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Safe hydrogen injection management at network-wide level: towards European gas sector transition

Shimmer

Safe Hydrogen Injection Modelling and Management for European gas network Resilience

D3.7 On the implication of subsea dispersion on overall risk assessment of severe H2 releases

VERSION	DATE	TYPE	DISSEMINATION LEVEL
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ABSTRACT

A modelling framework has been developed to assess the dispersion and dissolution of a bubble plume rising through the water column from an underwater gas leak. This approach is designed for multicomponent gases and forms a key part of a broader risk assessment for underwater gas releases. The study also outlines a general guideline for evaluating such risks. The methodology is applied to underwater releases involving hydrogen and hydrogen-natural gas blends. Findings indicate that the risk of fire, explosions, and increased hydrodynamic loads at the surface escalates with higher hydrogen content.

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Table of contents

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List of Abbreviations

Table 1: List of abbreviations

Term	Explanation
API	Application Programming Interface
CFD	Computational fluid dynamics
HDF5	Hierarchical Data Format version 5
HHV	Higher heating value
NG	Natural gas
LFL	Lower flammability limit
UFL	Upper flammability limit
LEL	Lower explosion limit
UEL	Upper explosion limit
T&D	Transport and distribution
QRA	Quantitative risk assessment

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Executive Summary

This report examines the safety implications of underwater gas leaks, also known as subsea gas releases, from faulty equipment, ruptured or damaged seabed pipelines transporting hydrogen or hydrogen-natural gas blends. Such leaks result in bubble plumes rising to the surface, posing safety risks that vary depending on the characteristics of the gas. These risks include fire, explosion, asphyxiation, and severe hydrodynamic loads on surface vessels.

A thorough safety assessment involves analysing factors such as estimating the gas release rate and duration, modelling the dispersion and dissolution of gas bubbles within the ocean column, how the gas surfaces, and evaluating atmospheric dispersion due to wind. This report focuses primarily on the behaviour of hydrogen and hydrogen-natural gas mixtures as they disperse in the water column and how they surface. These findings define the starting point for traditional atmospheric dispersion modelling which is part of established quantitative risk assessments (QRA) methodologies.

To support this assessment, a numerical model originally developed for single-component gases like methane and carbon dioxide was extended to accommodate multicomponent gas mixtures, including hydrogen and hydrogen-natural gas blends. The model is used to evaluate safety risks as hydrogen is increasingly introduced into existing natural gas pipeline systems. *Compared to methane, hydrogen is lighter, less soluble, more combustible, and easier to ignite*.

The analysis indicates that higher hydrogen content results in a more rapid plume ascent to the surface, increased combustion potential at the surface, and elevated hydrodynamic loads on nearby vessels. As a result, overall safety risks escalate with rising hydrogen concentrations.

This report documents Deliverable D3.7 *On the implication of subsea dispersion on overall risk assessment of severe H2 releases* in the SHIMMER project.

About the project: The European natural gas infrastructure provides the opportunity to accept hydrogen (H_2), as a measure to integrate low-carbon gases while leveraging the existing gas network and contributing to decarbonisation. However, there are technical and regulatory gaps that should be closed, adaptations and investments to be made to ensure that multi-gas networks across Europe will be able to operate in a reliable and safe way while providing a highly controllable gas quality and required energy demand. Aspects such as material integrity of pipelines and components, as well as the lack of harmonisation of gas quality requirements at European level must be addressed to facilitate the injection of H_2 in the natural gas network.

In this context, the SHIMMER project (Safe Hydrogen Injection Modelling and Management for European gas network Resilience) was selected for funding as part of the 2023 Clean Hydrogen Partnership programme. SHIMMER aims to enable a higher integration of low-carbon gases and safer H_2 injection management in multi-gas networks by strengthening the knowledge base and improving the understanding of risks and opportunities in H_2 projects.

It will do this by:

- Mapping and assessing European gas T&D infrastructure in relation to materials, components, technology, and their readiness for hydrogen blends.
- Defining methods, tools and technologies for multi-gas network management and quality tracking, including simulation, prediction, and safe management of network operation in view of widespread hydrogen injection in a European-wide context.
- Proposing best practice guidelines for handling the safety of hydrogen in the natural gas infrastructure and managing the risks.

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1 Introduction

1.1 Purpose of the document

This report addresses safety issues related to subsea release of hydrogen and hydrogen blends originating from punctured or ruptured pipelines at the ocean floor. Since hydrogen and natural gas can cause fire and explosions, operations in the vicinity of releases and leaks need to follow strict safety guidelines. These guidelines should be based on relevant and reliable quantitative data. A protocol on how to obtain such data is outlined in this report and special focus is given to the analysis related to the impact of gas dispersion and dissolution in the ocean.

1.2 Authorship and Intellectual Property Rights (IPR)

Key Results	**Asset (IP)**	**IPR Principle**	**Primary Exploitation Partner**	**Secondary Exploitation Partner**
Mathematical framework to assess dispersion and dissolution of bubble plumes of hydrogen blends resulting from subsea release of gas from damaged pipelines.	Adapted computational libraries to the SURE framework (SINTEF background) to account for multicomponent gases including hydrogen blends	Closed software library owned by SINTEF	SINTEF	
Risk guidelines and assessment of selected release scenarios	Qualitative and quantitative results	Open report and publication	SINTEF	ALL PARTNERS

1.3 Intended readership

The methods developed and results obtained should be of interest to pipeline operators, regulatory bodies, company personnel in charge of QRA and safety consultants performing or advising companies with respect to QRA, safety measures and emergency response planning and preparedness.

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2 Risk assessment of subsea release of H_2 blends

Pipeline transport of hydrogen is an integral part of the value chain for adopting hydrogen as an energy carrier in the green transition. Utilizing existing infrastructure for natural gas will enable a more rapid transition. However, this infrastructure is subject to material degradation when exposed to hydrogen. A mitigating action is to transport a blend of hydrogen and natural gas [1], [2]. This is subject to high risks if there is any damage to the pipeline infrastructure. Risks associated with leaks of hydrogen is related to fire and explosion and most incidents are related to pipelines [3]. This is also true for blends of hydrogen and natural gas which are both combustible gases. The risk is often assessed by estimating the concentration of these combustible components and oxygen.

In large scale production and transport of hydrogen, some of the transport will be in pipelines at the ocean floor. If there is considerable damage to the pipelines resulting in a partial or full-bore rupture, a significant amount of gas will be released into the ocean. This will rise towards the surface as a bubble plume. Some of the gas will be dissolved in the ocean and some will reach the surface and enter the atmosphere. This poses a threat to life and infrastructure at the surface since the gas can ignite if the concentrations are in flammable ranges. Thus, quantitative risk assessment needs to be performed for potential scenarios where gas might reach the surface. A vital step and output of a quantitative risk assessment is an estimate of the concentration of and distribution of harmful gases in the atmosphere.

The quantification of potential gas concentrations in the atmosphere is the final outcome of a multi-step analytical process. The step associated with the greatest uncertainty involves how the gas disperses and dissolves within the water column and subsequently reaches the surface. This work focuses primarily on assessing gas behaviour within the water column but also provides general guidance on estimating atmospheric gas concentrations and incorporating these estimates into a risk assessment framework.

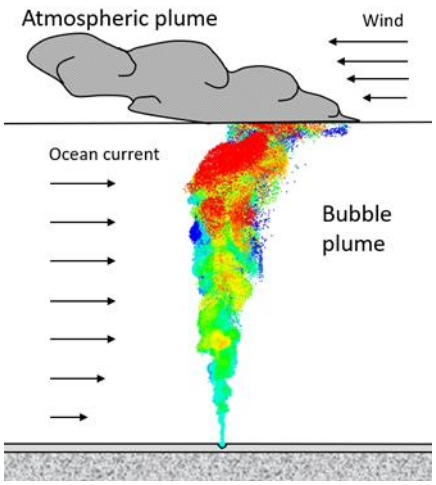

Figure 1: Underwater gas release.

2.1 Guideline for risk assessment

A risk assessment related to a subsea release of gas is often applied to assess the immediate danger for personnel and assets in the proximity of the release or to assess if an intervention operation to repair the damaged pipeline or evacuate staff is safe. This is among others based on assumed values of concentration of potential harmful gas. The emergency response is greatly enhanced if reliable estimates of gas concentrations are available. These can be estimated based on the following protocol:

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1) Identify release parameters including pipeline configuration, depth, oceanography and wind
2) Calculate release rate and duration of release
3) Calculate dispersion and dissolution of bubble plume in the ocean and how the gas surfaces
4) Calculate atmospheric dispersion giving concentrations of gases and resulting safety distances

This protocol is applicable to all gases. For hydrogen and hydrogen-natural gas blends (H2-NG blends) specific details on material properties are needed. Some details on each of the analyses steps are given in the following sub-chapters.

2.1.1 Release rate

The release rate is a vital input to further analysis of the scenario being assessed. The release rate is affected by pipeline characteristics such as inner diameter, pipeline length (or distance to nearest block valve), size of rupture/damage, line pressure and gas temperature. It is governed by gas dynamics and compressible flow and is often calculated by commercial flow assurance software such as LedaFlow[1] or Olga[2] which are designed to handle a much broader spectre of flow assurance issues. Some special purpose in-house codes are also applied to this.

The release is driven by the difference between the line pressure and the exterior pressure (i.e. ocean depth). As gas is released, the line pressure and the driving force decreases. Thus, the release rate is transient and decreases with time. Still, a constant release rate is often applied. This can either be caused by the lack of transient capabilities in software applied in the subsequent analysis or computational cost of assessing a very long-lasting release with a slow decay. When applying a constant release rate, it is necessary to assess which rate is most relevant for the operation to be risk assessed.

The release rate can be specified as a volumetric rate or a mass rate. A mass rate (e.g. kg/s) is more consistent since a volumetric rate also need a definition linking it to a density of the released gas.

2.1.2 Subsea dispersion

When gas is released from an underwater gas pipeline, gas well or some other underwater reservoir of gas, the gas will ascend in the water column as bubbles. Some of these releases are very small (i.e. leaks) resulting in a trail of individual bubbles rising towards the ocean surface – a bubble train. For more severe releases, the gas will rise as a cloud of bubbles – a bubble plume. The severe releases are those which causes a safety risk and are the focus of this study.

This can be assessed either with classical integral models for buoyancy driven plumes or by computational fluid dynamics (CFD). The integral models (e.g. [4], [5], [6]) assume a flow profile (often Gaussian) and operate at a low computational cost. Integral models are built on some assumptions that introduce tuneable parameters that are difficult to justify or validate. CFD (e.g. [7], [8], [9]) is based on fewer assumptions, but has a much higher computational cost.

The most important input variables to the subsea dispersion analysis is the gas composition, ocean depth of the release and the release rate. Other important input parameters are related to the state of the ocean e.g., profiles of temperature, salinity, ocean currents and to some extent dissolved gas components already present in the ocean water. Output from this analysis include:

- Rise time (time available to move surface vessels if an incident is discovered immediately)
- Surface flux of gas (input to atmospheric dispersion)
- Induced surface ocean velocities (impact on hydrodynamic loads)
- Fountain height

[1] https://ledaflow.com/
[2] https://www.slb.com/products-and-services/delivering-digital-at-scale/software/olga

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The authors have developed a CFD model to assess this for either CH_4 or CO_2 [9]. This was implemented as a series of user-defined-function in the commercial software ANSYS/Fluent. To assess underwater release of H_2 and H_2-NG blends, the modelling concept needed to be further developed to account for multicomponent gases and to include material properties for H_2. Ideally the model should also be made more available within an Open-Source-framework. An Open-Source approach was assessed using OpenFoam. It was concluded that this could be achieved, but not within the budget and time allocated for the task in the project. The OpenFoam assessment is documented in Appendix B. This can be explored further within a future project. Instead of adopting an OpenSource approach, the modelling concept linked to the commercial software was enhanced to include the above-mentioned features. This is documented in Appendix A.

The results from the subsea dispersion and gas surfacing analysis need to be exported in a format which can be imported as a boundary condition for the atmospheric dispersion analysis. This can be done by defining a file format or using a standard format which both the subsea dispersion code and atmospheric dispersion code is compatible with. An alternative is to report Gaussian parameters. It should however be noted that the true surface flux is not a perfect Gaussian. Due to the turbulent nature of the bubble plumes the surface flux varies with time and some kind of time averaging is needed. Time averaging over shorter times captures more of the dynamics while longer time averaging brings the profile closer to a Gaussian profile as seen in Figure 2. Short time averaging also captures local high peaks in the surface flux, but will require a series of consecutive fluxes to be exported to and imported into atmospheric dispersion analysis. If they are exported as Gaussian profiles, they should be exported relative to centre of mass defined by the surface flux of the respective time incident. Long time averaging will naturally move the centre of mass back to the centre of the release but not capture the maximum peaks of surface fluxes. It is more convenient to apply long time averaging and historically that is what has been applied. A sensitivity study on this choice has not been performed, neither conducted by others according to the authors knowledge.

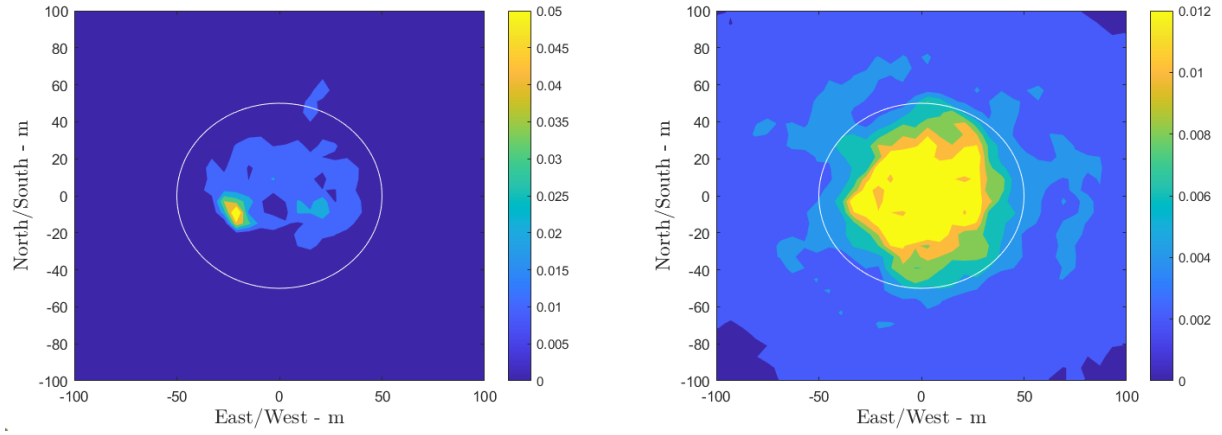

Figure 2: Surface flux (kg/m^{2}s) of H_2 averaged over 10 secs (left) and 100 secs (right) for a release of 106 kg/s from 300 m.

2.1.3 Atmospheric dispersion

As the gas enters the atmosphere it will be dispersed by wind. It will also tend to rise upwards due to buoyancy if the gas is lighter than air (e.g. NG, H2) or settle on the water surface if the gas is heavier than air (e.g. CO2). Wind, atmospheric stability, material properties (buoyancy) and amount of gas entering the atmosphere (surface flux) thus determines the concentration of the surfacing gas in the atmosphere. The wake formed by vessels or assets at the surface also influence the gas dispersion and should be included if they are close to the release. The concentration determines the risk for fire and explosions.

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Dispersion can be calculated by multipurpose CFD software, either commercial (e.g. ANSYS/Fluent, CFX, Star-CCM+) or open source (e.g. OpenFoam) or by special purpose software such as KFX[3] or FLACS[4] for explosion, fire and dispersion modelling. They will report the concentration of the surfaced gas in a geometrical domain in the proximity of the release source. Based on this the extent of the domain which falls between the lower flammability limit (LFL) and upper flammability limit (UFL) can be reported. Similar can be done for explosion limits (LEL and UEL) and asphyxiation limits.

2.1.4 Risk assessment

If a pipeline has ruptured there might be a need to evacuate personnel in the vicinity of the release and/or to repair the infrastructure. Such operations will require risk assessments to verify the safety of such intervention operations. Also, operations above subsea infrastructure with a possibility of dropped object which can damage the infrastructure should perform a risk assessment linked to potential underwater gas release. A comprehensive risk assessment will require input from the above analysis and apply it to estimate

- the regions between LFL and UFL and LEL and UEL to define exclusion zones,
- the rise time of the plumes to define how long time there is to evacuate and/or shut down all potential ignition sources,
- the duration of the release, thus the total time of possible exposure.

The risk assessment requires export of data between each of the above analyses. While each of these analyses have been thoroughly studied and explored, there are no standards for exporting data between them. This should be clarified, particularly for the data transfer from the subsea dispersion analysis to the atmospheric dispersion analysis.There exists one API between the present modelling framework in ANSYS/Fluent and KFX, the format is built on the open HDF5 file format standard.

2.2 Assessment of H2 and H2-NG blends

The above guideline on how to assess risk for an underwater gas release was developed for natural gas. Incidents with release of natural gas caused a series of studies on the topic [10]. Driven by the green transition, the potential for large-scale subsea pipeline transport of CO_2 and H_2 has increasingly come into focus. H_2-NG blends are also part of this potential scenario. In principle the same protocol and analyses should be applied for H_2-NG blends with updated material properties. A significant difference is that H_2-NG blends constitute a multicomponent gas mixture. In principle natural gas alone is also a multicomponent gas mixture, but due to the high amount of CH_4 in natural gas, it has often been assumed as a single component gas. The analysis of a multicomponent gas becomes more complicated. E.g. some commonly used risk criteria's are based on the concentration of a single gas component.

When comparing the properties of H_2 and CH_4 as listed in Table 2, we see that H_2 is a much lighter gas than CH_4. The mass-based heating values is higher, and the volume-based heating value is lower. When analysing release from a pipeline where the content is shifted from pure CH_4 to pure H_2 without changing the line pressure, it is seen that the volumetric release rate increases, and the mass-based release rate decreases with increasing H_2 content. The released higher heating value is still roughly the same. This is documented in Appendix A. Since H_2 is less soluble in water than CH_4, less H_2 will dissolve in the ocean and thus the surfacing gas has a higher heating value when surfacing. It will also surface faster since H_2 is lighter and thus more buoyant. This indicates that the risk increases as the H_2 content increase in the pipeline.

[3] https://www.dnv.com/software/services/plant/kfx-computational-fluid-dynamics-cfd-simulation-software-for-fires-and-dispersions/
[4] https://www.gexcon.com/software/flacs-cfd/

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Table 2: Properties for methane and hydrogen

	CH_4	H_2
Molecular weight – g/mol	16.04	2.01
Density (STP) – kg/Nm^3	0.717	0.0899
Higher heating value – MJ/kg	55.5	141.8
Higher heating value – kWh/Nm^3	11.05	3.54

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3 Conclusions and further work

A modelling concept on how to assess dispersion and dissolution of a bubble plume migrating upwards in the water column from an underwater gas leak has been developed for a multicomponent gas. This is a vital analysis in a set of several analyses for quantitative risk assessment of an underwater gas releases. An overall guideline for assessing risk is also outlined. This is applied to underwater releases of hydrogen and hydrogen-natural gas blends. The study demonstrates that the risk for fire, explosions, and higher hydrodynamic loads on the surface increases with increasing hydrogen content.

Additional work should be pursued. This includes how to export data from the subsea dispersion analysis to the atmospheric dispersion analysis. No systematic studies exist on how the time averaging of the surface flux should be performed. How does the Gaussian profile fitting and time averaging influence the estimated risk? This should be clarified.

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A Appendix A - Underwater release of hydrogen-natural gas blends

Manuscript as submitted to International Journal of Hydrogen Energy

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The transport of hydrogen and hydrogen-natural gas blends through subsea pipelines introduces significant safety risks in the event of pipeline damage or rupture. Such incidents can lead to the release of gas, forming a bubble plume that ascends to the ocean surface. Elevated surface concentrations of hydrogen and hydrogen-natural gas may pose serious hazards to life and infrastructure. Risk assessments typically involve a sequence of analyses, with gas migration and dissolution in the marine environment representing the greatest source of uncertainty. This study presents a transient, three-dimensional computational fluid dynamics model developed to quantify the surfacing gas volume, its composition, and spatio-temporal distribution for a multicomponent gas. The model aims to improve the accuracy of quantitative risk assessment related to subsea hydrogen transport.

INTRODUCTION

Hydrogen is an attractive energy carrier for the green transition. The distribution of hydrogen through pipelines is partly envisaged in existing infrastructure for natural gas. This might save costs but has a negative impact on material integrity due to steel embrittlement and more. A compromise is to transport a blend of hydrogen and natural gas [1], [2]. While this reduces the risk of failure due to material degradation, leaks and pipeline ruptures may still occur due to external factors. This can potentially result in fatal incidents related to hydrogen's flammability, explosiveness and asphyxiation characteristics. Hydrogen has been the cause of many incidents and fatalities, and most of these are related to piping and pipelines [3].

The large-scale production of hydrogen will require corresponding large-scale transport solutions, including the likely use of subsea pipelines for part of the distribution network. If a pipeline is damaged such that a hole, crack or full bore opening releases gas, the gas will rise to the surface due to buoyancy. At substantial release rates, the gas ascends as a bubble plume, undergoing dispersion and dissolution in the water column. Upon reaching the atmosphere, it is subject to wind-driven dispersion. This process is illustrated in Figure 3. The resulting atmospheric concentration of hydrogen—or a hydrogen-natural gas blend—determines the associated risk potential.

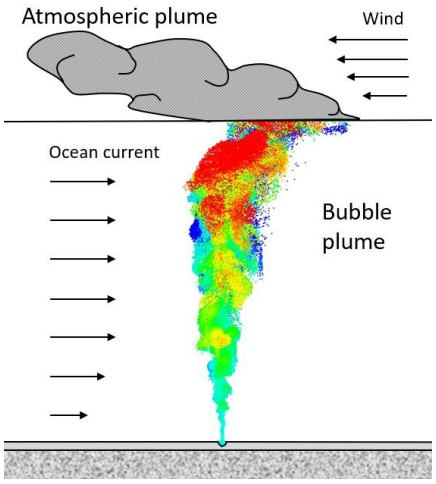

Figure 3: Underwater release with bubble plume and atmospheric plume

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Assessing safety and risks associated with underwater release of hydrogen or hydrogen blends rely on quantitative input from several analysis. This includes predictions on how the gas migrates and dissolves in the ocean before it reaches the surface and how the gas is dispersed into the atmosphere. This has historically been studied for release of methane and natural gas in relation to risks in natural gas extraction and export. Modelling approaches initially focused on so-called integral models which assume a profile, either Gaussian or top-hat, for the velocity and bubble volume fraction [4], [5], [6], [11]. More recently full three dimensional CFD (computational fluid dynamics) models have also been applied [7], [8], [9].

For pure hydrogen transport, existing models for methane and natural gas can be applied by replacing material properties for methane with hydrogen. However, many plans for hydrogen transport are based on using existing infrastructure for natural gas. As mentioned above, these pipelines are envisaged to transport a blend of hydrogen and natural gas. This necessitates mathematical models accounting for gas bubbles consisting of multiple species. If that capability is in place, it will also be worthwhile to account for stripping of oxygen and nitrogen from the ocean to the bubbles. Oxygen and nitrogen are present in the ocean due its large interface with the atmosphere and biological processes producing nitrogen. This can potentially affect the composition of the bubbles entering the atmosphere.

To address the abovementioned challenge a mathematical modelling framework based on CFD [9] has been modified from tracking single component gas to tracking multicomponent gas bubbles. Material properties of hydrogen, nitrogen and oxygen have been added. The modified framework has been applied to study the fate of underwater release of hydrogen blends.

MATHEMATICAL MODELLING FRAMEWORK

Conservation of mass, momentum and energy governs the evolution of composition, motion and temperature of bubbles and nearby ocean waters. This is expressed mathematically by conservation laws. Here we apply an Eulerian-Lagrangian CFD model developed by Cloete et.al.[7] and enhanced by Olsen & Skjetne [9] including gas dissolution and a VLES turbulence model. The bubbles are tracked in a Lagrangian framework in which Newton's second law provides a force balance on the bubbles. This is mathematically expressed by

$$\frac{d\vec{u}_b}{dt} = \frac{\vec{g}(\rho_b - \rho_w)}{\rho_b} + \vec{F}_D + \vec{F}_{VM} \qquad \text{Eq.(1)}$$

Here $\vec{u}_b$ is bubble velocity, $\vec{g}$ is gravity, ρ_b is bubble density, ρ_w is local sea water density, and $\vec{F}_D$ and $\vec{F}_{VM}$ represent drag force and virtual mass force. The first term on the right-hand side represents buoyancy. The drag force between bubbles and ocean water is given by

$$\vec{F}_D = \frac{18\mu}{\rho_b d_b^2}\frac{C_D \mathrm{Re}}{24}(\vec{u}_w - \vec{u}_b) \qquad \text{Eq.(2)}$$

where C_D is drag coefficient, Re is Reynolds number, d_b is bubble diameter and u_w is local velocity of ocean water. Since the drag force includes a velocity difference between bubble velocity and local ocean velocity, the bubble motion is coupled to the ocean velocity. The ocean velocity is also governed by conservation of momentum. This is mathematically expressed in an Eulerian framework by the Navier-Stokes equation also

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including a drag term coupling back to the bubble velocity. This ensures a two-way coupling between bubbles and ocean water. Further details, including turbulence model and bubble size are given by Olsen & Skjetne [9]. Energy is also exchanged between bubbles and ocean since bubbles might be released at a different temperature than the temperature of the ocean water. This is calculated by equations conserving energy for bubbles and ocean water resulting in a temperature field.

The temperature field affects material properties important to motion and mass transfer.

Mass transfer or gas dissolution is driven by the ocean's ability to dissolve gas species. For many relevant gas components gas dissolution in water is significant. The earlier versions of this framework only accounted for a single gas component. Assessment of multicomponent gases thus requires an enhanced mathematical framework. Mass transfer from a gas bubble to the surrounding ocean is limited by the diffusion and convection of species on the liquid side of the interface. The mass transfer rate $\dot{m}_i$ of species i, can be expressed by the Ranz-Marshall equation [12]

$$\dot{m}_i = \pi d_b^2 \, k_i \left(c_i^{sol} - c_i^w\right) \quad \text{Eq.(3)}$$

Here $d_b$is the bubble diameter, k_i is the mass transfer coefficient, c_i^{sol} is solubility of species i in the ocean and c_i^w is the local concentration of the species in the ocean. If the bubble consists of multiple species of gas it is important to apply the partial pressure p_i of the species in question when extracting the solubility

$$c_i^{sol} = c_i^{sol}(p_i, T) \quad \text{Eq.(4)}$$

It is assumed that the fugacity coefficient of a species in a mixture is equivalent to that of the species by itself. The partial pressure is given by the molar fraction x_i or the mass fraction Y_i of species i in the gas bubble

$$p_i = x_i P = \frac{Y_i/M_i}{\sum Y_k/M_k} P \quad \text{Eq.(5)}$$

where P is local total pressure and M_i is the molar weight of species i. The generalisation to a multicomponent gas is primarily given by the use of partial pressure instead of total pressure in Eq.(4). In addition, the updated mass of a bubble now involves a sum of the contribution from all species expressed by

$$m_{i,j} = m_{i,j-1} + dt \dot{\cdot} m_{i,j-1} \quad \text{Eq.(6)}$$

where j indicates timestep number and dt indicates the numerical timestep. The total mass of a bubble is the sum of the mass of each species within the bubble

$$m_j = \sum_i m_{i,j} \quad \text{Eq.(7)}$$

At the end of each timestep the molar fractions are updated according to

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$$x_{i,j} = \frac{m_{i,j}/M_i}{\sum m_{i,j,k}/M_k} \qquad \text{Eq.(8)}$$

It should be noted that a modification of the code architecture is needed when tracking *n* species instead of one. This also adds a substantial larger set of material properties.

Material properties

Gas properties which affect the fate of the bubble plume are primarily density, solubility and diffusivity. Gas viscosity only has a minor impact on bubble size and is given by Wilke's equation [13] for a gas mixture. The density of the gas species involved directly affects the buoyancy of the gas. It is assumed to be represented by an ideal gas. In reality this assumption is not adequate for higher pressures typically at depths of 300 meters and deeper as seen in Figure 4. For this comparative study, this assumption is acceptable. The density of the multicomponent gas (gas mixture) is the sum of all gas species weighted by their molar fraction

$$\rho = \sum_i x_i \rho_i = \sum_i \frac{x_i P M_i}{RT} \qquad \text{Eq.(9)}$$

Here the assumption of ideal gas has been applied in the last expression. This can be modified to account for real gases.

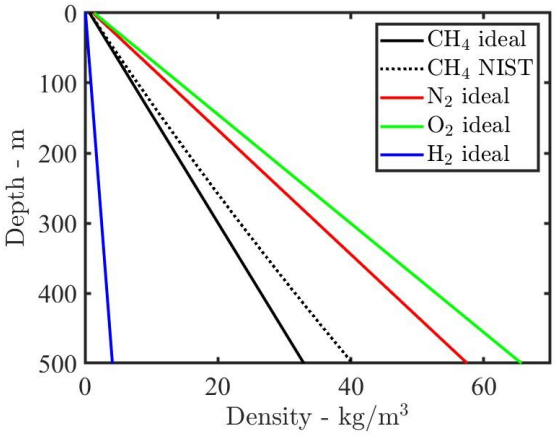

Figure 4: Gas density as function of depth at 5°C for ideal gas and proper data from NIST for CH_4.

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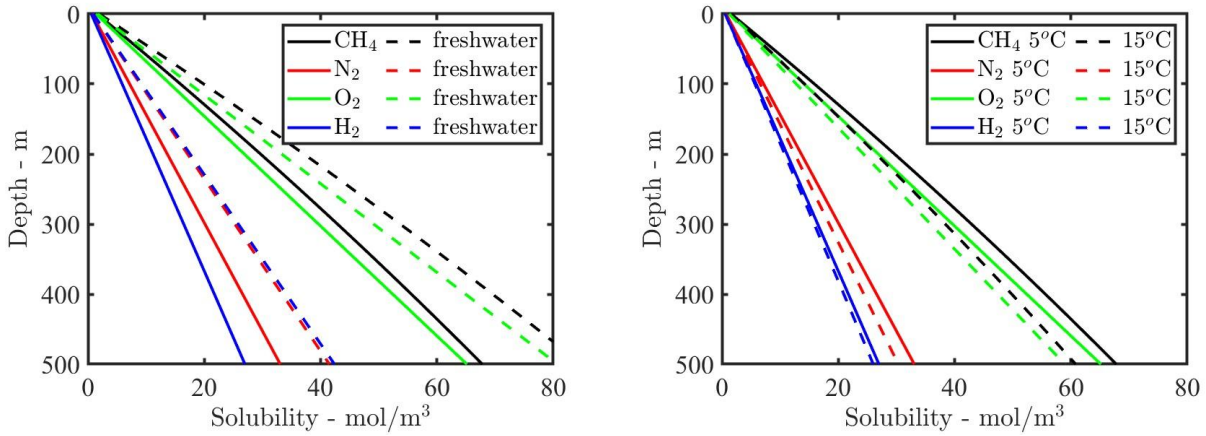

Figure 5: Solubility for CH_4, N_2, O_2 and H_2 as function of depth at 5ºC for a salinity of 30 PSU. Left plot compares with freshwater values. Right plot compares with higher ocean temperature.

As seen from Eq.(3), solubility governs how much of the released gas can be dissolved in the ocean. It varies with temperature, pressure and salinity. For hydrogen and methane we apply the correlations derived by Wiesenburg & Guinasso [14]. For nitrogen and oxygen we apply the correlations for pure water (freshwater) from Perry's handbook [15] corrected for salinity according to Hamme & Emerson [16] and Garcia & Gordon [17] for nitrogen and oxygen, respectively. Plots of solubility as functions of ocean depth (i.e. pressure) is seen in Figure 5. Methane has the highest solubility and hydrogen the lowest of the four species. Solubility decreases with increasing salinity and temperature. It increases with pressure i.e., ocean depth.

Diffusivity affects the transport of species away from the bubble interface. The mass transfer coefficient which is part of Eq.(3) is a function of the diffusivity of the species in focus. The correlation for diffusivity favoured by Hayduk & Laudie [18] is applied. This was derived by Othmer & Thakar [19] and revised to

$$D_i = \frac{13.26 \cdot 10^{-5}}{\mu_w^{1.4} V_i^{0.589}} \qquad \text{Eq.(10)}$$

where D_i is the diffusivity (cm^2/s) of species i, μ_w is the viscosity (cP) of the sea water and V_i is the molar volume of the species.

Model implementation

The mathematical model is implemented as a library of *user-defined-functions* specially developed to capture the governing physics outlined above and in the work of Olsen & Skjetne [9]. This library is linked to the commercial CFD code ANSYS/Fluent which handles the numerical methods and model simulations. In ANSYS/Fluent a VOF (volume of fluid) method is applied to track the interface between ocean and atmosphere, tracking of multiple species is activated and the energy equation is enabled to solve for temperature. As mentioned above, this is coupled to parcel based tracking of bubbles.

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The library of *user-defined-functions* includes macros for drag, mass transfer, turbulence, bubble size and removal of bubbles entering the atmosphere. Functions for material properties are also an integral part of the library. All details implemented in these libraries are documented above and/or in previously published work [9].

Model validation

For a mathematical framework to be applied to quantitative risk assessment (QRA), it is critical that the framework is trustworthy. This is done by validating model results with relevant observations. While many experiments have been performed, most of these are in a lab with small scales or in the ocean with very small release rates [10]. Some of these experiments are more relevant than others and the preceding version of the modelling framework has been compared against the observations in these experiments and shown to be consistent [9]. The updated version documented above has been compared to observations of a controlled 17 kg/s of natural gas release from a depth of 138 m through a valve with an effective opening of 1 inch. This release was linked to a pigging operation for which a release permit was obtained to conduct a field experiment.

By using this scenario as a validation case and a test on how gas composition affects the behaviour, a series of case studies was conducted. When comparing different gas compositions, it is also important to define how the release rate is specified. This could involve using a consistent total mass flow rate or a consistent volumetric flow rate across all scenarios. Here we have chosen to keep the pipeline operating conditions similar for all scenarios since the study is motivated by safety if hydrogen and hydrogen blends are transported in existing pipelines for natural gas. These are then assumed to be transported under the same conditions as methane (natural gas) with the same pipeline dimensions and same pipeline pressure. With a pipeline pressure of 160 bara and a release valve with an opening of 1 inch, the release conditions are as listed in Table 3. The release rate varies with hydrogen fraction in the gas blend. Due to the narrow release valve, the release rate is dictated by release area, compressibility and the speed of sound of the gas mixture, i.e. choked flow.

Table 3: Release rates and conditions for test pipe

Hydrogen content		Release density	Volumetric release rate	Mass release rate
Molar fraction	Mass fraction	kg/m^3	m^3/s	kg/s
0.00	0.00	10.4	1.64	17.00
0.50	0.11	5.9	3.21	18.77
0.89	0.50	2.3	4.44	10.26
1.00	1.00	1.3	4.79	6.22

These scenarios were assessed by running numerical simulations with the model described above. Some of the results are seen in Figure 6 and Figure 7. Figure 6 shows how fast the front of the plume travels towards the

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surface. It is seen that gas composition affects the rise time of the plume. Hydrogen is lighter than methane. This makes hydrogen more buoyant. There is also a distinct difference between a blend of 50% mol H_2 and 50% mass H_2. Thus, it is important to specify the unit of how the gas blending or gas composition is defined. This is illustrated by Figure 7.

It also seems that the model is consistent with the observed evolution of the plume front. This provides some validation for the model. The earlier version of the model has also been tested against several other observations and experiments with air and methane [9] and shown to be reliable. No experiments have been performed with hydrogen or hydrogen blends to the authors knowledge. Ideally the model should be compared against such experiments. However, it should be noted that assessments of potential natural gas incidents have historically been based on models validated by experiments on air bubbles.

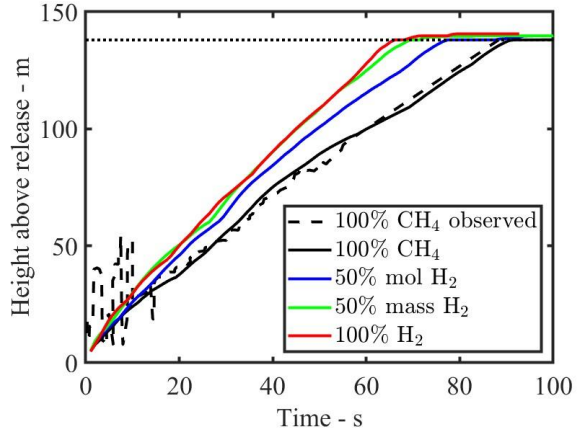

Figure 6: Model predictions of plume rise as function of time for various gas blends compared to observations on a release of CH4

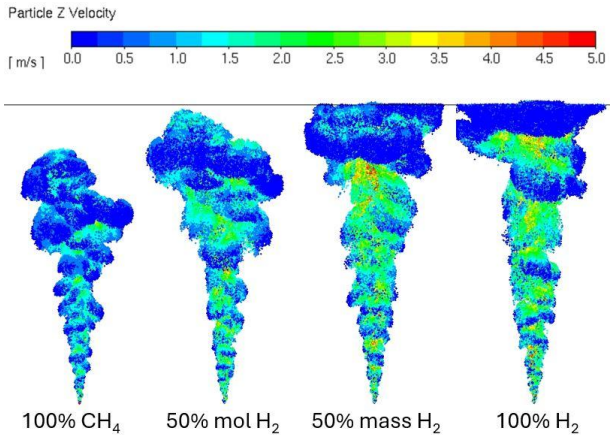

Figure 7: Bubble plumes for various gas blends 75 secs after initiation of release coloured by bubble vertical velocity.

CASE STUDY ON EXPORT LINE

The modelling framework described above can be applied to assess realistic release scenarios. Again, we focus on comparing releases of different gas blends based on similar pipeline operating conditions. The reference is a pipeline releasing 300 kg/s of methane from 300 meters in a typical export pipe with a 4-inch release area, e.g., from a faulty subsea valve or resulting from an unintended impact. This is not an initial release rate but is representative for a typical release rate when the pressure in the pipeline is around 100 bara and possible interventions may be underway. The calculated release scenarios are seen in Table 4.The trend is that the mass rate decreases with increasing hydrogen content and the volumetric rate increases. The higher heating value (HHV) is the upper limit of the available thermal energy output by complete combustion. This is higher for hydrogen (141.8 MJ/kg) than methane (55.5 MJ/kg). Due to the higher value for hydrogen, the HHV of the release varies little even if the total release rate decreases with increasing hydrogen content.

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Table 4: Release rates, conditions for pipeline rupture and surfacing results.

Hydrogen content		Release density	Volumetric release rate	Mass release rate	Buoyancy release flux	Release HHV	Rise time	Surface flux	Dis-solution	Top HHV	Surface velocity
% mol	% kg	kg/m^3	m^3/s	kg/s	m^3/s^4	GJ/s	s	kg/s	%	GJ/s	m/s
0.0	0.00	21.7	13.8	300.0	6279	16.65	139.8	127.4	57.6	7.05	4.74
4.0	0.01	21.0	14.0	294.7	6628	16.49	120.7	134.2	54.6	7.53	4.76
50.0	0.11	12.2	18.4	225.0	15018	14.65	128.7	126.5	43.8	8.59	5.45
100.0	1.00	2.7	39.0	106.2	144221	15.06	87.0	84.6	20.2	12.01	6.58

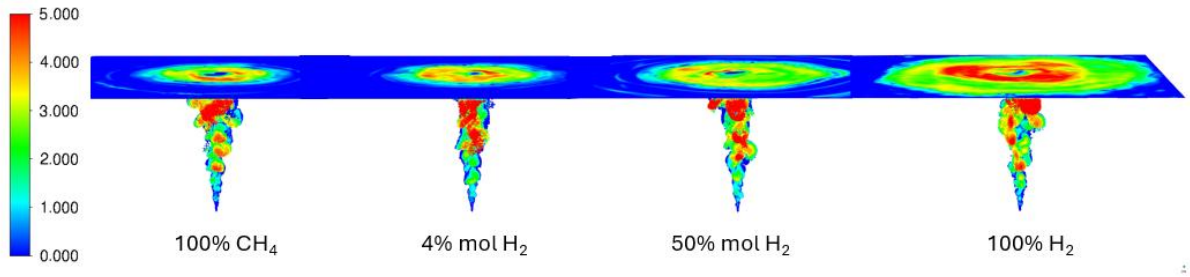

Figure 8: Bubble plumes coloured by distance from plume axis and radial surface velocities coloured as indicated by colormap for various gas blends 200 secs after initiation of release.

The resulting plumes are depicted in Figure 8. Qualitatively it seems like more hydrogen content promotes a stronger and more buoyant plume. This is confirmed by the buoyancy flux of the releases as listed in Table 4. Figure 9 show plots of time-varying surfacing rates and HHV at the surface for all scenarios. **Error! Reference source not found.** a) represents the scenarios with either pure CH_4 (100% mol CH_4) or pure H_2 (100% mol H_2) releases. The release with 100% mol H_2 surfaces 87 secs after initiation of the release which is shorter than that of a pure CH_4 release which surfaces after 140 secs. This is explained by the higher buoyancy of H_2 in comparison to CH_4. Due to turbulence the surfacing rates fluctuate. At an equivalent release rate, methane dissolves more in the ocean than hydrogen. 58% of CH_4 is dissolved compared to 20% of H_2 (average of surfacing rate for the last 300 secs of observation). This is caused by the higher solubility of CH_4 compared to H_2.

The surface rate for the scenario where a small fraction of H_2 (4% mol) is added to the CH_4 stream is plotted in Figure 9 b). Due to the low hydrogen content, the hydrogen surface rate is plotted against a second y-axis with a different scale. The release surfaces after 121 secs and 55% of the gas is dissolved in the ocean. This deviates almost insignificantly from the release of pure CH_4. For the release of 50% mol H2, the surface rate is seen in Figure 9 c). The release surfaces after 129 s and 44% of the released gas is dissolved. The gas dissolution is 46% for CH_4 and 26% for H_2 indicating that the bubbles changes composition as they rise to the surface and thus obtaining a higher concentration of H_2 at the surface. Initial release rate, initial gas composition and gas dissolution dictates the surfacing rate and the surfacing composition. This is reflected by the higher heating value of the surfacing gas. This is plotted in Figure 9 d). Even if the release rate decreases with increasing H_2 content, the HHV increases with increasing H_2 content due to the higher heating value of H_2 compared to CH_4. Time averaged values of these results are listed in Table 4. Also, the time averaged maximum surface velocity is given in the table. This indicates the agitation at the ocean surface caused by the gas release and the strength of the hydrodynamic loads which can be imposed on surface vessels. This is an additional risk which needs to be assessed. An increase in hydrogen content increases the surface velocity and

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hydrodynamic loads. This is attributed to hydrogen being more buoyant than methane as indicated by the buoyancy flux of the releases given in Table 2.

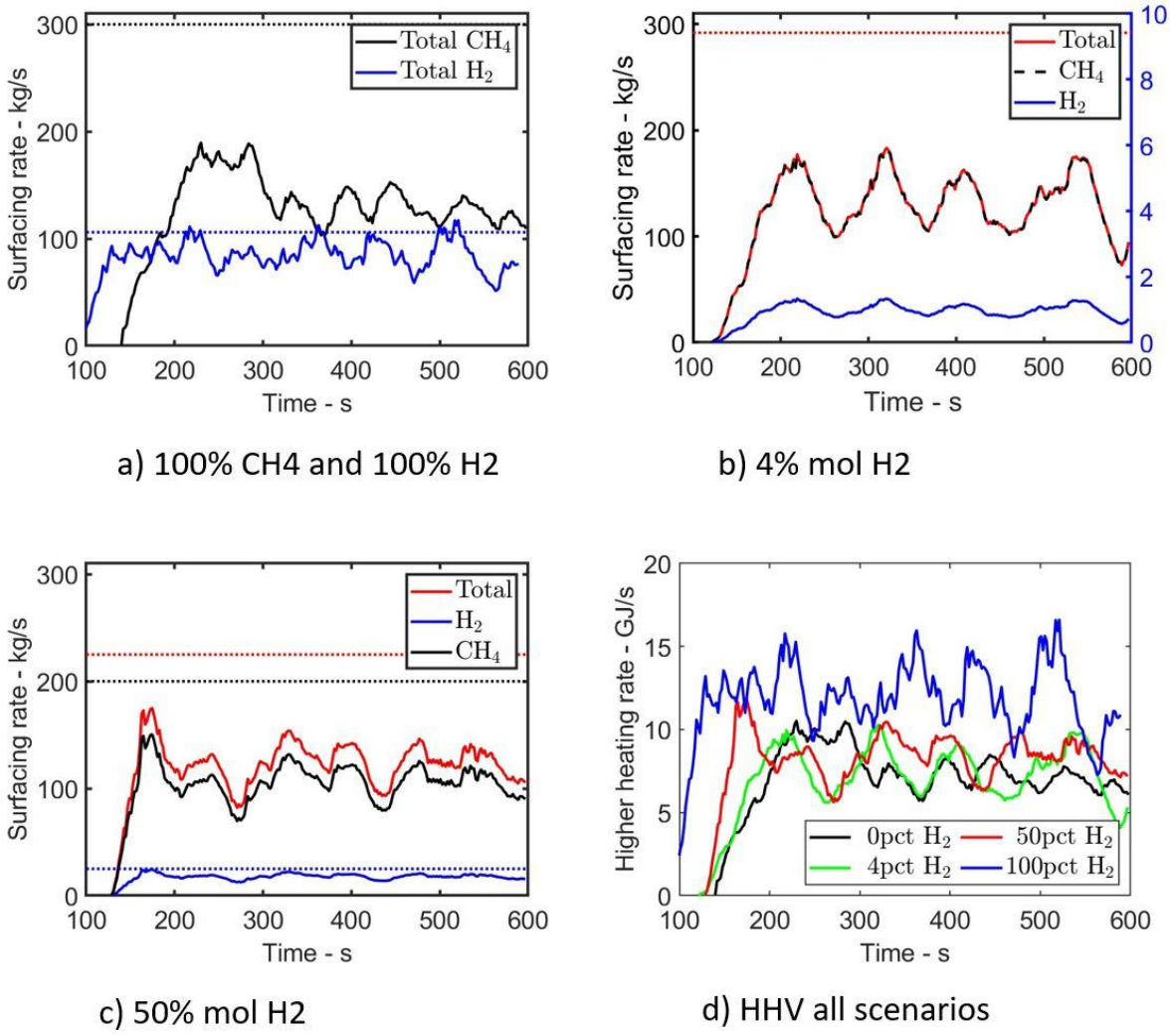

Figure 9: Time varying surfacing rates and HHV. a) Surface rate for scenarios of 100% mol CH_4 and 100% mol H_2, b) for 4% mol H_2, c) for 50% H_2 and d) HHV for all scenarios. The dotted lines are the release rates.

Figure 10 shows 2D contour plots of the total surface flux and higher heating flux as distributed at the ocean surface. Even by averaging for 100 secs, the flux does not represent a smooth curve consistent with the historical assumption of reporting this as a Gaussian profile. It is also seen that the surface flux decreases with increasing H_2 content in the released gas blend. Even if more of the CH_4 is dissolved in the ocean than H_2, the effect of gas dissolution does not compensate for the reduced mass release rate associated with increasing H_2 content. A similar comparison can be made for the higher heating flux as seen in Figure 10 b). Here the higher heating value of H_2 compared to CH_4 causes the higher heating flux to increase with increasing H_2 content even if the mass release rate decreases. This indicates that the risk related to gas concentrations in the atmosphere above the release increases as the H_2 content of the gas blend increases.

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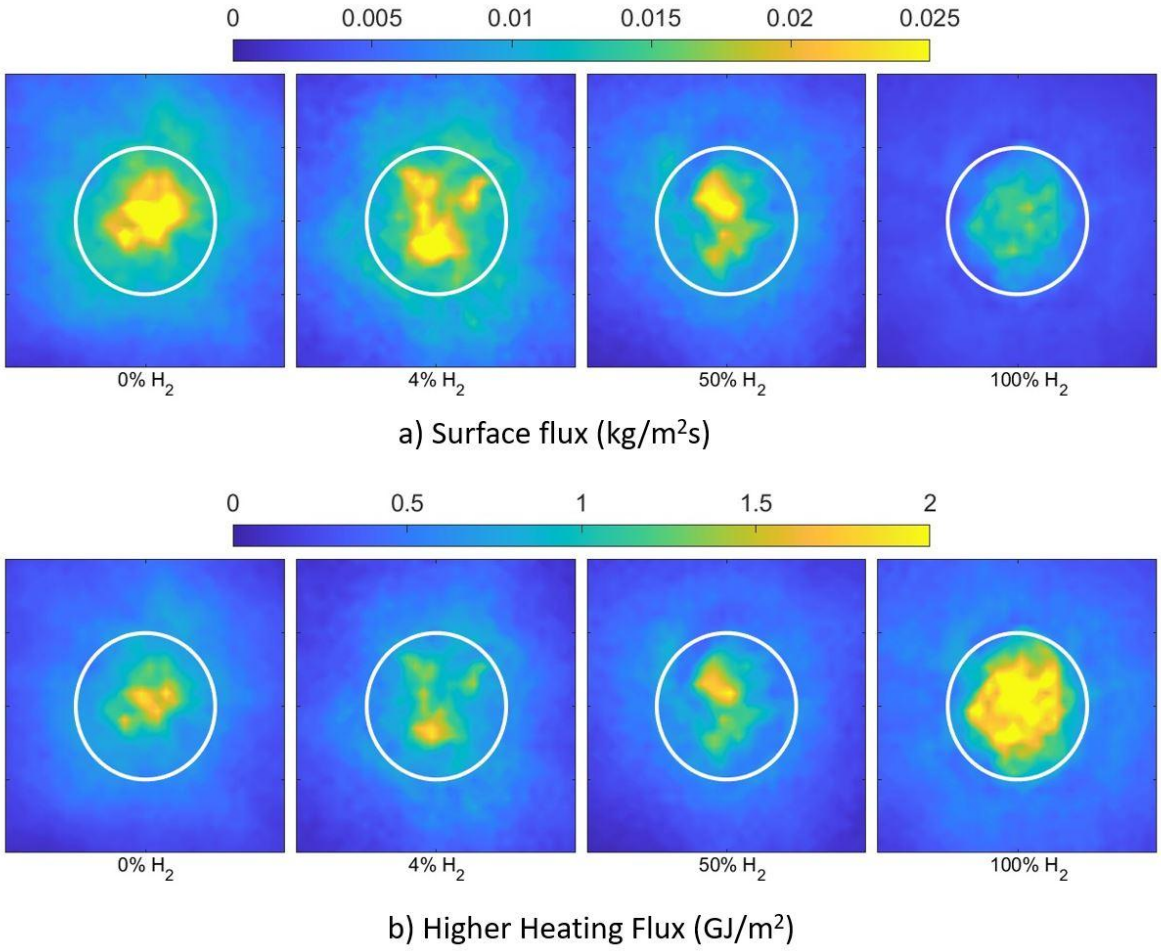

Figure 10: Contour plots of total surface flux (a) and higher heating flux (b) averaged for 100 secs for the analysed scenarios. Width and height of plots represents 200 m. The white circle has a radius of 50 meters.

Stripping of nitrogen and oxygen

The above assessments account for mass transfer of hydrogen and methane primarily as gas dissolution to the ocean. If the dissolved concentrations of the species accumulate to levels above the saturation limit, the mass transfer will be reversed, and the bubbles will receive gas as can be concluded by Eq.(3). This also implies that nitrogen and oxygen naturally occurring in the ocean will be transferred into the bubbles as they migrate upwards, sometimes referred to as stripping of dissolved gases.

In order to assess the impact of this, the scenario with 50% mol H_2 was assessed by also accounting for stripping of nitrogen and oxygen. The concentration of these gases in the ocean will vary with season and geographical location. In this study we have assumed that their concentrations are given by equilibrium with the atmosphere (i.e. no biological effects). This gives a constant molar concentration of $1.03 \cdot 10^{-5}$ for N_2 and $5.53 \cdot 10^{-6}$ for O_2. The driving force for stripping is higher closer to the surface since the pressure is lower and thus the solubility is lower. A scenario with similar conditions, but the release occurring at a depth of 500m was also assessed. The analyses shows that the composition of the bubbles changes as they move upwards. Due to

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difference in solubility the composition of CH_4 decreases and H_2 increases as bubbles move upwards. Closer to the ocean surface the stripping of N_2 and O_2 becomes more significant and starts affecting the overall composition of the bubbles. This is seen in Figure 11 where the molar concentrations of the bubbles are plotted. The changes in the bubble composition are more significant for the scenario with a release from 500m since the bubbles are exposed longer to mass transfer.

While the molar fraction of H_2 increases significantly as the bubbles rise to the surface, the mass fraction is still relatively low. This implies that the surface flux of H_2 is low compared to CH_4. This is seen in Figure 12 where the surface flux of the different gas components is seen. Note that the fluxes of the stripped N_2 and O_2 are in fact higher than that of H_2. This is primarily caused by the low density of H_2. The time averaged results seen in Table 3 document that roughly the same amount of CH_4 and H_2 reaches the surface from 300 m whether stripping is accounted for or not. However, the total surface rate increases with stripping since also N_2 and O_2 is brought to the surface. From 500 m more of the released gas dissolves since the bubbles are exposed longer to mass transfer. The heating rate is also not directly affected by stripping of N_2 and O_2 since they have no contribution to the higher heating rate (heating value = 0). Thus, the averaged higher heating rate is quite similar for the release from 300 m both with and without accounting for stripping of N_2 and O_2. The release scenario from 500 m has a lower higher heating rate since more of the released CH_4 and H_2 has been dissolved due to the longer residence time compared to the release from 300 m.

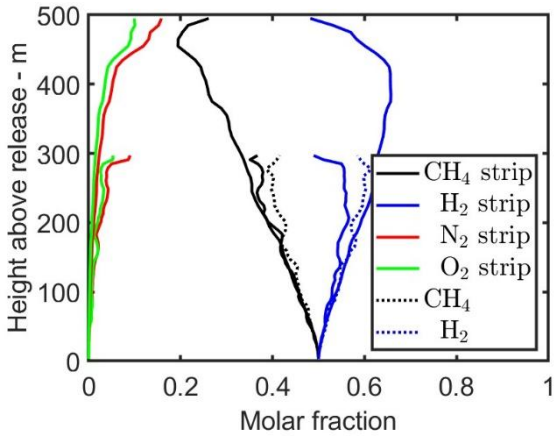

Figure 11: Gas composition of bubbles as function of height above release for releases with and without stripping of N_2 and O_2 from 300m and 500m.

Table 5: Surfacing data on 225 kg/s release

	Surface rate		HHV
	Total	CH_4+H_2	
	kg/s	kg/s	GJ/s
300 m, no strip	126.5	126.5	8.59
300 m, strip	205.5	131.1	8.86
500 m, strip	147.2	64.2	4.49

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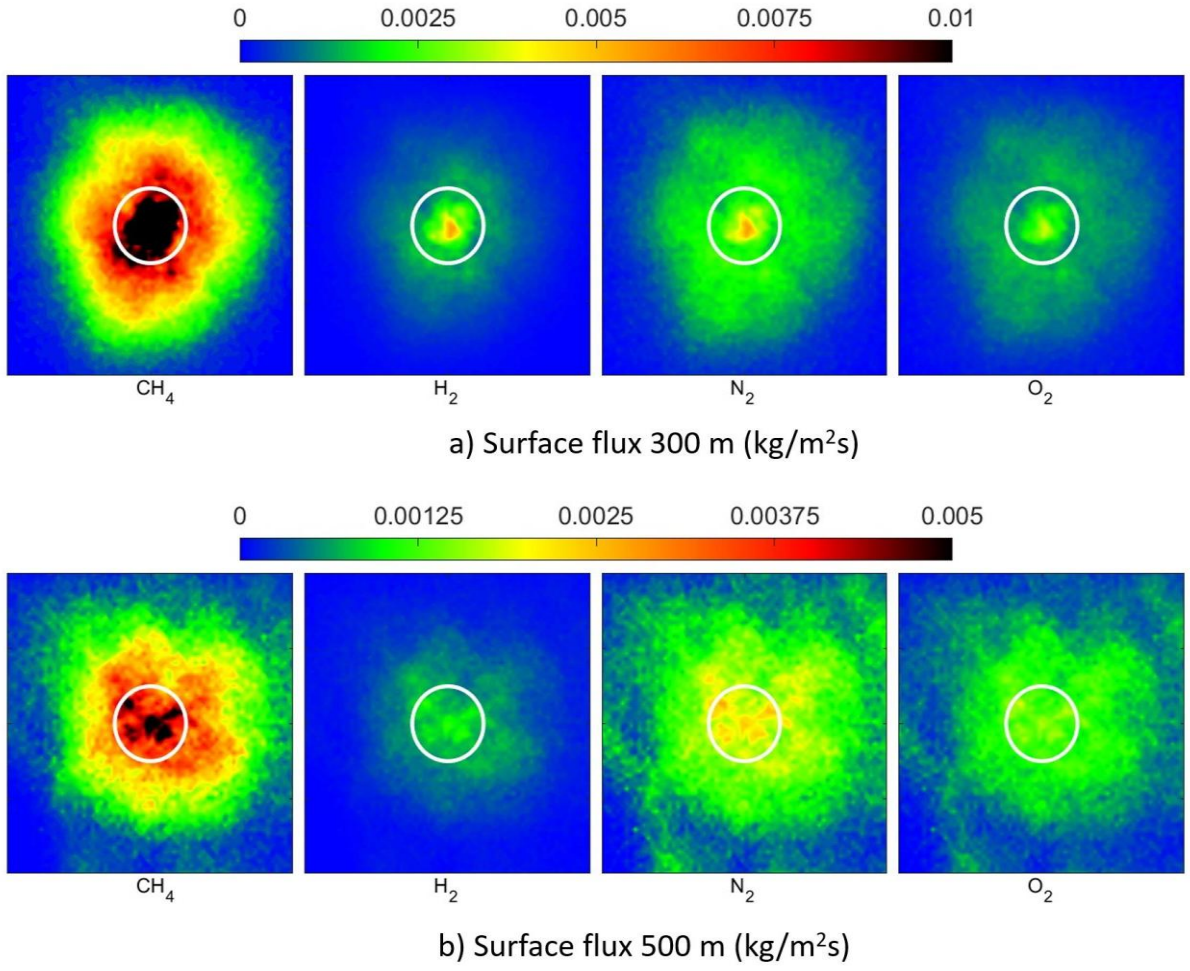

Figure 12: Surface flux of the individual gas components averaged between 500 and 600 secs after initiation of release from 300 m (a) and 500 m (b).

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CONCLUSIONS

A transient 3-dimensional numerical model for analysing the fate of an underwater gas release from a damaged pipeline has been further developed to account for gas mixtures consisting of multiple gas components. The model is consistent with observations of single component CH_4 releases. It has been applied to study release of hydrogen gas blends, i.e. hydrogen mixed with natural gas (here considered as pure methane).

Results show that the gas bubbles change its composition as they migrate upwards towards the ocean surface to contain more hydrogen and less methane since methane is more soluble in water than hydrogen. The bubbles also strip the ocean for nitrogen and oxygen naturally occurring in the ocean and thus provide the bubbles with a nitrogen and oxygen content. Overall, the higher heating value reaching the ocean surface is less than the value released due to gas dissolution. When comparing scenarios with different hydrogen content, it is seen that a higher hydrogen content results in higher heating rates and higher hydrodynamic loads at the ocean surface when emanating from pipelines with the same operating conditions. The risk thus increases as the hydrogen content increases in the gas mixture.

While it can be argued that the risk correlates with the higher heating surfacing rate, the appropriate procedure to assess the risk is to export the calculated surface gas rates to a numerical simulation of the atmospheric dispersion of the gas components and then assess the atmospheric concentrations. This has not been the focus of this study. Other future enhancements include performing release experiments with hydrogen and hydrogen blends and comparing the numerical model with the observations.

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B Appendix B – Open source-based approaches for modelling of subsea gas release

This appendix presents the findings of an initial assessment aimed at evaluating the capabilities of OpenFOAM in modelling subsea gas release scenarios. The context of this study is rooted in earlier simulations conducted using ANSYS Fluent with additional UDF (User defined functions) developed over several years for this specific application. The primary goal was to find out whether similar results could be achieved with OpenFOAM's built-in solvers, thereby offering a potentially cost-effective and open-source alternative, and to determine if similar results can be improved by also creating custom OpenFOAM-based solvers.

Our investigation focused on two different simulation approaches: the Lagrangian and the Multiphase Eulerian frameworks. The initial insights gained from this assessment will contribute significantly to our knowledge of subsea gas release simulation with OpenFOAM and help guide future research in this area.

OVERVIEW OF METHODS EVALUATED

Lagrangian-based approaches

The Lagrangian-Eulerian consists in principle of introducing continua to represent the water and the air on the surface, while modelling the gas released from underwater as discrete particles representing bubbles, while controlling their size and shape via other models. The motion of these particles is coupled with the momentum equation leading to the formation of rising plume. This approach has been successfully used by SINTEF after the development of significant customization and refinement in ANSYS Fluent. The method is attractive because of its relatively low computational cost, but it is more technically challenging to implement in a physically consistent way.

OpenFOAM offers a set of libraries to implement Lagrangian methods in its source code, and several pre-built solvers that show how these libraries can be implemented for different requirements. For most applications, the pre-built solvers can be used directly as they cover most of what is typically expected, such as different particle injection methods and drag models. These pre-built models also include reaction and multiphase applications. For more information on the included capabilities, one should refer to the documentation (OpenCFD, u.d.).

For the application to sub-sea gas release experiments, we aimed at fulfilling the following requirements:

1. Capability of resolving at least two immiscible phases (in addition to the Lagrangian particles) so the water surface movement can be modelled.
2. Capability of introducing particles at different injection models.
3. Particles must have variable density to resolve the effect of hydrostatic pressure on the bubble size.
4. Support for turbulence models.
5. Ability to merge particles with the air surface.

The Lagrangian solver that was deemed closest to these requirements was **MPPICInterFoam**, a solver based on the particle-in-cell method that also includes immiscible multiphase support through the VOF method (MPPICInterFoam, u.d.). Although this solver was the closest alternative, OpenFOAM in general does not support a few features that are necessary and thus require modification to the libraries that control the Lagrangian particle physics. These modifications included the incorporation of variable density with hydrostatic pressure and the implementation of phase merging algorithms. These changes were partially implemented, and it was observed that with further work, this approach could be modified to replicate methodologies available in other software entirely. The formulation of the VOF method used in this solver is also incompressible, but it can be modified to support compressible

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In addition to the particle-in-cell method, other Lagrangian approaches were also tested, such as the discrete bubble method. However, these were deemed too complex and had other limitations. The discrete bubble method, for instance, involves tracking individual bubbles in a fluid, which can become computationally expensive and complex for large numbers of bubbles.

Eulerian-Eulerian approaches

The Eulerian-Eulerian approach consists of using an Eulerian multiphase model to resolve all the phases, taking special care of phase properties. In Eulerian multiphase models, it is possible for a phase to represent particle clouds, and the focus is shifted to track the spatial distribution of volume fraction occupied by the particles, as opposed to their individual position and momentum. This approach is typically more computationally expensive than the Lagrangian-Eulerian one, although it is simpler conceptually. Each phase's properties, including particle size and drag models can be specified individually.

OpenFOAM offers a multiphase Eulerian family of solvers capable of resolving arbitrary numbers of phases with different properties and drag models for each, including chemical reactions. Initially, however, we tested only two-phase flow. The most comprehensive of these solvers is **multiphaseEulerFoam**, which is used in this comparison.

A known challenge with this approach was the computational expense needed to resolve adequate lateral spreading arising from turbulence. Another limitation is that fully resolving the gas inlet can be computationally expensive given the mesh resolution required and the use of a Large Eddy Simulation (LES) turbulence model. These limitations are partially offset by the additional flexibility provided by this formulation, making it attractive for subsea gas release applications. It is, however, possible to envision limitations when needing to resolve very large domains.

TESTING RESULTS AND OBSERVATIONS

For testing both approaches, a box-shaped computational domain was built and discretized using a regular grid, which was refined in the regions where the gas plume was expected to spread. The domain was built to accommodate water to 30m in depth, leaving a space for air of 10m in height as shown in Fig. 1.

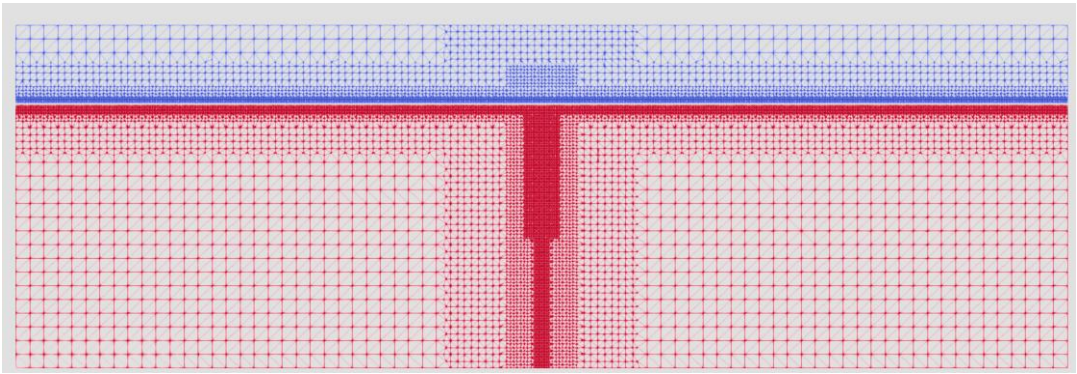

Figure 13. Computational domain showing discretization and refinement. Red zones represent the space occupied initially with water and the blue zones represent the air.

At the bottom of the domain, air was injected with different inlet sizes and mass flowrates. The injected air was allowed to rise due to buoyancy and the spreading patterns were observed.

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Eulerian-Lagrangian

For the Lagrangian simulations, initially bubbles were injected into the domain as particles with a constant *patchInjection* method introducing mass flowrates of 1.2 kg/s. Bubbles of different sizes and initial conditions can be injected in the options relevant to the injection method.

Although the bubble population is coupled with the momentum equation via the particle-in-cell method, it was noted that typically inserting only bubbles shows very laminar behavior, and the bubble cloud shows only simple, mushroom-shaped distributions. Increased spreading and more turbulent behavior were observed when using a mixed injection of Eulerian air and Lagrangian particles, shown in Fig. 2.

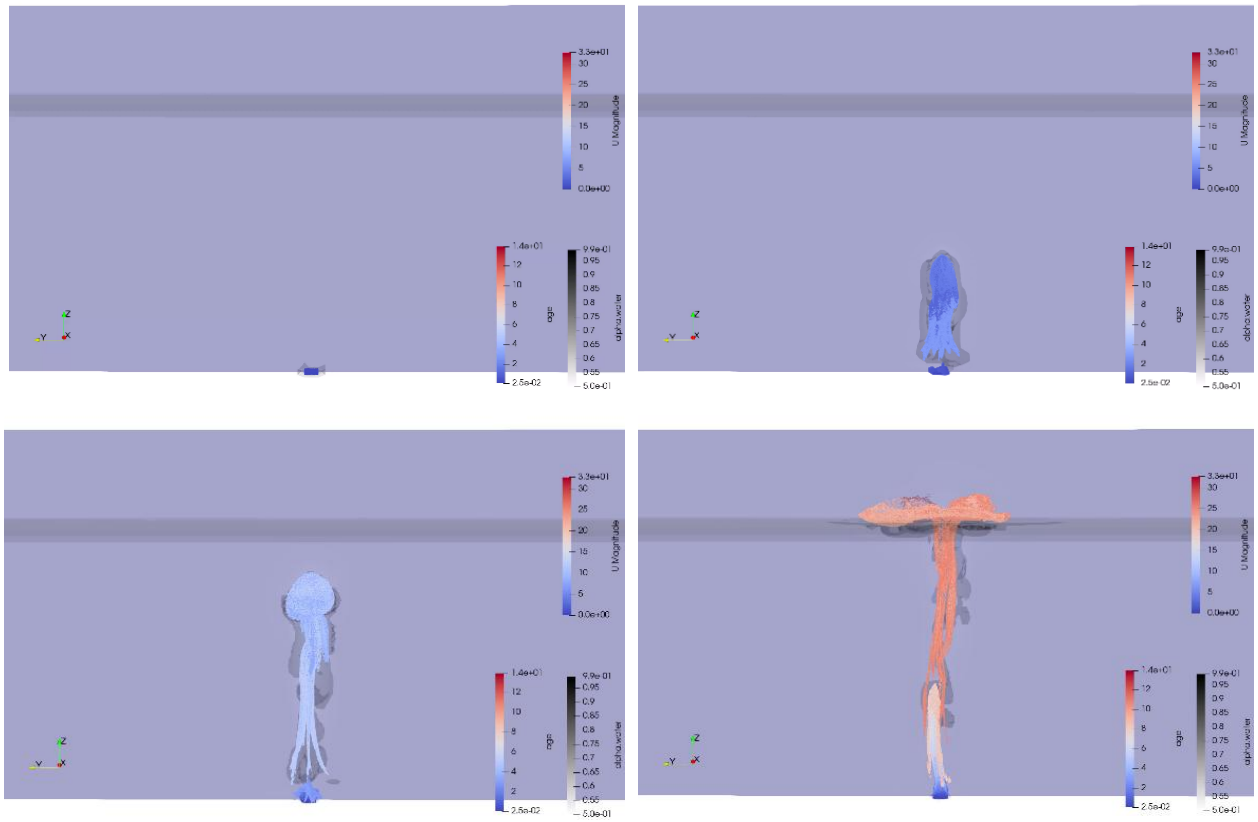

Figure 14 Mixed plume formed by cloud of Lagrangian particles carried simultaneously by an Eulerian injection of air (grey background)

One of the main limitations of the MPPICInterFoam approach is that particles are injected with a constant density. This was addressed by introducing our own modifications to the Lagrangian particle tracking libraries included in OpenFOAM. To achieve this, a state equation was introduced in the domain, and then applied to each particle, forcing it to adopt a density matching temperature and pressure conditions at its position.

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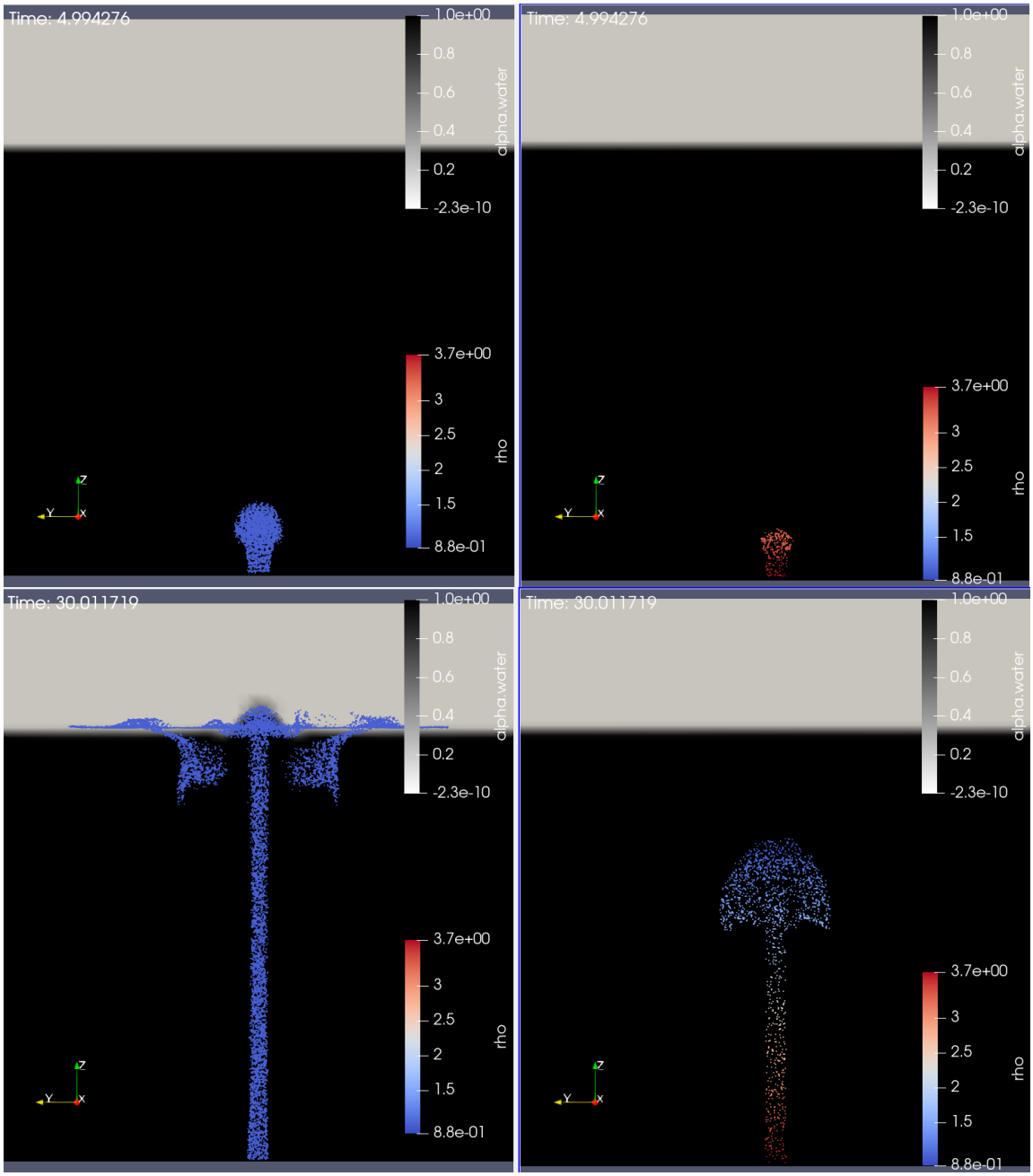

Figure 15. Snapshots of the Lagrangian particles after 1s (top row) and after 30 seconds (bottom row), shown with cases of constant particle density (left column) and variable (right column)

The introduction of a model to modify the density of the particles was done to both overcome this limitation and to familiarize ourselves with the customization of the Lagrangian libraries. In Figure 3 we show a comparison of a rising plume tested, showing snapshots after 30s. The discrepancy indicates that the introduction of variable density is fully coupled with the momentum equation. Our observation is that with further work, it is possible for us to customize this library further to introduce more sophisticated features and specialized, purpose-built sub-models.

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One possible limitation in the current implementation is also that the drag force is calculated in an Eulerian framework using the bubble volume fraction field. Another current limitation is that the air particles do not disappear when they re-join the air phase. Both are relatively simple to overcome but require additional development.

Eulerian-Eulerian

For the assessment of the Eulerian-Eulerian approach, the inlet size had to be defined, and it was fixed at 10cm for testing purposes. It was initially observed that resolving the inlet size with enough accuracy is necessary to obtain any spreading in the gas plume. This comes at the cost of increased grid density near the inlet and may be unfeasible for extremely large domains. Nevertheless, it is possible to do this with enough resolution allocated.

In the Eulerian-Eulerian approach, the main parameters that can control the spreading dynamics of the plume are the following:

1. Bubble size -can be set as constant or variable, coupled to the thermodynamic model chosen.
2. Virtual mass
3. Gas density model
4. Friction model

For testing purposes, the typical Schiller-Nauman model was used to model phase friction in all cases, although many other well-known models are also available.

All tests were carried out using an LES turbulence model, as it was noted that RANS-based methods are unable to capture the shear profile accurately, leading to unphysical lateral spreading.

The observed advantage of the Eulerian-Eulerian approach is that the merging of the phases and the mass transfer dynamics are resolved with a less heuristic-driven approach, and physically consistent results are achieved more easily, although it does come at a higher computational expense. An example of the gas plume rising in an Eulerian-Eulerian framework is shown in Figure 4 showing that the gas can form spreading patterns that qualitatively look realistic.

A limitation observed was that the rising times observed were slightly shorter and less dependent on the mass flow rate than expected, however, there are other reasons why this may be the case, and these may be mitigated by improved thermodynamic model or improvement of the drag models and particle size models. For example, the drag models could be refined to better account for the interaction between the gas and the surrounding fluid, and the particle size models could be improved to represent the size distribution of the gas bubbles more accurately.

The lateral spreading of the plume is also linked to the bubble size distribution and the virtual mass settings provided. An example comparing the difference in spreading can be seen in Table 1, where the difference in effective bubble size yields substantially different lateral distribution profiles for the same mass flowrates.

With adequate improvements, the Eulerian approach could potentially provide a more accurate and flexible method for modelling subsea gas release.

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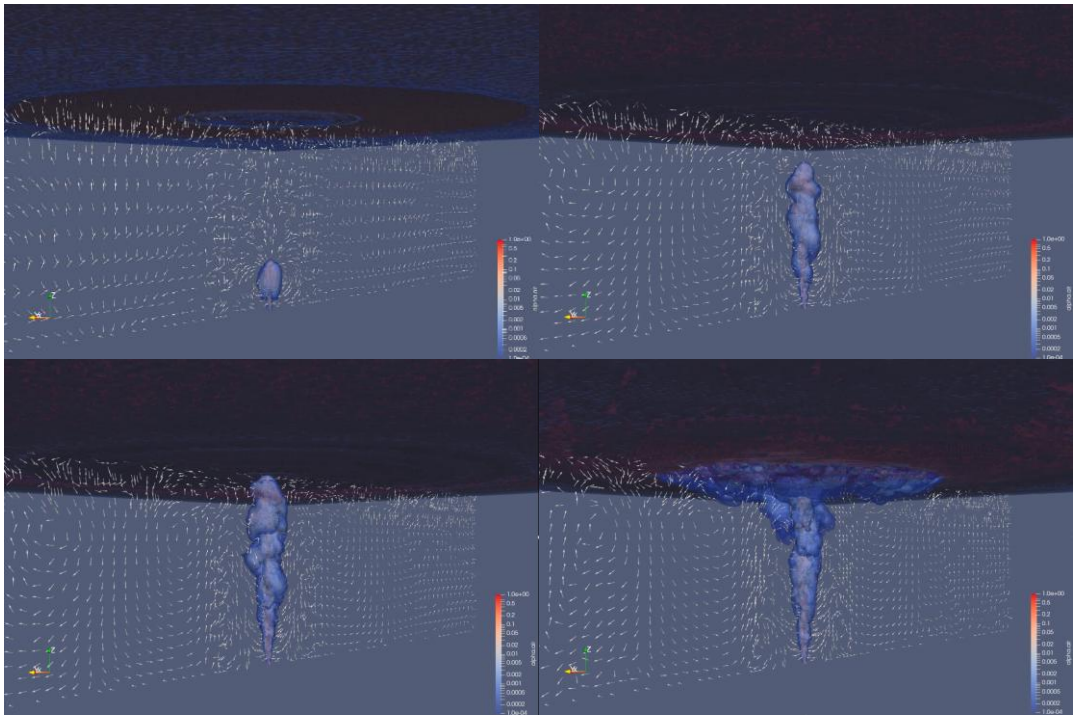
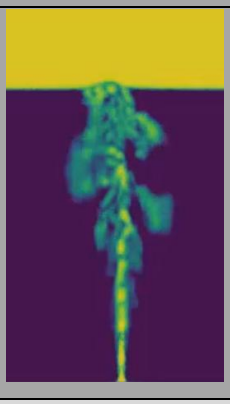
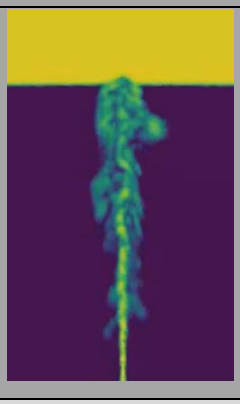


Figure 16. Snapshots at different time of an Eulerian air release at 1.2 kg/s

Table 6. Plume shape at rise time for different mass flowrates and bubble diameters

	Mass flowrate	
	1.2 kg/s	0.4 kg/s
Constant bubble diameter (1E-3m)		
	Bubble size	
	1E-4 m	1E-2 m

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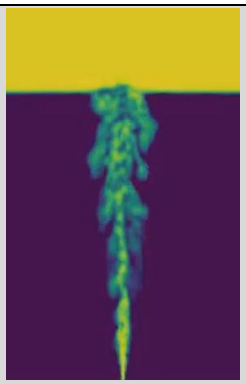
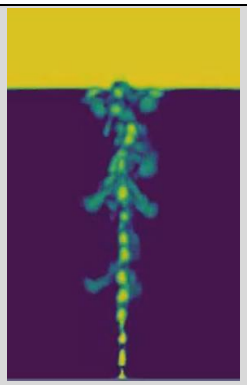
Constant mass flow rate 0.6 kg/s		

CONCLUSIONS

In general, both the Lagrangian and Multiphase Eulerian approaches can be implemented in OpenFOAM and achieve a similar capability to what is available in Fluent. However, more work is necessary to fully replicate the model capabilities that have been produced before using ANSYS Fluent. In the case of the Eulerian-Lagrangian approach, additional modifications to the source code are necessary to cover mass transfer and hybrid turbulence modelling capabilities developed before using the VLES method. In the multiphase Eulerian approach, no significant changes to the source code are expected, but application-specific parameter optimization might be necessary to achieve results with a similar level of quality. The main details that should be improved are the inclusion of detailed thermodynamic models to cover control over the bubble size dynamics and compressibility.

Additional approaches such as VOF (single momentum equation -multiphase) may also be tested at the expense of losing capability to include the bubble dynamics, but coupling this with an Eulerian framework like **MPPICinterFOAM** is also possible.

Other Lagrangian-Eulerian approaches have been made available via third party solvers, for example models based on the *discrete bubble method* like *atomizationFoam* or *VOFDBMcavitaitonFoam* (Linmin Li, 2023), however there is insufficient information to test these approaches thoroughly. These could be used however as a starting point to create a custom Lagrangian-Eulerian approach capable of fully replicating or improving other existing techniques.

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