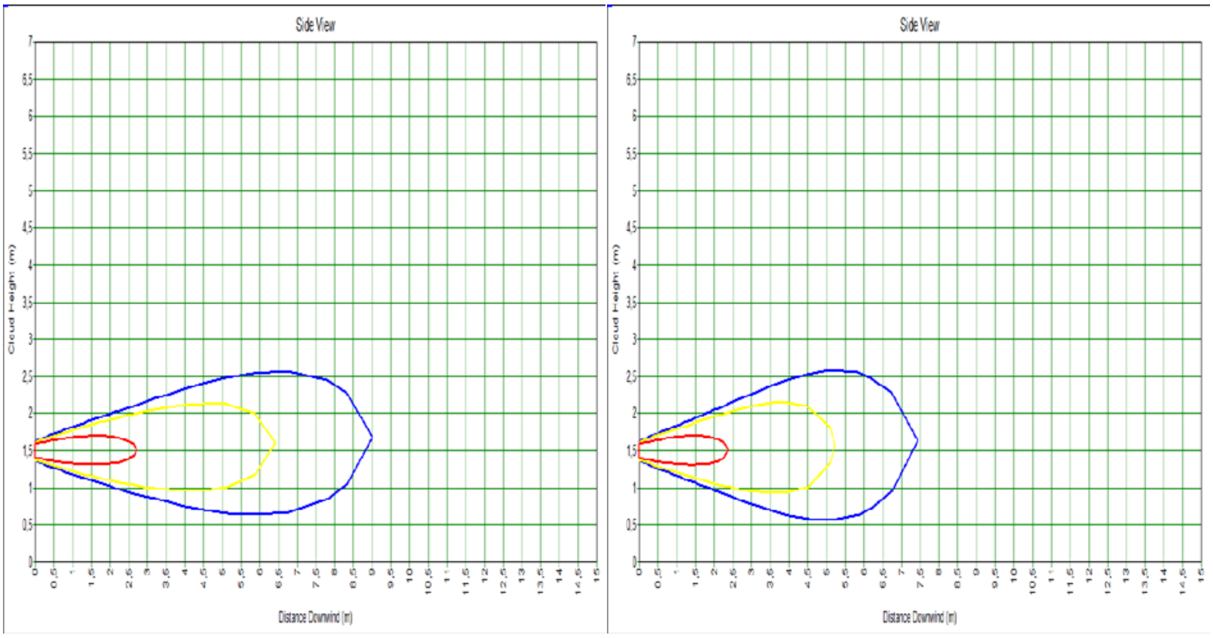


Figure 7-23 *Domain (up to 2.2 Vol%, LFL_2) of methane ATEX-like release (0.59 kg/s with discharge velocity of 255.7m/s) for steady state plumes for left ground roughness of 0.5m and right 1.5m. Wind conditions are 5.0 m /s of D stability.*

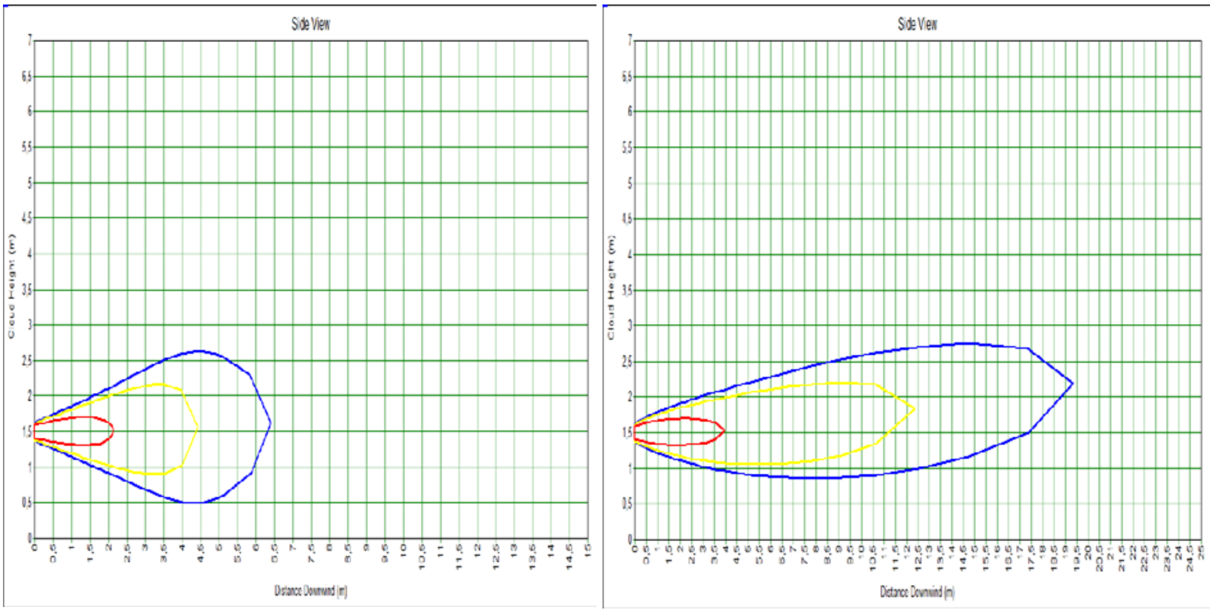


Figure 7-24 *Flammable (up to 2.2 Vol%, LFL_2) domain of methane ATEX-like release (0.59 kg/s with discharge velocity of 255.7m/s) for steady state plumes for left ground roughness of 3.0m and right 0.2mm. Wind conditions are 5.0 m /s of D stability.*

7.4.5 PHAST; Centerline approach for various ground roughness values

We can see from the illustrations above that changing the ground roughness in PHAST will change the extent of concentration decay of the jets to a large extent. The change in ground roughness is seen strongest at high wind speeds simulated.

Form the figures we clearly see that the concentration decay for the various simulation follow the same trend. However, for method 2 the simulation with the lowest ground roughness value of 0.2 mm reaches a downwind concentration of LFL_2 at 17.37 meters. The highest ground roughness value of 3000mm reaches 12.10 meters.

Below the plots show the impact of increased or lowered ground roughness value on the concentration lengths of the given plumes. Both method1 and 2 has been used to show these differences. The impingement choice in the model is also used with method1 and 2. The concentration up to the LFL_2 has again been the lowest concentration of interest.

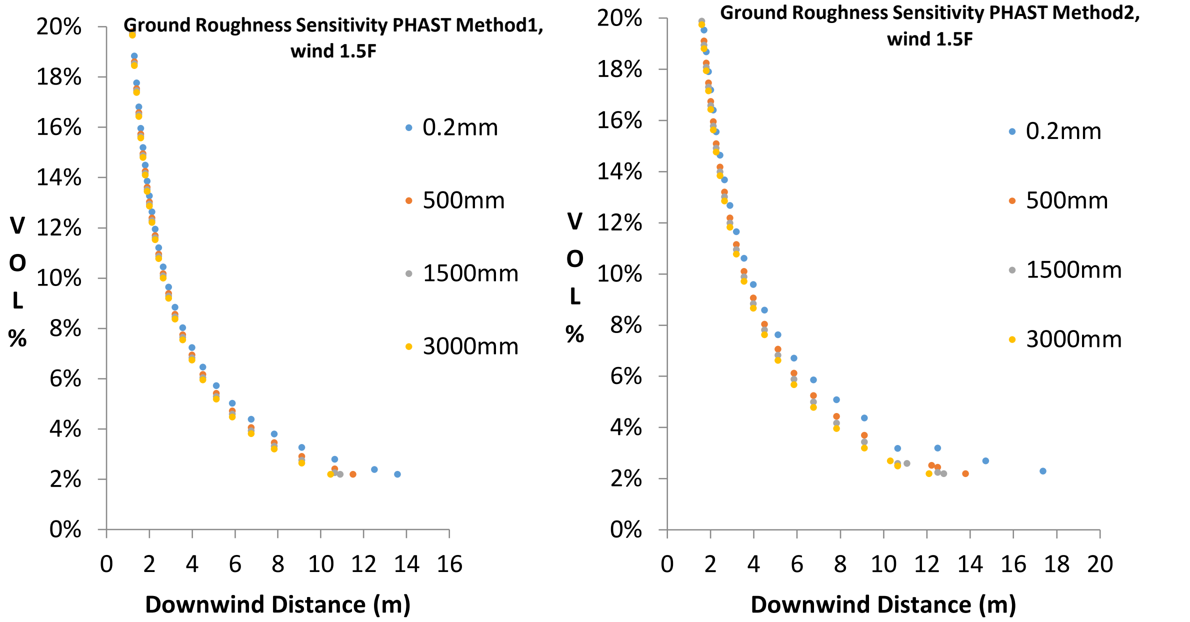


Figure 7-25 *Non Impinging Jet concentration as a function of Ground Roughness sensitivity for ATEX case Method1 and Method2 at 1.5F.*

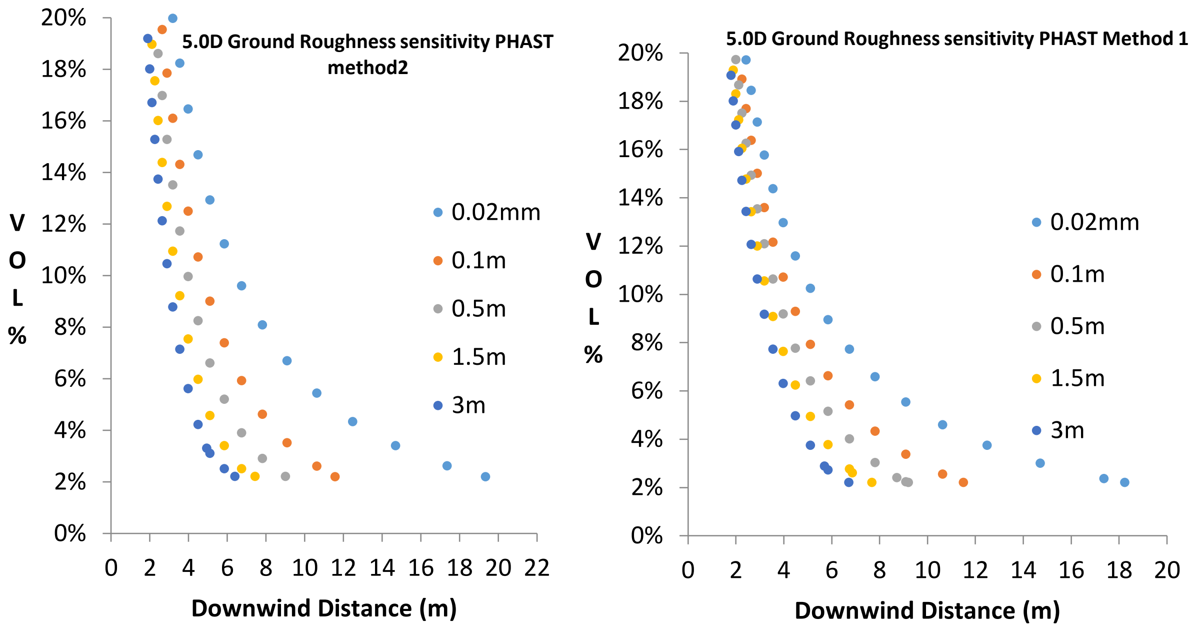
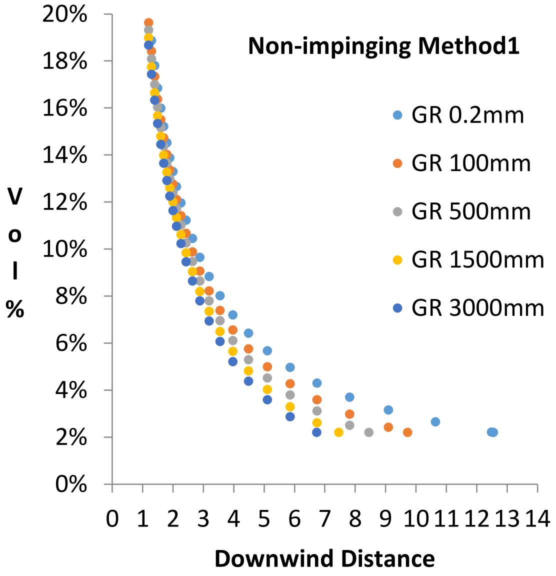


Figure 7-26 Impinging jet Concentration decay as a function of Ground Roughness sensitivity of ATEX leak method 1 and 2 at 5.0D.



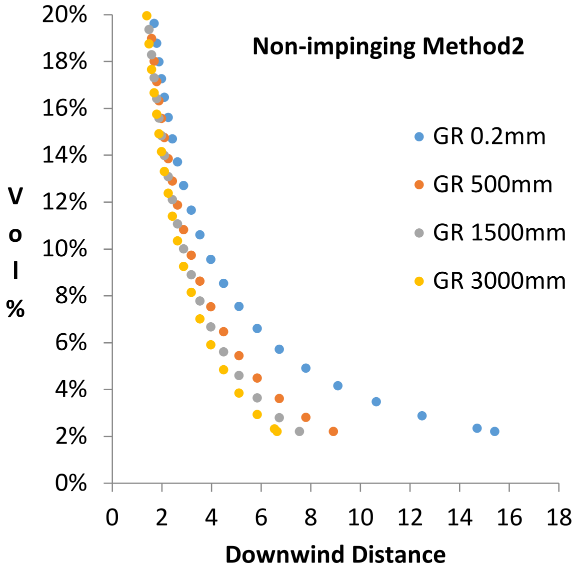


Figure 7-27 *Non-Impinging Jet concentration as a function of ground roughness for ATEX case Method1 and Method2 at 5.0D.*

7.5 RESULTS; Large flow rate release 9.48 kg/s

The section 7.5.1 show the results for the large release of 9.48 kg/s for the three different sized geometries.

7.5.1 FLACS; Low congested pipework

FLACS simulations shown below show the flammable mass of the dispersion plumes of methane, concentration up to LFL, 4.4 Vol%. The lower the wind speed the more buoyant plumes are seen for the FLACS and PHAST cases. The results given by FLACS shows that a plume of this relative high mass flow rate impinging into a pipework will fill the entire geometry with flammable concentration up to the LFL value for all the different simulations run for the various wind conditions chosen.

Table 7-6 *Overview of wind conditions for simulations in FLACS for medium geometry*

Sim nr	Wind condition (m/s) and stability class
010200	1.0F
010201	1.5F
010202	3.0F
010203	3.0B
010204	5.0D
010205	5.0B
010206	10.0D

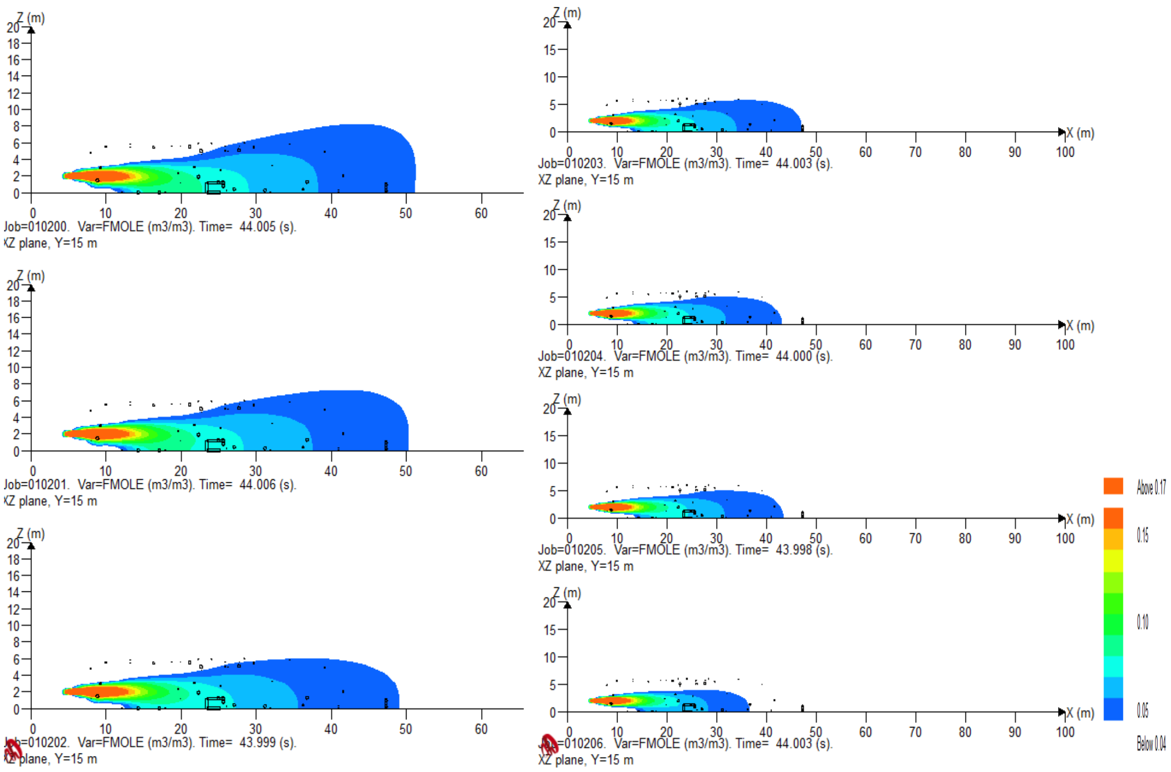


Figure 7-28 *Large jets impinging into small geometry Packing density of 0.7. Concentration up to LFL values, 4.4Vol%. All simulations run in FLACS is shown here for the different wind conditions and stability classes.*

For FLACS the low wind speed makes the makes the plume more buoyant seen from job 010200. Higher wind speed gives larger dilution and lower buoyancy as seen from the 0100204-05 cases.

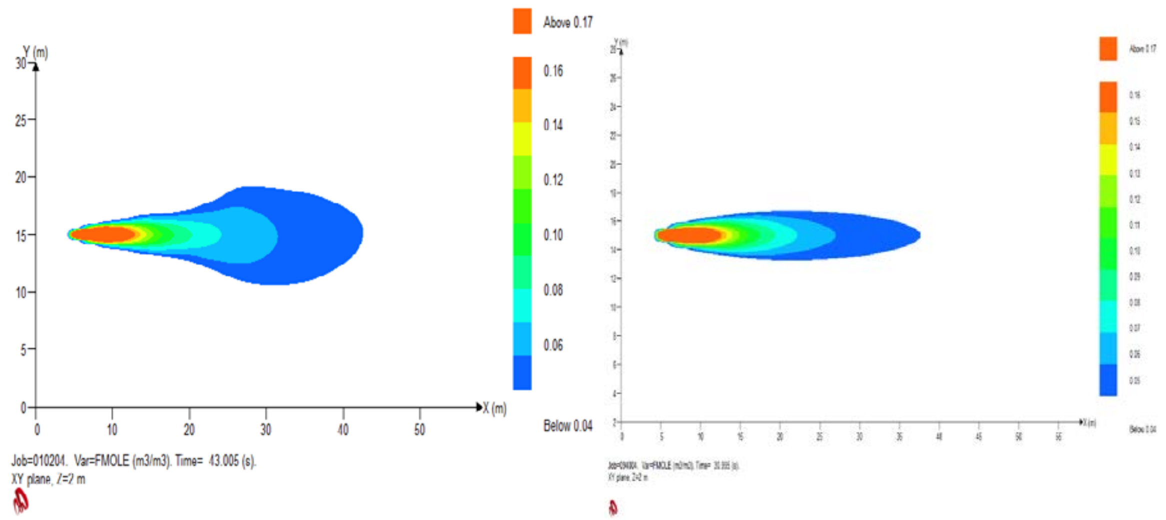


Figure 7-29 *FLACS simulations. Left figure jet impinging into pipework seen from above (pipework removed from picture). Right picture is a free jet same seen from above without geometry. Concentration decay up to LFL, 4.4 VOL%.*

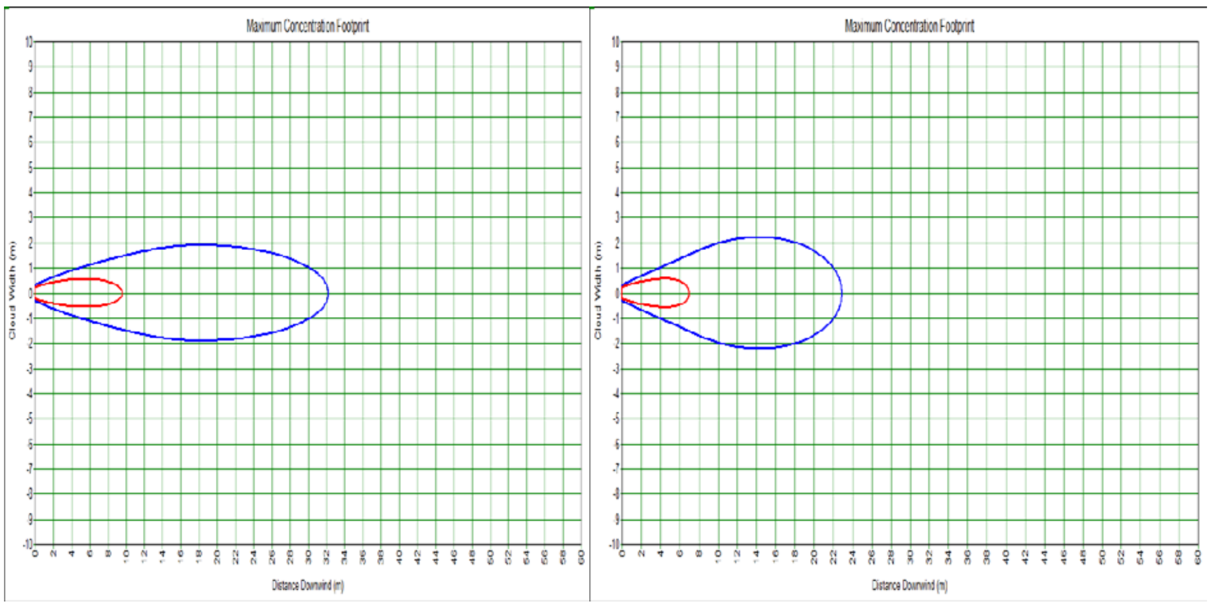


Figure 7-30 Cloud width plots; *PHAST free jet to the left with ground roughness 100mm. Picture to the right is same jet with 3000mm ground roughness. Wind speed 5.0 m/s, stability class D.*

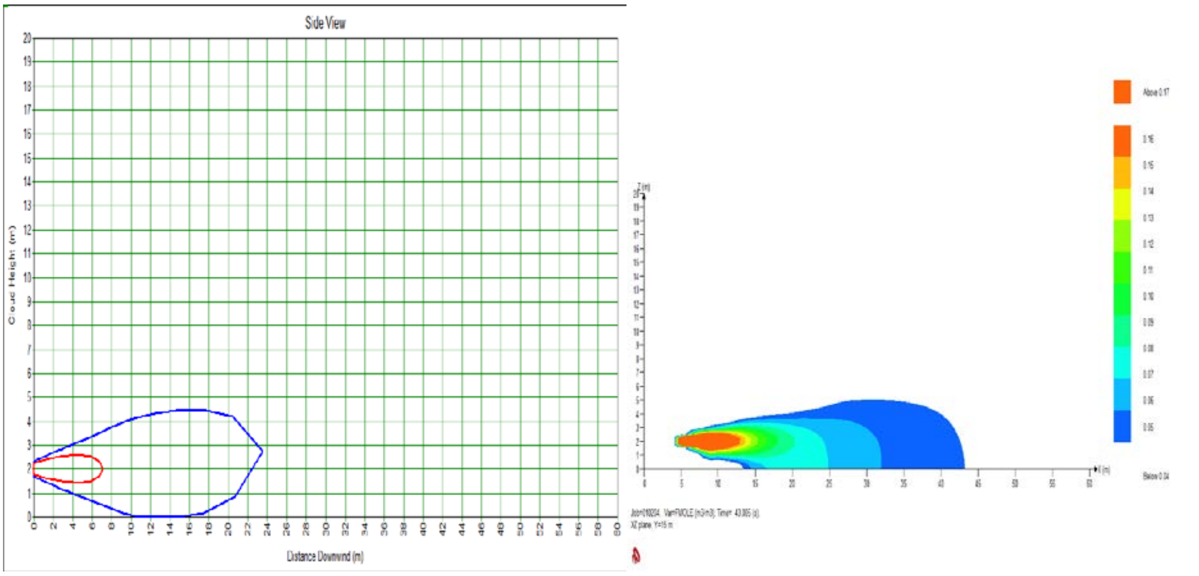


Figure 7-31 *Left figure is a Comparison plot with ground roughness of 3000mm in PHAST. Right figure is a FLACS simulation with small geometry. Wind speed 5.0 stability class D.*

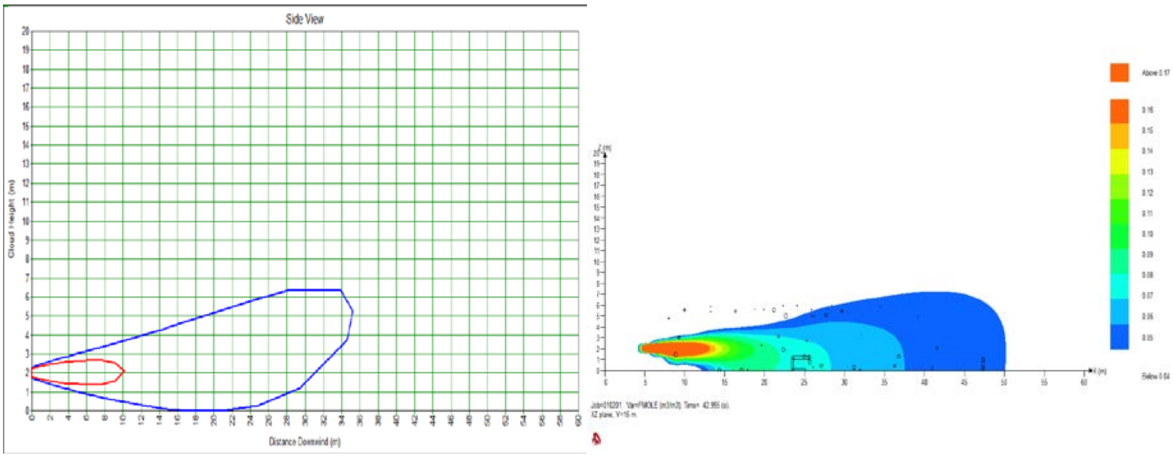


Figure 7-32 *Comparison of FLACS and PHAST. Left figure is PHAST with ground roughness of 3000mm. FLACS jet is shown in large geometry, PD=1.4m/m^3. Wind conditions of 1.5 m/s with stability class F.*

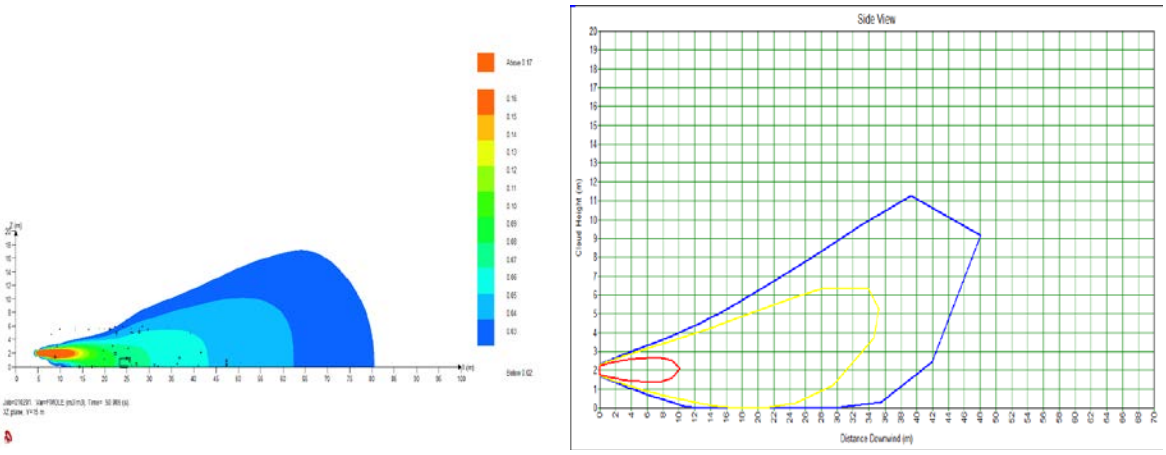


Figure 7-33 *FLACS 1.5F up to LFL2 values. Not steady state, the FLACS plume keep on growing in the LFL$_2$ (2.2 Vol%) concentration regime. PHAST jet show some of the same characteristics as FLACS. PHAST ground roughness of 3000mm.*

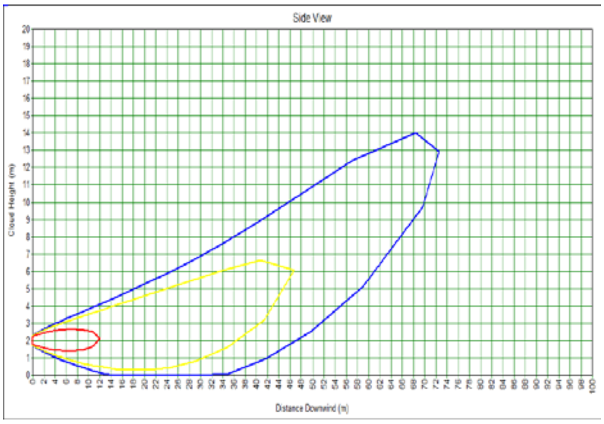


Figure 7-34 *PHAST Impinging Jet 1.5F Ground Roughness of 0.2mm.*

7.5.2 FLACS; Medium congested pipework

Table 7-7 *Overview of wind conditions for FLACS simulations*

Sim nr	*Wind condition*
010200	***1.0F***
010201	***1.5F***
010202	***3.0F***
010203	***3.0B***
010204	***5.0D***
010205	***5.0B***
010206	***10.0D***

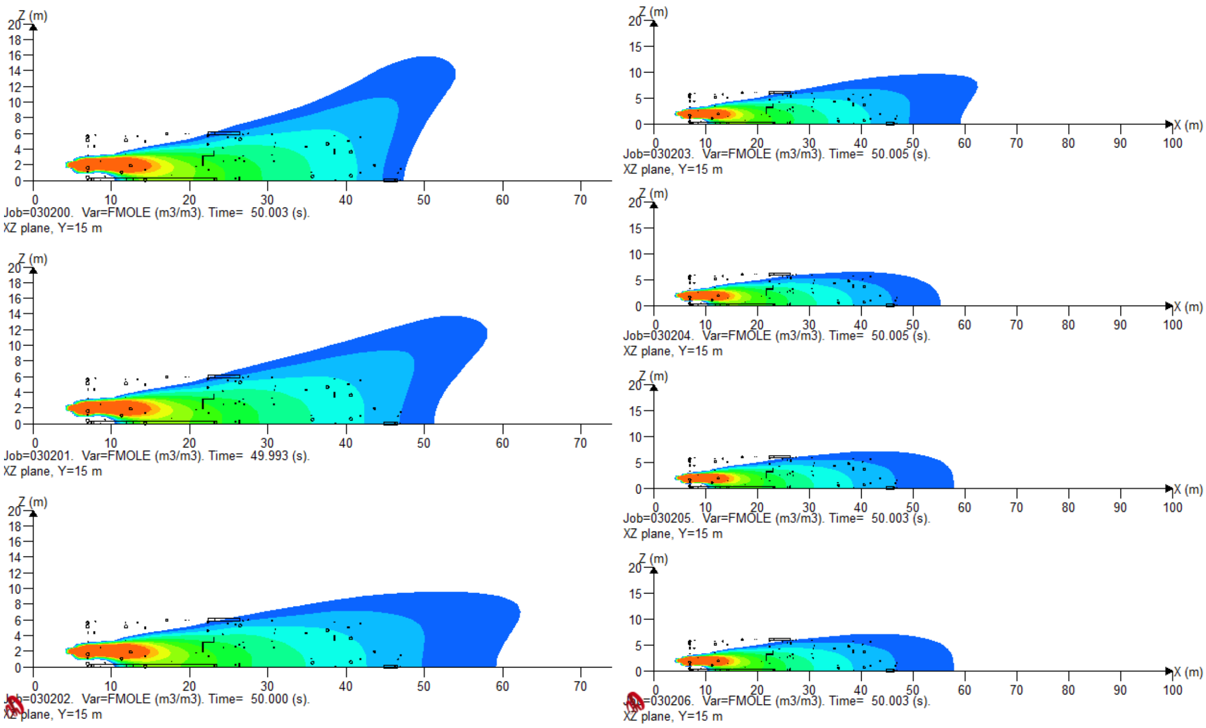


Figure 7-35 *Flammable (up to 4.4 Vol%) domain of methane release in medium geometry steady state plumes.*

7.5.3 FLACS; Highly congested pipework

Table 7-8 *Overview of wind conditions for simulations in FLACS shown in figure x.x below for medium geometry*

Sim nr	*Wind condition*
030200	***1.0F***
030201	***1.5F***
030202	***3.0F***
030203	***3.0B***

030204	***5.0D***
030205	***5.0B***
030206	***10.0D***

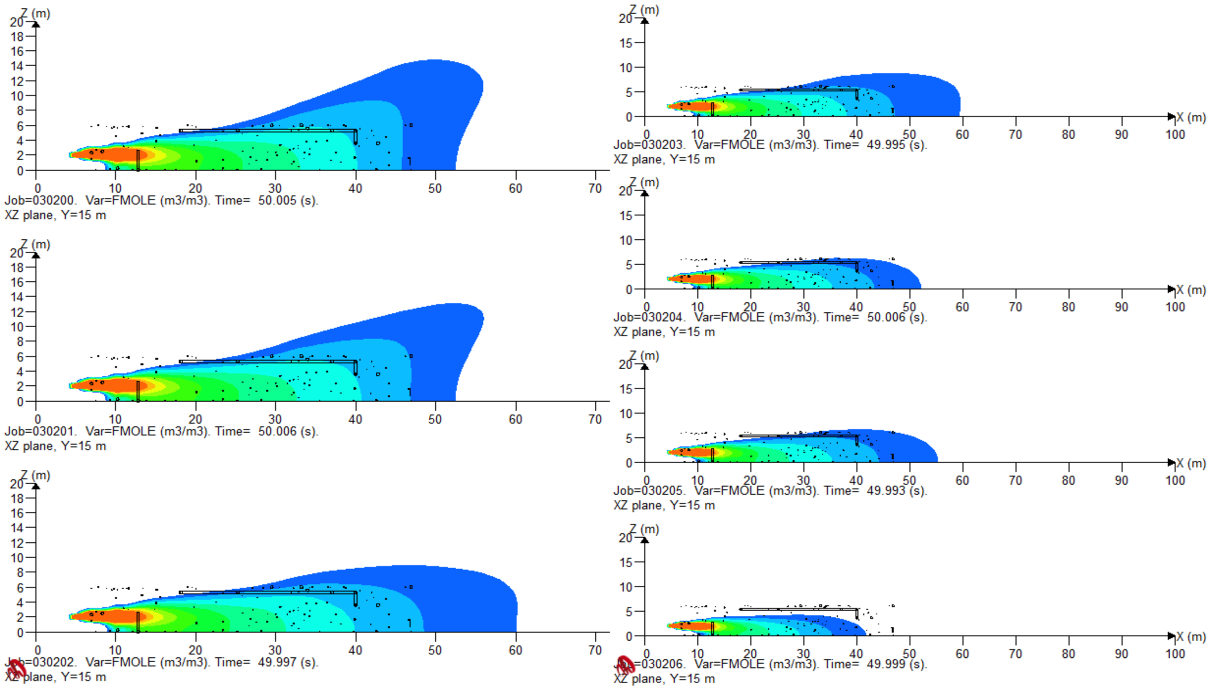


Figure 7-36 *Flammable (up to 4.4 Vol%) domain of methane release in large geometry for steady state plumes with different wind conditions.*

Similar trend as seen for releases within medium geometry. The low wind speeds causes the interaction between the gas jet and the geometry to give a buoyant plume. This is especially observed, at wind speed 1.0m/s with stability F.

7.5.4 PHAST large leak scenario; attempts to account for congestion

The figures below show the simulations with wind conditions of 1.5F and 5.0D run in PHAST with impinged velocity factor at default value (0.25) with various ground roughness values with the four different values. For the PHAST scenarios a total of 56 simulations were run for the large leakage scenario (9.48 kg/s).
The PHAST simulations for 1.5F is compared against FLACS simulations 030201 shown above in Figure 7-36. FLACS simulation 030204 is compared against PHAST simulations in Figure 7-39 and Figure 7-40.

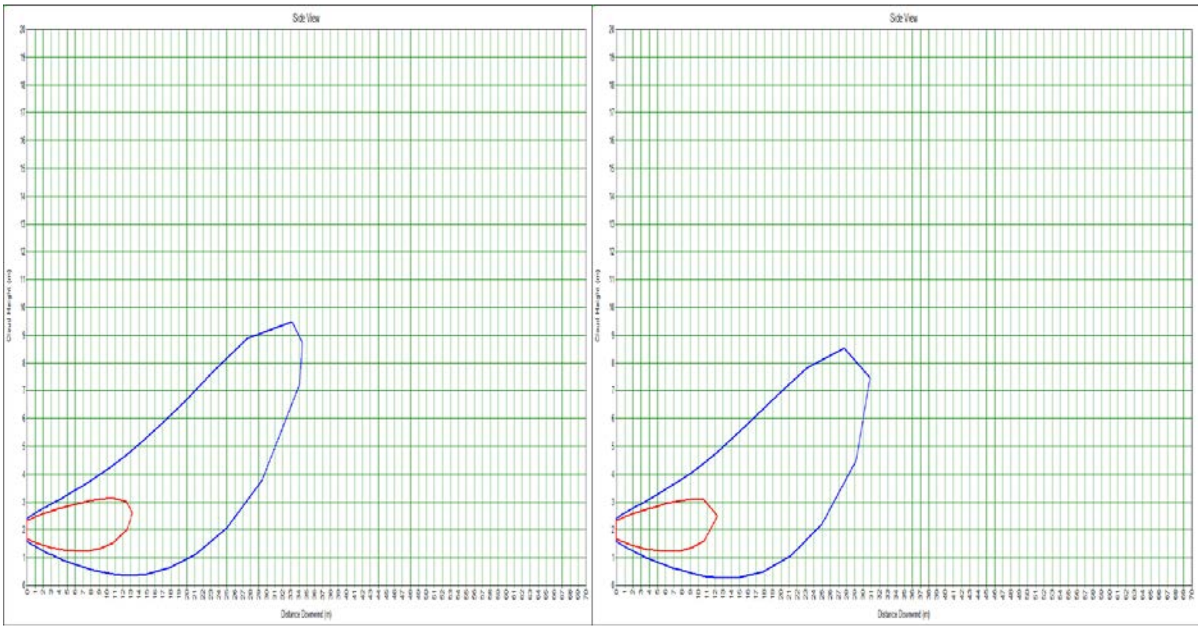


Figure 7-37 *Flammable (From 4.4 Vol% up to 16.5 Vol%) domain of methane release (9.48 kg/s with discharge velocity of 251.1m/s) for steady state plumes for left ground roughness of 0.5m and right 1.5m. Wind conditions are 1.5m /s of F stability.*

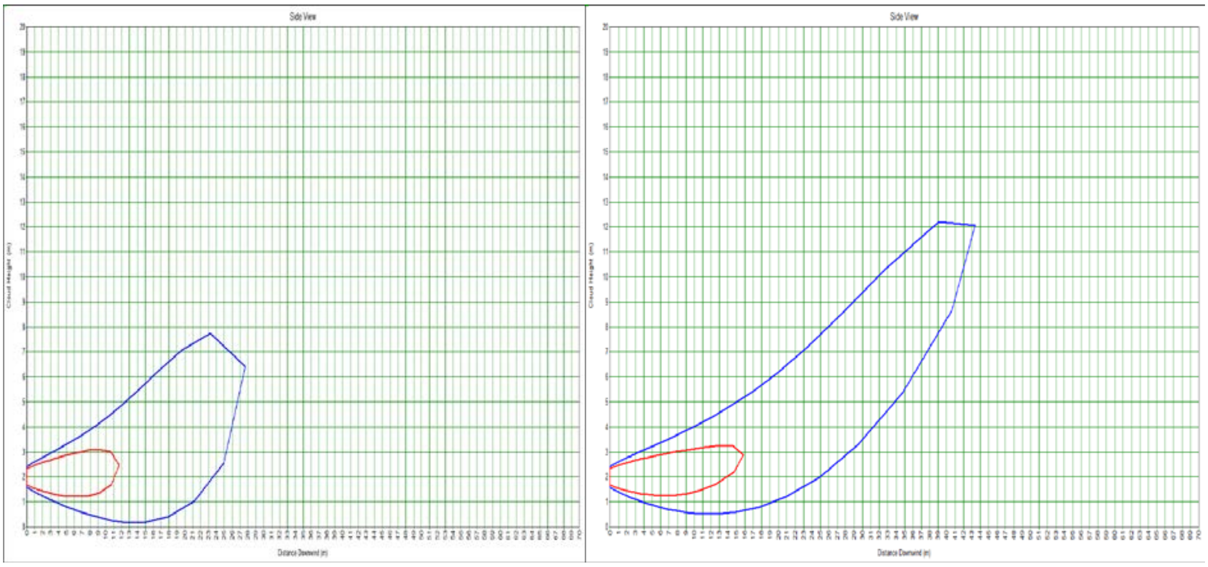


Figure 7-38 Flammable (up to 4.4 Vol%) domain of methane release (9.48 kg/s with discharge velocity of 251.1m/s) for steady state plumes for left ground roughness of 3.0 m and right 0.2mm. Wind conditions are 1.5m /s of F stability.

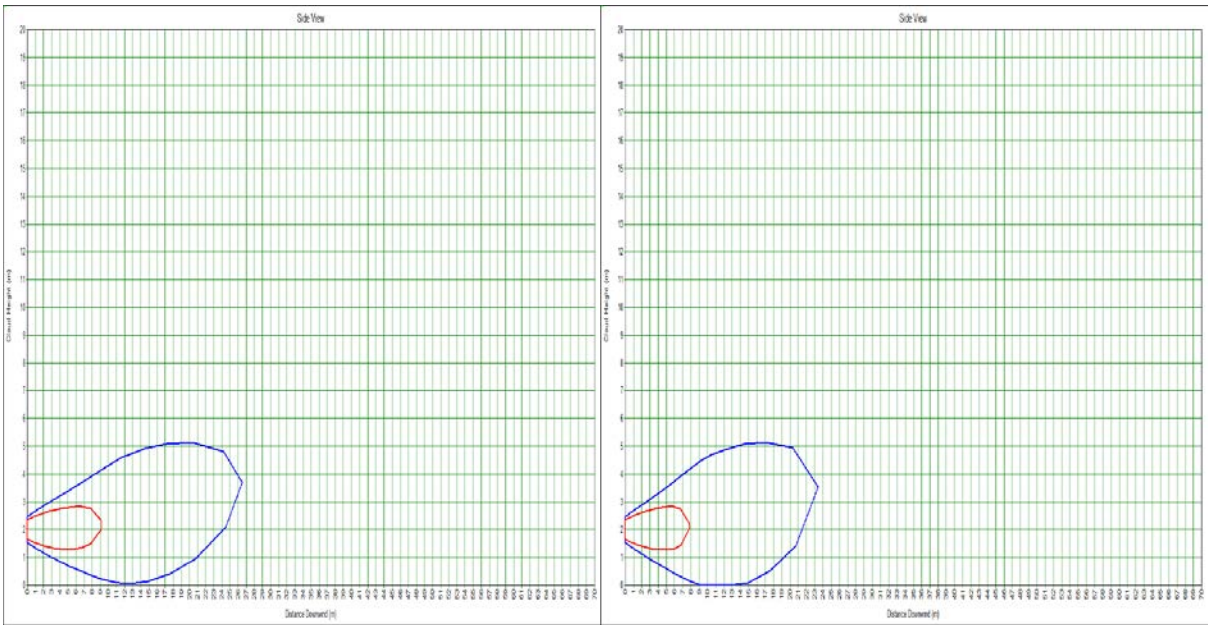


Figure 7-39 Flammable (up to 4.4 Vol%) domain of methane release (9.48 kg/s with discharge velocity of 251.1m/s) for steady state plumes for left ground roughness of 0.5 m and right 1.5m. Wind conditions are 5.0m/s of D stability.

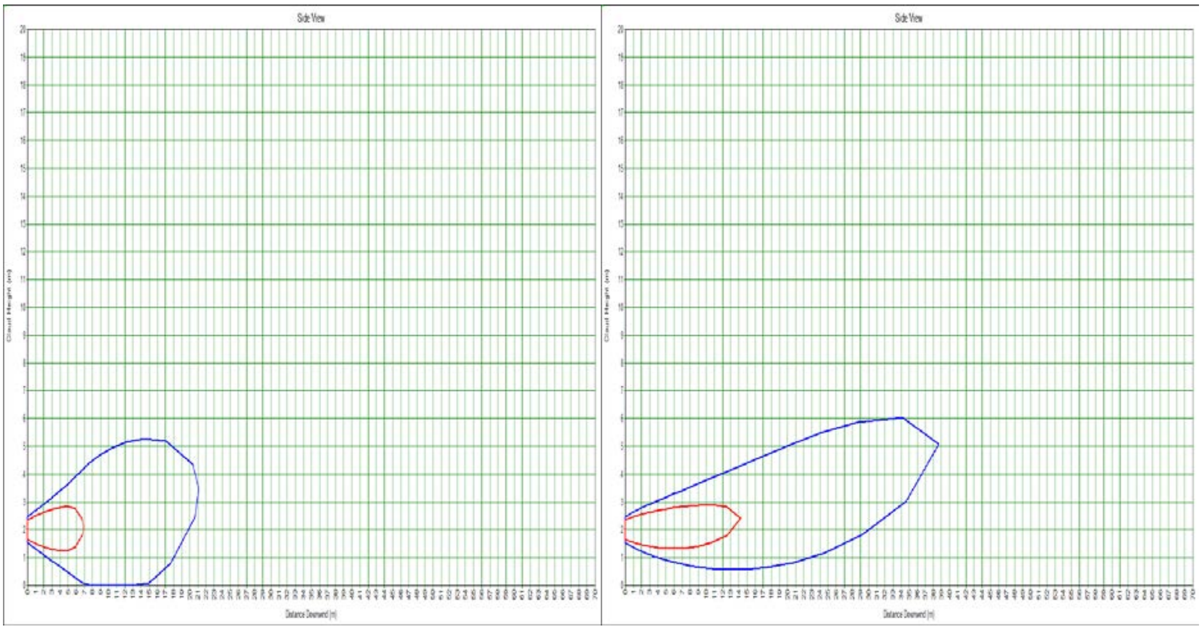


Figure 7-40 Flammable (up to 4.4 Vol%) domain of methane release (9.48 kg/s with discharge velocity of 251.1m/s) for steady state plumes for left ground roughness of 3.0 m and right 0.2mm. Wind conditions are 5.0m/s of D stability.

7.5.5 PHAST; Large leakage Centerline approach for different ground roughness values

An analysis was done for both the defined method1 and 2 in PHAST by plotting the concentration decay profile for various ground roughness values given from the dispersion report. The changing of ground roughness value was also performed together with the horizontal impinging choice in PHAST. The wind scenarios 1.5F and 5.0D are shown below in figures below.

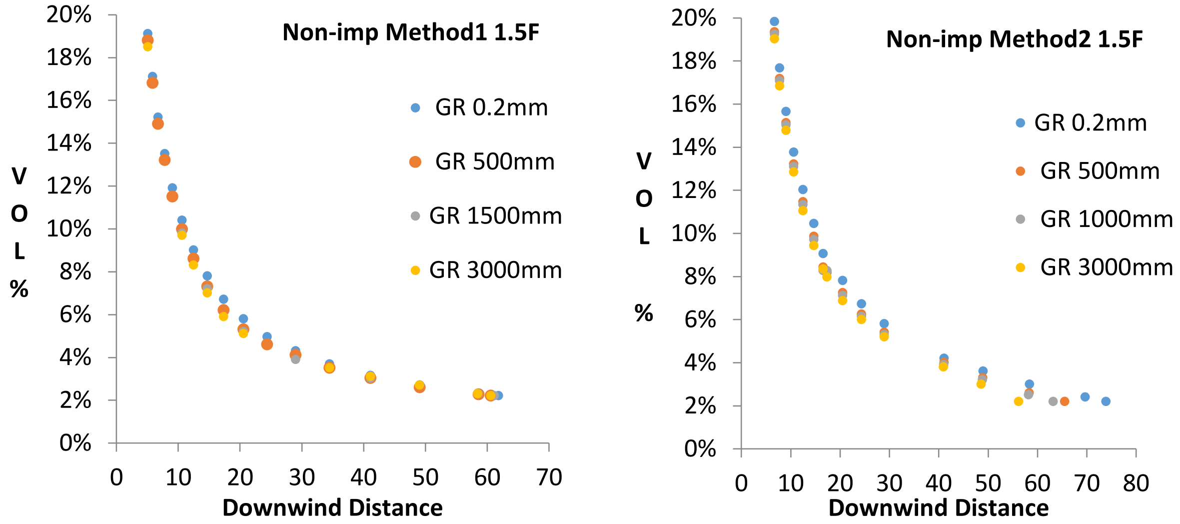


Figure 7-41 *Large leak 9.48 kg/s, Concentration decay up to LFL_2 of non-impinging jet as a function of ground roughness sensitivity of large leak method 1 and 2 with windspeed of 1.5F*

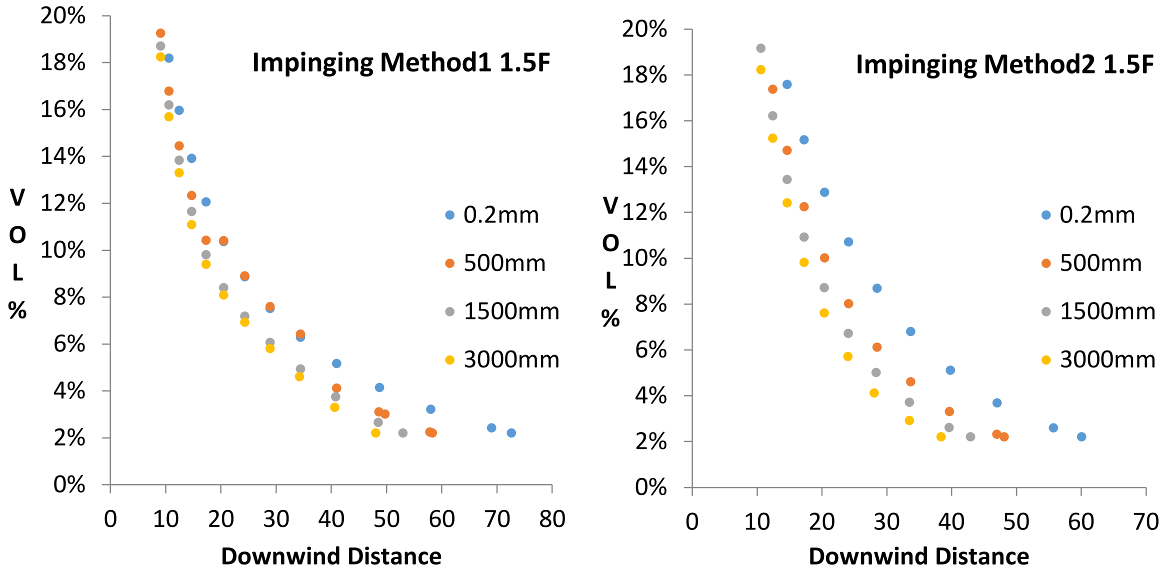


Figure 7-42 *Large leak 9.48 kg/s, Concentration decay up to LFL_2 of Impinging jet as a function of ground roughness sensitivity of large leak method 1 and 2 with windspeed of 1.5F*

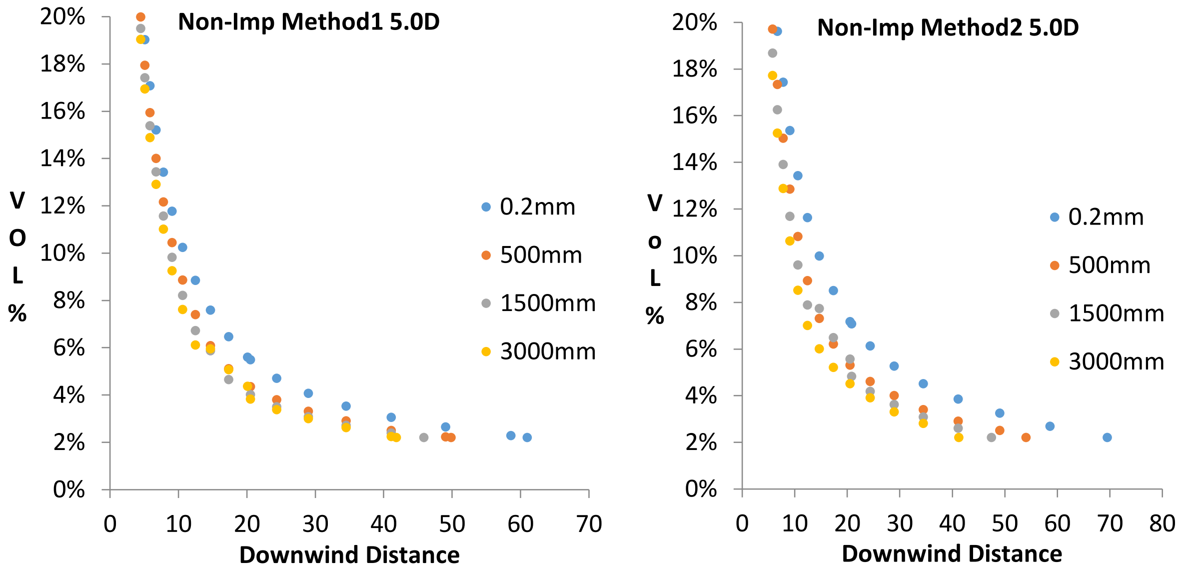


Figure 7-43 *Large leak 9.48 kg/s, Concentration decay of non-impinging jet as a function of ground roughness sensitivity of large leak method 1 and 2 with windspeed of 5.0D*

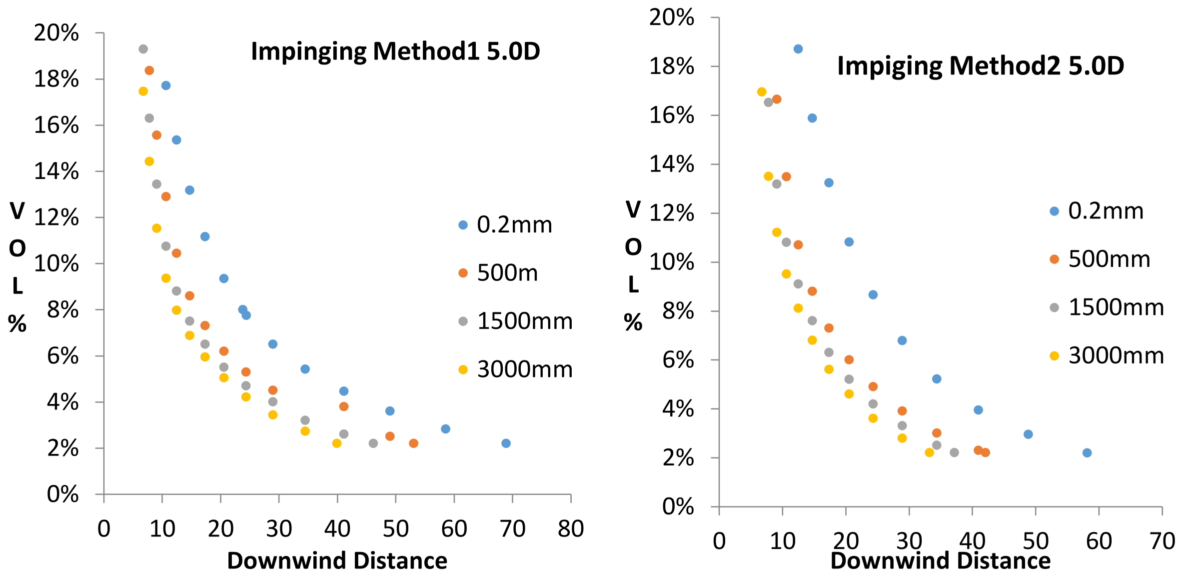


Figure 7-44 *Large leak 9.48 kg/s, Concentration decay of impinging jets as a function of ground roughness of large leak method 1 and 2 with wind speed of 5.0D.*

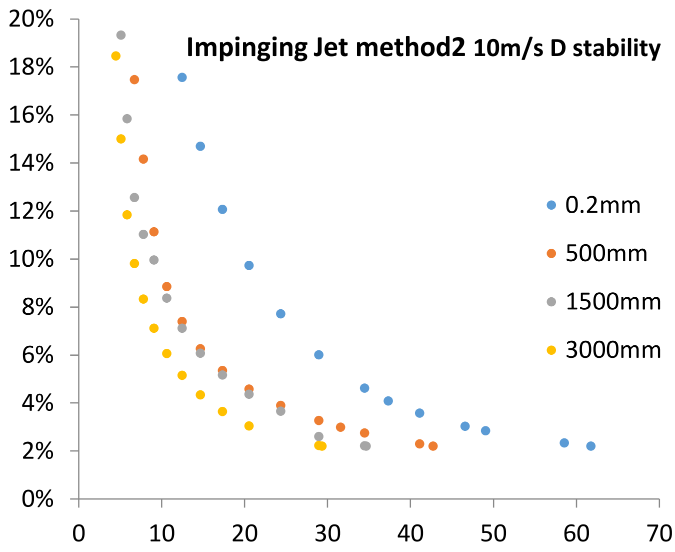


Figure 7-45 *Large leak 9.48 kg/s, Impinging jet of method2 with external wind field of 10m/s stability D for various ground roughness values.*

The plots above show how the ground roughness influences the concentration decay along the concentration centerline in PHAST. The results show that for higher wind speeds the effect of ground roughness decreases the spreading distances in the downwind direction of the leakage. The higher the wind speed the stronger this effect is seen. The horizontal impingement choice in PHAST gives the strongest implications on the downwind dispersion compared to the non-impinging choice. Method2 shows more effect of ground roughness than method1.

Ground roughness will also have an impact on the sideway spread of the dispersion in PHAST. The illustrations below show the effect of different ground roughness on plume spread. As already established the ground roughness will give lower concentration values downwind of the leakage. The sideway / lateral spread is showing a different characteristic behavior. High values for ground roughness will cause the plume to disperse sideways as shown below in Figure 7-46. The illustration gives the difference in plume behavior for 0.2mm and 3m ground roughness values in PHAST. This effect was seen strongest for higher wind conditions in the range of 5m/s for the simulations run in the framework of this report.

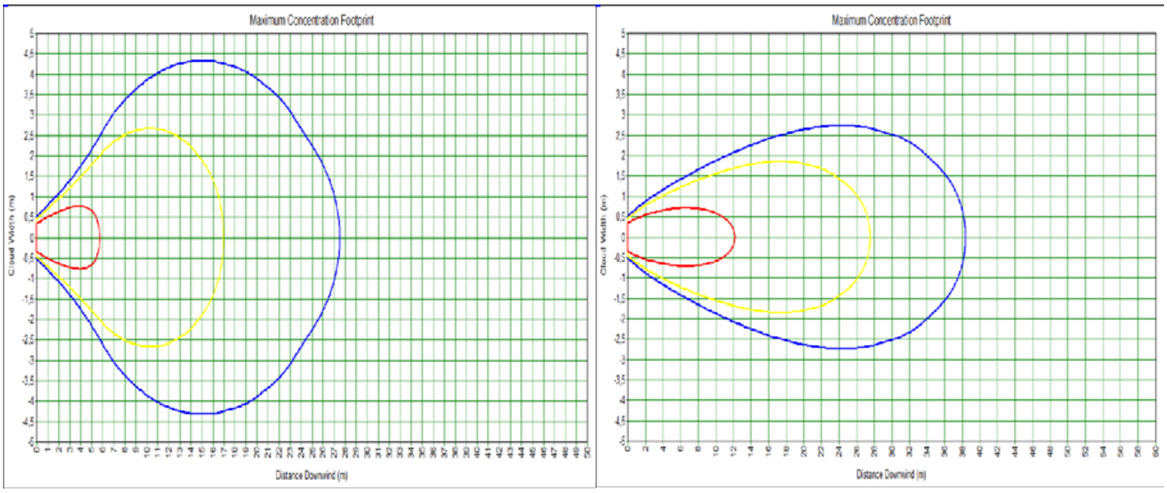


Figure 7-46 *Impinging Jet Lateral spread of plume due to different ground roughness. Left picture has ground roughness of 3m and right picture has 0.2mm. Wind condition of 5.0B are shown here. Red color indicates ULF range, yellow LFL and blue LFL_2 concentration range.*

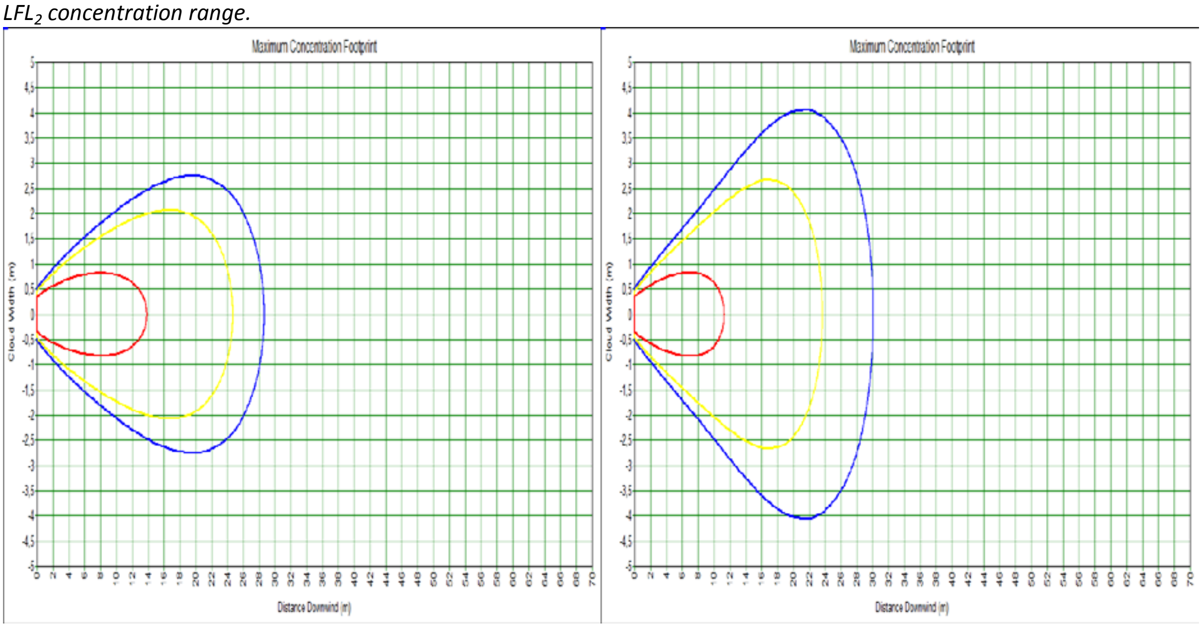


Figure 7-47 *Impinging jet Lateral spread of plume due to different ground roughness. Left picture has ground roughness of 0.2mm and right picture has 3m for similar jets. Wind conditions of 1.5F is shown here.*

Figure 7-47 show the horizontal spread / cloud width spread of the plume seen from above. These plots show the implication of the ground roughness value on sideway and downwind spreading of gaseous releases. The value chosen for roughness is two cases at both end of the ground roughness scale in PHAST of 0.2mm to 3000mm.

The yellow and red line indicates the UFL and LFL concentration range. These values are not very affected by changing of the ground roughness values. Seen from the figures above the concentration in the LFL_2 range is mostly affected.

7.6 Flammable mass study for jet dispersion in congested environments

7.6.1 ATEX-like release flammable mass comparison for the congested flows

A flammable mass comparison was performed for the results given by the simulations the simulations run for the congested flows. Both method 1 and 2 in PHAST were compared to the simulations done with small, medium and large congestion in FLACS.
An expectation would be that the congestion will increase the amount of flammable gas within the same volume compared to free field jet due to accumulation caused by lower wind speeds inside the array of pipe obstacles, and by that giving lower dilution and mixing of the plume with ambient air.

For the ATEX-like case, shown in 0, the PHAST method2 results was in good agreement with the FLACS results. For the methane jets impinging into pipework geometries the congestion introduced a higher flammable mass for almost all the plumes examined. The function horizontal impingement was used in PHAST and various roughness lengths were used to see what effect this had on the flammable mass accumulation. Flammable mass values were extracted in the late explosion report in PHAST and in the fuel file in FLACS.

Two effects were seen for the ATEX-like leaks for the large pipework congestion. The PHAST values are in the range of 50 percent of the highest values given by the FLACS simulations, data for flammable mass is given in Table 7-9.

A tunnel effect in FLACS made the ATEX-like leak behave as a perfect free jet without impinging into any pipes. The flammable mass from this leak was in good agreement with the free jet releases.

A blocking effect made the leak impinge with the pipe and cause the leak to behave as a highly buoyant jet, seen in Figure 7-48.

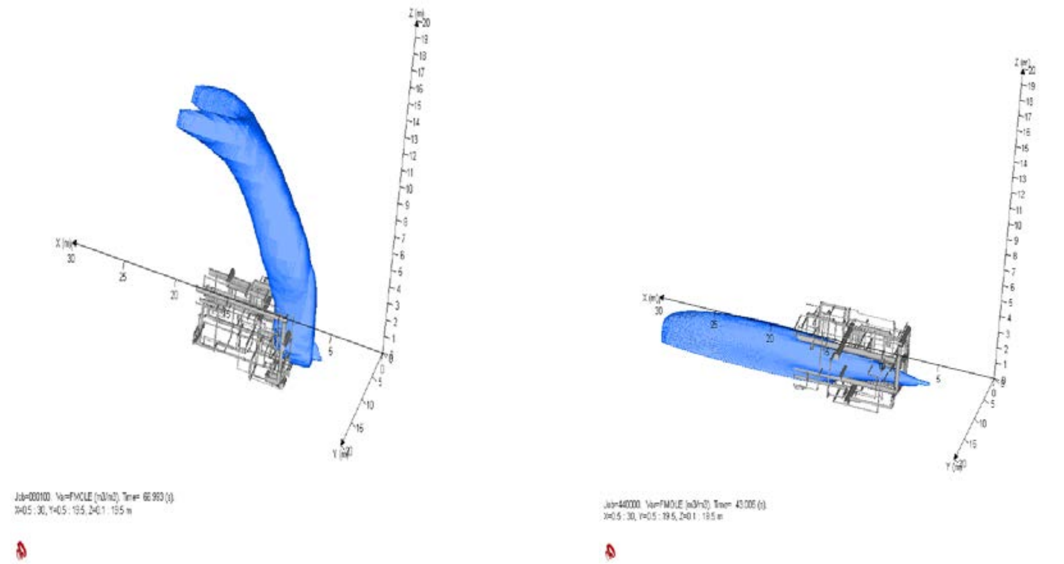


Figure 7-48 *Blocking and tunnel effect for large geometry. Concentration decay up to LFL_2.*

Table 7-9 *Flammable mass Comparison ATEX-like case FLACS and PHAST , Ground Roughness of 10cm for all cases.*

Wind speed stability class	PHAST Impinging Method1 (kg)	PHAST impinging Method2(kg)	FLACS PD=0,7	FLACS PD=1,0	FLACS Tunnel PD=1,4	FLACS Blocking PD 1,4
1.0F	0,32	0,58	1,15	1,22	0,11	1,5
1.5F	0,3	0,54	1,1	1,18	0,11	1,35
3.0F	0,24	0,4	0,86	1,25	0,105	1,05
3.0B	0,18	0,29	0,7	1,05	0,095	1,25
5.0D	0,15	0,23	0,38	0,551	0,0841	0,355
5.0B	0,14	0,2	0,44	0,62	0,083	0,65

Table 7-10 *PHAST ATEX scenario Flammable mass calculations for various ground roughness values of impinged and non-impinged jets for 1.5F.*

ATEX scenario	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)
Ground Roughness (mm)	**METHOD1 Non-impinging**	**METHOD2 Non impinging**	**METHOD1 impinging**	**METHOD2 Impinging**
0.2mm	0,05	0,14	0,32	0,55
500mm	0,05	0,12	0,28	0,51
1500mm	0,05	0,12	0,27	0,47
3000mm	0,05	0,11	0,25	0,45

Table 7-11 *PHAST ATEX scenario Flammable mass calculations for various ground roughness values of impinged and non-impinged jets for 5.0D.*

ATEX scenario	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)
Ground Roughness (mm)	**METHOD1 Non-impinging**	**METHOD2 Non impinging**	**METHOD1 impinging**	**METHOD2 Impinging**
0.2mm	0,04	0,10	0,20	0,30
500mm	Not given in PHAST	Not given in PHAST	Not given in PHAST	Not given in PHAST
1500mm	Not given in PHAST	Not given in PHAST	Not given in PHAST	Not given in PHAST
3000mm	Not given in PHAST	Not given in PHAST	Not given in PHAST	Not given in PHAST

From the tables above the following trends was seen for PHAST;

- Changing ground roughness will not have a large impact on the flammable mass calculations given by the simulations. The trend shown is that for larger ground roughness the values for flammable mass will be reduced.
- Higher flammable mass is seen for PHAST method2 compared to method1.
- The higher the wind velocity in the jet domain the lower the flammable mass.

From the tables above the following trends was seen for FLACS.

- The higher the wind velocity the lower the flammable mass.
- For small jets the flammable mass values will greatly depend on how the jet interacts with the geometry. To different extreme cases were seen for these simulations, the blocking and tunnel effect. For the blocking-effect the flammable mass was large compared to the PHAST values. For the tunnel-effect the calculation of flammable mass was comparable with the free jet scenario.

7.6.2 Flammable mass comparison large leakage scenario 9.48 kg/s

Flammable mass was calculated for the large releases in both FLACS and PHAST. Both method one and two was used in PHAST and the horizontal impingement was used. The values for flammable mass was three to four times as high with the impingement used in PHAST compared to not using this parameter.

The FLACS simulations that were used for flammable mass were the same simulations as used for part three. The approximate flammable mass was found in the FUEL file.

A comparison for flammable mass was then done to compare the various congested environments in FLACS with the PHAST simulations for horizontal impingement and the free jets.

Table 7-12 *Flammable mass comparison for large release scenario of 9.48 kg/s. Ground roughness 10cm in PHAST. Default value of 0.25 for the impinged velocity factor was used in PHAST.*

Wind and stability class	PHAST Impinging Method 1	PHAST impinging Method 2	FLACS PD=0,7 (kg)	FLACS PD=1,0 (kg)	FLACS PD=1,4 (kg)
1.0F	22,29	32,30	31,80	89,0	86,0
1.5F	20,04	28,15	28,0	93,0	84,0
3.0F	17,07	20,78	22,0	89,0	75,2
3.0B	12,25	15,21	17,80	80,0	65,0
5.0D	10,66	13,17	13,70	50,0	42,7
5.0B	9,09	11,55	12,50	53,0	44,6
10.0D	5,89	7,6	7,50	52,0	16,5

A very close relationship between the values given for FLACS and PHAST method2 for a packing density of 0.7 when using impinging (default value 0.25) velocity factor.

Table 7-13 *PHAST Large scenario flammable mass calculations for various ground roughness values of impinged and non-impinged jets for 1.5F. Method1 and method2 was also used in PHAST.*

Large scenario	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)
Ground Roughness (mm)	**METHOD1 Non-impinging**	**METHOD2 Non impinging**	**METHOD1 impinging**	**METHOD2 Impinging**
0.2mm	3,57	9,93	21,97	31,62
100mm	3,50	9,59	20,04	28,15
500mm	3,42	9,33	19,79	25,72
1500mm	3,32	9,38	20,13	23,65
3000mm	3,32	10,20	20,68	21,15

Table 7-14 *PHAST Large scenario Flammable mass calculations for various ground roughness values of impinged and non-impinged jets for 5.0D.*

Large scenario	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)	FLAMMABLE MASS (kg)
Ground Roughness (mm)	**METHOD1 Non-impinging**	**METHOD2 Non impinging**	**METHOD1 impinging**	**METHOD2 Impinging**
0.2mm	2,81	6,63	12,65	16,57
100mm	2,40	5,47	10,66	13,17
500mm	2,13	4,91	9,67	12,58
1500mm	1,97	4,51	9,11	12,09
3000mm	1,82	4,43	9,08	12,14

8 Realistic scenario

8.1 Background / method

So far, this report has described differences / similarities of FLACS and PHAST for free and impinging jets. Far field effects and comparison against experimental results have also been examined through the Kit Fox experiment. Now the focus will now shift to a realistic scenario of an offshore module. Information gathered from the initial comparisons was used for the comparison in this realistic environment. Two different mass flow rates were chosen, a relative small and a medium large leakage.

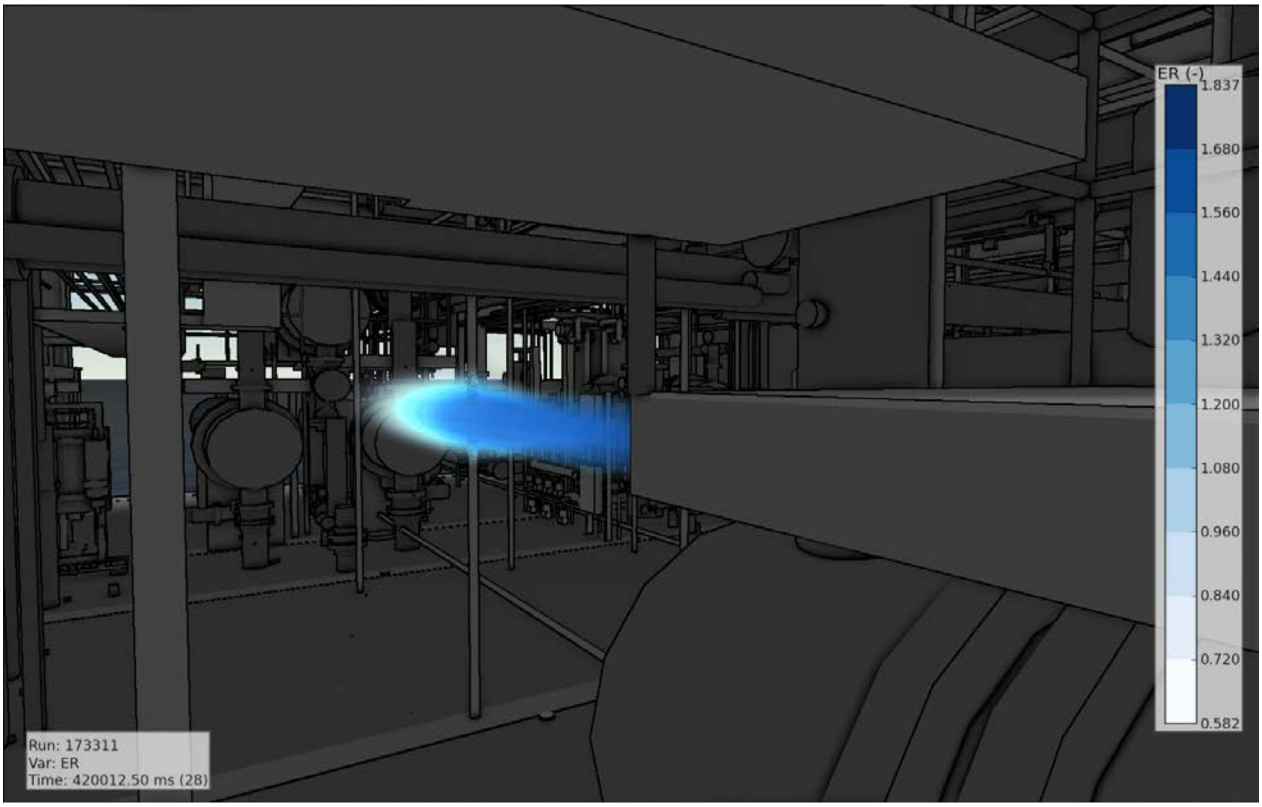


Figure 8-1 *Simulations of a gas leakage at an offshore module performed at GexCon of 0.75 kg/s. (Flammable range plottet in terms of equivalence ratio). Indicating the difficulty of detecting this type of leakage with gas detection devices.*

There is a need for a real case in this report to challenge the appreciation of the main findings so far and to transfer the theoretical topic into applications. This is done as a case study of a gas leakage at an offshore module to challenge the outcomes from FLACS and PHAST. The module consists of segregating walls, pipes and process equipment. The leakage shown is from a process vessel.

Two different gas leaks are simulated at 0.75 kg/s and 7 kg/s. Initially the simulations are performed in FLACS. The user-defined discharge (method2) in the PHAST model used for the comparison, as this has proven to be most comparable with the FLACS model throughout this report.

8.2 Results of case study

An attempt to represent a realistic gas leakage on offshore platform is performed for different leakage rates (0.75 kg/s) and (7 kg/s) in accordance with two of the leakage classes defined in NORSOK Z-013 [18].

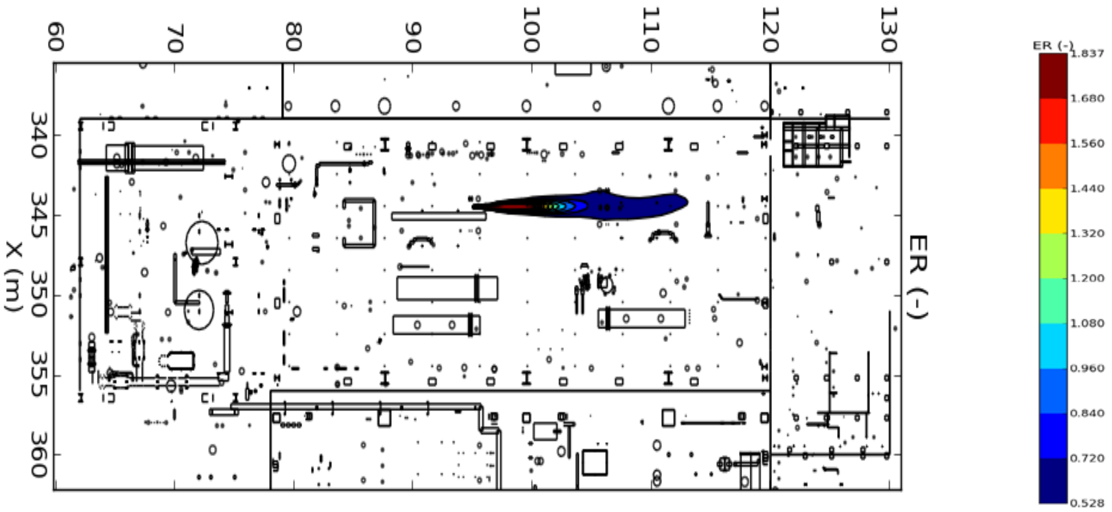


Figure 8-2 *Small jet 0.75 kg/s leak, discharge velocity of 204.62 m/s. Equivalence ratio legend to the right. A value close to 1.0 will be stoichiometric. Higher or lower equivalence ratio defines the mixture to be rich / lean.*

Figure 8-2 is the representation of the 0.75 kg/s leak simulated in FLACS. This type of small leak may be represented in PHAST model similar to the FLACS leakage, within 20-30% deviation for concentration decay. When using the PHAST model for these scenarios the user will extract the results in all directions in 3D to account for all possible leakages.

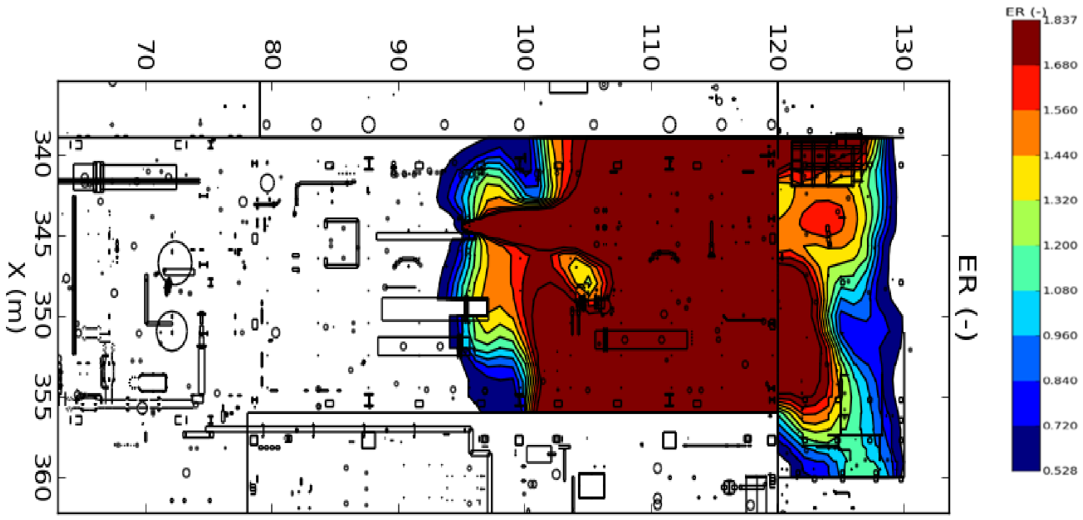


Figure 8-3 *Flammable range plotted; Medium leak 7.0 kg/s, Discharge velocity of 204.62 m/s. Equivalence ratio legend to the right. A value close to 1.0 will be stoichiometric. Higher or lower equivalence ratio defines the mixture to be rich / lean.*

Figure 8-3 show the 7.0 kg/s leak, for the FLACS simulation. When the jet dispersion is dominated by the wall interaction, and the gas complete fills the module with flammable concentration of gas.
This simulations performed in FLACS was not transferable to the PHAST model. The concentration decay / flammable mass will not be correctly represented by PHAST, and thus a CFD code is required for this scenario.

8.3 Conclusion for the realistic scenario

The simulations performed in FLACS illustrates the differences between the two models for real scale engineering applications.

The two different leaks represents different scenarios in terms of concentration decay, spread and flammable mass.

Large leakage rate, 7.0 kg/s;

The large leak shown in Figure 8-3 is highly influenced by the environment / congestion in which the jet travels. For this type of leak the PHAST model in not able to produce a similar plume, nor will the model be able to give adequate flammable mass for this type of leak. For the environments where the congestion and geometry drive the plume spread, the PHAST model is not recommended as a tool for consequence assessment, whatever reasonable deviations of comparisons have been observed for a similar leak rate range in the earlier section of this report.

No attempt to simulate a comparable plume in PHAST was performed for this leak.

Small leakage rate 0.75 kg/s;

The small leak run in FLACS is possible to model in PHAST. The PHAST user will be confident that the results gained from the model will be within 20-30% deviation from the FLACS jet in concentration decay for a free un-impinged jet. This involves using same input to the dispersion model in FLACS and PHAST as this has proven to be most comparable. Flammable mass will also be relative similar.

The PHAST user may also account for a leakage in every possible scenario, evaluating both impinging and non-impinging jets. This can be done by deriving the same jet in all possible directions in 3D. To match a CFD tools flammable mass calculation the impinging choice within the PHAST model must also be used.

The conclusions given above for the two different leaks are aligned with the earlier conclusion given in this report. Small leaks with a relative low mass flow rate (ATEX-regime) may be possible to model in an integral model without corrupting the risk assessment to a large extent. Large leak with interaction with walls are not possible to simulate in integral modelling and a CFD approach is to be preferred.

9 Final Discussion/Further work

General discussion;

As a CFD tool, the range of applicability covered by FLACS is subsequently wider compared to the integral model PHAST. Still, over a given selective range of parameters, the FLACS and PHAST results from a reference case can be compared with similar range of confidence.

Throughout this report, FLACS has demonstrated more conservative patterns than the PHAST model, giving longer spreading distances and larger flammable mass for most of the simulations runs.

The integral model PHAST was unable to give comparable results for flammable potentials when the effect of congestion (packing density values higher than 0.7) was introduced for the large leaks simulated.
The corrective effect of ground roughness used in PHAST to account for increased congestion hasn't been showed successful as this approach could not account for the range of congestions chosen. However, small leaks like the ones considered in the ATEX approach frame did not give widely different plumes or flammable mass calculations. These leaks are not expected to give large deviation in terms of consequence assessments following dispersion.

The simulations performed as part of this work was not compared to experimental results for free or impinged jets. This implies being unable to promote the one tools over the other with great confidence. Uncertainty in the results was therefore not evaluated for either FLACS or PHAST. However, the FLACS model proved most conservative for most cases and is to be preferred when low congestive effect are seen to affect the dispersion over an experimental case.

When working with PHAST as a tool for risk assessment, the shortcomings of the model must be understood / appreciated by the user. PHAST has a limited way of handling wind. Situations where the external wind field is below 1 m/s and where wind direction expected is blowing against the leak, the PHAST UDM model is not recommended as a consequence assessment tool.

The PHAST model has been widely validated against large experimental cases in the open field. Hence, it is important to emphasize that these limitations will either be translated into over-conservatism or discrepancies. The threshold between using the simplified methods as a preliminary screening for further advanced assessments or as a direct approach is often very narrow and has to be further clarified.

Guideline development;

The goal of this study was to develop data supporting guidelines and recommendations improving accurate use of simulation tools for flammable gas dispersion modeling depending on environments. The goal was also to illustrate what was the sensitivity of increasing the congestion level over the flammable range. Eventually, the objective was to address to what extent a simplified integral tool like PHAST could account for such congestion, - in a safety engineering perspective. Indeed, besides modelling tools, safety engineers relate to "real industrial plants" and, to some extent, more insight on effects of congestion and confinement is needed before ruling out these parameters from consequence assessment when arguing conservatism is guaranteed.

To fully understand how the set-up and the subsequent results from an integral model can be representative and somewhat account for geometry effects, the modeler needs a method to introduce the geometrical effects and quantify how flow interacts with geometry. One way of attempting to do this, as done in this report, is to use a CFD model able to account for these effects and perform a comparison. In the CFD code, a virtual congested geometry is elaborated based on a parameter called the "packing density". The packing density is adjusted for several different pipework geometries and thus used within the CFD code FLACS. The fundamental question is to know how the modeler should relate to the congestion level using the parameters within the PHAST integral model.

Is it at least manageable to match the results assessed with CFD versus empirical results for given specific cases?

Discharge modelling;

In light of this report, results from the simulations were the most similar when the PHAST user bypassed discharge modelling and used the properties gained from the FLACS jet utility and implemented this in the PHAST dispersion model. The only source of deviations studied between FLACS and PHAST was therefore the dispersion models themselves. Using the whole chain of discharge and dispersion models in PHAST gave results that were not as comparable with FLACS. Deeper investigation reveal that these differences in result`s are mainly due to FLACS and PHAST`s different discharge models. FLACS uses choked flow following Rankine-Hugoniot relations, while thermodynamic laws drive discharge modelling in PHAST.

For example the NORSOK Z-013 [18] used for risk and emergency preparedness analysis in the Norwegian sector gives certain mass flow rates that are to be examined in risk analysis. In an analyst perspective the concept mass flow rate is fully dependent on the hole size and the pressure and temperature characteristics of the containment. A simple example illustrates this phenomenon;

"A 2" leak from a containment at 90 bar can achieve the same flow rate (NORSOK rate) as a leak from 6" containment with limited / no differential pressure. Two widely different cloud potentials are expected in this respect, with widely different physical characteristics."

PHAST can easily be used to get a picture of how different cloud behavior can originate from the same mass flow rate by varying the said parameters and quickly rerunning simulations. This can efficiently aid safety engineers in showing different cloud behavior for the same mass flow rates. How PHAST will represent the dispersion plume, namely if it is dense or buoyant may also help the modeler in grid assessment and by that saving time / cost.

Furthermore, integral models can be implemented within CFD codes to give quick input to the modeler on how the simulations should be performed in CFD. By doing so the integral model will no longer be a stand alone tool, but a tool used preliminary screening or in cooperation with a CFD model.

Eventually, a safety engineer needs to understand the complete chain of assessments (based on intial discharge modelling) to be able to suggest valuable assessments and further improvements, within the big picture.

Applications of dispersion modeling in safety engineering;

The discussion regarding the differences between FLACS and PHAST is not efficient unless it covers topics which are of interest in the safety sciences. For this discussion, obviously the explosion risk and gas detection should be addressed in this context. Side assessments of stack releases are also given.

- **Explosion risk perspective (ATEX-like case and large leakage scenario);**

To focus on the impinging jets into the various congested pipework's the various mass flow rates indicates widely different explosion risks in a comparison perspective. The small leaks in FLACS were largely dependent on the geometry itself since the leak may be completely blocked or unblocked / free jet behavior. The blocked jet will give the highest flammable mass in FLACS. When using the impinged velocity factor in PHAST this gave the highest flammable mass.

For explosion risk the differences between the models for the small mass flow rate are not considered large enough so that a different explosion consequence would be given (potential explosion overpressure for the different models are expected to be relatively similar).

For explosion risk, a large leak (in this study 9.48 kg/s) gives a different perspective than the ATEX case and FLACS are to be preferred when packing density values are higher than the 0.7 m/m^3 value. The low congestion (0.7m/m^3) pipework gave almost perfect match between the models in terms of flammable mass. However, the simulations run with medium and large (PD 1.0 and 1.4) geometry, in FLACS gave flammable mass three times as high, indicating large differences in the consequence if this gas cloud will be ignited. The 0.7 value cannot be seen as a "breaking point" were the models start to deviate as not enough simulations in this range of packing density was run to strengthen this conclusion.

FLACS has thus an ability to produce gas clouds that are significantly larger than the PHAST model and is therefore considered to be more conservative than the PHAST model for the simulations performed in this report.

- **optimize gas detection layout assessment;**

Earlier mentioned small leaks in the range of 1 kg/s is the most common gas leakages mass flow rates experienced in the Norwegian oil and gas sector. Leaks of this relative small character, and up to 2-3 kg/s and below is important when considering gas detection. The focus area of the industry is now shifting towards detecting small leaks, even lower than the 1 kg/s leak. Normally alarm limits are set at 10-20 % of the LFL value, which is low concentration values compared to the ones examined in this report. The focus area is to detect the gas leakage before the gas cloud reaches a potential before it can threat the integrity of the installation called a dimensional gas cloud potential.

Today ATEX certification plays a major part in the industry due to equipment placed in hazardous zones in offshore / onshore installation must have this certification and follow electric appliances requirements. This to avoid ignition sources in hazardous classified areas. The ATEX-like leak should in this context be used. The underlying idea is that pieces of equipment have to be excluded from a given area around this type of leakage since they are challenging to detect due to limited size and extents.

How can we use the PHAST model for optimization for gas detection layout? The IP15 for area classification is sometimes uses standardized table with generic values varying with pressure range. Often, the values used have initially been calculated by using integral models. In respect of the work performed in this report a leak of ATEX-like character should be evaluated as both impinging and non-impinging by using the information extracted from the IP 15 standard. The jet must again be multiplied in every possible direction to account for all scenarios in 3D.

On the other hand, the process of gas detector layout optimization for design purposes against large leakages should always focus on the realistic scenarios development, typically the potential leak points within process area at the studied installation and subsequent dispersion patterns. Large leaks in the range of 7.0-9.5 examined in this report represents a somewhat different type of gas cloud as these cloud are significantly larger in terms of concentration spread and flammable mass than the small leaks examined. These type of leak sizes are used to establish design requirements for a facility, and is therefore considered aside from the ATEX-like leaks.

At that point, more complex dispersion patterns are expected as per seen in chapters 7 and 8 and it sounds difficult to avoid using advanced CFD modelling for this purpose.

- **Stack releases;**

Another field of interest might be the elevated stack releases where both of the tools can decently be used. This is often the release type at high elevation with different wind velocities than ground level. Both FLACS and PHAST can be used for these kind of releases, shown in chapter 5. However, if geometry will interfere with plume or wind conditions are expected below 1 m/s, some restriction in the PHAST model should be addressed. Low wind speed, below 1 m/s, may contribute to exhaust gases coming down to ground level from the stack release. This may again contribute to alarms going off, especially at nighttime when the turbulence of the ambient air is in a stable wind regime [8].

Further work;

- More extensive comparisons for congested environments to show the where the models start to deviate significantly is needed. In this report, for the large leaks the “breaking points” was seen in the area of a packing density 0.7 is FLACS. More analysis should be performed for this packing density value to support or reject this conclusion.

- In this report the flow rates examined came from the same class of containment pressure / temperature, identical input for FLACS / PHAST simulations. However, different cloud behavior can originate from different containment / stagnation conditions and this may give different physical characteristic behavior of gas leakages. A further analysis evaluating same mass flow rates for different storage conditions should be performed to see how well the results from models corresponds for a wider set of variables.

- Consequence assessments; A comparison analysis examining consequence assessments for the same scenarios should be performed for CFD / integral models. Emphasize on different consequences; Jet fire, explosion risk and other types of hazards.

- Discharge; initially some discrepancies were seen between FLACS and PHAST for discharge modeling. Some further work can therefore be valuable to do a review on the simple discharge to list and describe the simple model.

- Discharge; Analysis of the implications if having different input for dispersion from discharge modeling (effects on initial air entrainment depending on velocity).

10 Conclusion

This report describes a comparison of the CFD code FLACS and the empirical integral tool PHAST for flammable gas dispersion. Concentration profiles have been compared for methane and propane free jets with varying mass flow rates and wind conditions. Further analysis of impingement of methane jets into various congested pipework geometries in FLACS have been carried out and compared against different parameters in the PHAST model. Flammable mass comparison of the methane free and impinging jets have also been performed for the two tools.

A large scale experimental trial of the Kit Fox experiments have been simulated by both the models and compared against experimental observations.

Eventually, two realistic gas leakages with variable mass flow rate on an offshore module have been simulated and results compared for the two models.

Initial feedback from benchmarks;

A consistent result throughout the work has shown that the user defined discharge utility in PHAST must be used when comparing PHAST and FLACS for dispersion in open field. Indeed, this particular method has shown more comparable results with the FLACS model when it comes to discharge assessment and estimation of the input for dispersion modelling. Using this method to assess the source term for dispersion leads to more comparable results afterwards for both near and far field and for both concentration decay and flammable mass, as indicated by almost all the simulation batches run within the framework of this report.

Free jets with different mass flow rates and wind conditions:

For free jet releases where the two tools should compare well given the limiting assumption of a wind aligned with the release, the results presented in this report give a broad insight of the differences among the two models in the open field for concentration decay downwind the release assuming slightly varying input. The models may deviate up to a range of 50%. However, most of the simulations performed with similar source terms are within a 20% deviation for concentration profile decay for UFL, LFL and LFL_2 values of downwind concentration along the centerline. For the methane simulations the results were more comparable than for the propane results. The models compare best under circumstances where the models have a relative low external wind speed.

Overall, one can conclude that there is good agreement for methane and propane free jets for concentration decay, when the dispersion model in PHAST is used and the discharge properties are extracted from the jet utility in FLACS. This overall agreement between the models is assumed for the mass flow rates and wind criteria chosen for the simulations performed in this study.

Comparison in congested environments (Packing density compared against ground roughness);

- **Small Jets/ ATEX-like scenario:**

Jets impinging into pipework geometries gave results which indicate that the jet-size compared to the size of the impinging geometry is important, especially for small jets. The behavior of the FLACS jets simulated in this work can be divided into two extremes independent cases. The 0.59 kg/s was so small compared to the obstruction close to the leak that a complete blockage can result. The other extreme is that the jet may not impinge in any manner, displaying the jet as a free jet with equal concentration decay and flammable mass as the free jet without geometrical impingement, in the range of PHAST validity. However, depending on the location of this hypothetical release, PHAST is obviously unable to represent the occurrence of this impingement effect to the extent shown in FLACS, when using default values for the parameters within the model, (0.25 for the impingement velocity factor). When reducing this impingement value to its lowest extent the blocking effect may also to some extent also be seen in PHAST model. However, detailed evaluations regarding the impingement velocity factor value in the PHAST model was not fully performed as part of this study and will be difficult to consider on a case by case basis in an industrial application.

- **Large Jets:**

The large leakage impinging into different geometries showed throughout the FLACS simulations that the dispersion completely filled the entire domain of geometry with flammable concentration touching ground at higher concentration than PHAST for almost all cases run. The PHAST jets are smaller than FLACS for all the cases run indicating that FLACS is more conservative than the PHAST model for the scenarios run for the framework of this report.

Flammable mass comparison;

Flammable mass was compared for free methane jets and jets impinging into pipework geometries. The simulations in PHAST and FLACS indicate that PHAST will give comparable values for free jet releases if the discharge modelling in the two models are similar, jet utility in FLACS is used.

However, when accumulative effects of the geometrical objects in the flow path occur the models start to deviate both for downwind concentration and for the flammable mass calculations. The simulations performed in this report indicates that the effect of congestion may give different results in terms of flammable mass due to the complexity of interaction between plume and geometry. The local wind speeds are greatly influenced by the geometry and the dilution of gas jet is affected, and the entrainment of air into the mixture may also be lower.

For large releases the values for flammable mass using the dispersion model in PHAST together with horizontal impingement at default value of 0.25, gave perfect match when the packing density of the FLACS environment was 0.7 m/m^3. The flammable values given by the PHAST model was not comparable with the FLACS results for geometries of a packing densities at 1.0 m/m^3 and above. In terms of hazard interpretation this deviation is an important illustration of the differences between the models. However, too few discrete assumptions in the packing density were performed to see this 0.7 m/m^3 value as a “breaking point” for congestive effects between the models.

Ground roughness was used further as a parameter to see if PHAST could account for accumulative mass due to congestion. The results show that increasing ground roughness decreased the flammable mass calculations. This is contradictory to what was expected since the opposite effect was seen in FLACS. However, the intrinsic trend will highly be connected to the parameter of interest for this aspect.

Sensitivities in PHAST to account for increased congestion (assessments of concentration decay and flammable mass);

The sensitivity in PHAST was tested in order to see how some parameters could be used or “tweaked” to account for an increased congestion compared to the range of validity in open field. This was mainly done to clarify the threshold were the range of applicability is significantly violated and to see until which extent the results can be reasonably used. Some conclusions were given for dedicated parameters like ground roughness and impinged velocity factor aiming at representing these effects.

The following conclusions was extracted from the work performed;

- In PHAST the ground roughness parameter cannot be used as a means to account for pipework congestion of a given packing density in FLACS. When using the ground roughness values in PHAST compared to the packing density, the lowest value for ground roughness in PHAST gave the most comparable plumes with the FLACS model. Increasing ground roughness will reduce the flammable mass in the calculations in PHAST. In FLACS the opposite effect was seen to a certain extent (increased pipework congestion – increased flammable mass). However, the ground roughness value in PHAST does have a large impact on the dispersion profiles / spreading lengths.

- The wind criteria is important for ground roughness. When simulating at higher external wind velocities the effect on concentration decay form ground roughness was higher.

- Assuming a horizontal impingement in the PHAST model (resulting in a simple velocity decay) this changes the appearance of the jet and makes the jet more buoyant. The flammable mass values also increase significantly compared to a free jet in PHAST. However, the values seen for flammable mass was significantly lower than the values seen in FLACS for medium and high packing density values for the large leakage rate, indicating widely different risk assessments. For the small jet the differences between FLACS and PHAST in terms of flammable mass may not overall contribute to large deviation in the risk assessments. However, this was not fully examined in detail as part of this work.

Final remarks;

Eventually, 500 PHAST calculations and 100 FLACS simulations have been performed during this thesis.

The analysis results in the following main conclusions:

1. Discharge modeling is critical and a particular attention must be paid to it to achieve comparable results between CFD compared to integral models.
2. PHAST and empirical models have usually a limited range of validity for dispersion modelling compared to FLACS / CFD models due to limitation in supported wind velocities, limitations in wind orientations compared to leakages and lack of accuracy to handle obstacles and real geometries.
3. However, FLACS and PHAST compare relatively well together for leakages when both tools used in their range of applicability – ensuring that the discharge modelling and dispersion input are aligned within the two tools. FLACS and PHAST results have also even been satisfactory evaluated against experimental large scale trials in the open field.
4. The FLACS model develops larger plumes in terms of downwind concentration / crosswind spread and local effects of congestion can give results that will interact with more ignition sources than expected in the PHAST model, thereby giving a higher explosion probability / risk.
5. When it comes to introduce the influence of geometry and deviate from the range of applicability of PHAST in this field:
    a. The relative size leak compared to the congestion is of importance. Small and large leaks show different behavior cloud behavior in interaction with geometry.
    b. Ground roughness cannot be used to represent real congestion that is represented in a CFD model.
    c. Recommendations are that PHAST can only be used preliminary for small leaks within congested environments and that results in the ATEX-range is multiplied is every possible direction to account for all scenarios.

More generally, when performing the work with this thesis a significant experience has been gained in understanding the mechanism of gas dispersion and industrial hazards in general. The use of two recognized and worldwide used consequence assessment tools has permitted to gain some insight over the practicalities of consequence assessments, of models, assumptions and limitations.

Underestimating size of gas cloud size something that should not be dealt with lightly. The simulations performed during this work have indicated that the PHAST model represents the same dispersion phenomena as the FLACS model with smaller plumes and also significant lower flammable mass in congested environments. This report has not gone into the depth regarding the risk assumptions connected to this. However, this should be known to the modeler of flammable gas dispersion when using the PHAST model as a substitute for a CFD model. Failing to estimate correct dimensioning gas cloud may again contribute to unsafe design.

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27 *www.gov.uk; Buncefield; Why did it happen? The underlying causes of the explosion and fire at the Buncefield oil storage depot*, Hemel Hempstead, Hertfordshire on 11 December 2005; Report referenced 4.2.2014.