From Gases and Evaporators risk assessmeNt towards an Integrated management of sea and land pollution incidentS

MANIFESTS is a project co-funded by the European Union Civil Protection - DG-ECHO, developed in cooperation with RBINS, CETMAR, IMT Mines Alés, INTECMAR, IST, the UK Security Agency as associated partner and coordinated by Cedre.

Co-funded by the European Union

D2.4 - Underwater gas release module

15/07/2025

Work Package 2	
Task 2.3	
Date	15/07/2025
Version	1
Author/s	LUDOVIC LEPERS, SÉBASTIEN LEGRAND
Partners	INSTITUTE OF NATURAL SCIENCES

Co-funded by
the European Union

Index

Co-funded by
the European Union

Co-funded by
the European Union

1. Introduction

In the event of an underwater release of hazardous and noxious substances (HNS), the behaviour of the released gas can vary significantly depending on both the chemical involved and the surrounding environmental conditions. This variability introduces considerable uncertainty for emergency responders, who require as much reliable information as possible to effectively manage such incidents.

These scenarios are not merely theoretical. Real-world incidents, such as the Nord Stream pipeline rupture, have demonstrated the potential for underwater gas releases. Moreover, the formation of a gas cloud at the water's surface can pose serious risks to nearby stakeholders, including coastal populations, especially if the incident occurs in a port or harbor. In addition to public safety concerns, the environment itself may be affected, both by the dissolved underwater plume and by the atmospheric dispersion of gas. These risks highlight the necessity of accurately estimating both underwater and atmospheric plumes.

Within the MANIFESTS GENIUS project, this challenge is addressed through a holistic approach that integrates theoretical analysis, modelling, and both laboratory and mesoscale experimentation. The project's objectives include enhancing the decision support system (DSS) developed during the initial MANIFESTS project and strengthening best practices, tool assessment, and training. By deepening the understanding of the risks coming from gas cloud dynamics, estimating their behavior, and potential mitigation strategies, the project seeks to support informed decision-making in emergency response. A key focus is also placed on disseminating these advancements to relevant stakeholders to encourage the adoption of improved protocols in real-world operations.

As part of the project, a dedicated underwater gas release module has been developed. This module simulates the ascent of gas from an underwater source—such as a pipeline or vessel hull—through the water column and estimates the resulting surface expression and atmospheric behaviour. The source code for this model is available at [https://github.com/naturalsciences/SubSeaGasLeak], where it can be downloaded and used by interested institutions. Alternatively, it can be accessed directly through the MANIFESTS DSS platform (login required).

This report provides a detailed overview of the gas rise model. It presents the governing equations, describes the required user inputs, and explains the outputs generated by the simulation.

2. Model description

2.1. Model availability

The gas bubble rising model, developed as part of the MANIFESTS GENIUS project, is designed to simulate the ascent of gas bubbles from an underwater release and estimate their behaviour as they reach the surface. The model goal is to supports risk assessment and decision-making in emergency response scenarios involving hazardous and noxious substances. It has been designed to simulate underwater hole in vessels tanks and underwater pipeline.

The model is available at [https://github.com/naturalsciences/SubSeaGasLeak] under the European Union Public License (EUPL). This open-source license allows users to freely use, modify, and improve the model. For full licensing details, please refer to the EUPL license provided in the repository.

The model can be used as a “stand-alone” software, and run on a computer, or it can be integrated on a computing server, from which user can run simulation through a web interface for instance. Refer to section 2.3 for more information.

2.2. Model overview

This section provides an overview of the physical processes represented in the model. For a detailed description of each process, refer to section 5. The primary objective of the model is to simulate the ascent of gas through a water column. This is a complex task due to the dynamic nature of the system, which involves multiple interacting phases. To address this complexity, the model divides the system into distinct components: the gas source, the rising plume, the water column, and the atmosphere.

The source represents the point at which the gas is released, such as a rupture in a pipeline or a hole in a vessel. It defines the initial velocity and size of the gas plume at the release location. The user must provide key information about the source, including the chemical flow rate. As this parameter can be difficult to estimate directly, the model offers an option to calculate it based on predefined scenarios. Specifically, it can estimate the flow rate assuming one or two holes in a tank, or a single hole in a pipeline.

Once the gas is released, it begins forming a plume. The plume is modelled as a series of Lagrangian elements, each released sequentially. These elements are represented as cylindrical volumes composed initially of pure gas. Each element contains gas bubbles and is assumed to be entirely gaseous. At the beginning of their trajectory, elements rise with the initial velocity defined by the source (jet phase), which gradually decreases until they reach the terminal velocity characteristic of the bubbles (advection phase).

As the elements ascend through the water column, the gas bubbles begin to disperse. This dispersion is represented in the model by allowing the volume of the elements to increase, reflecting the growing separation of individual bubbles as water enters the space between them.

During the ascent, gas exchange begins between the bubbles and the surrounding water. The water column is discretized into a series of horizontal layers, each assumed to have a uniform dissolved gas concentration. Horizontal advection due to water currents and vertical diffusion between layers are both modelled to simulate the transport and mixing of dissolved gases. The model is capable of simulating multiple gases simultaneously, distinguishing between the gas released at the source and gases already dissolved in the water column.

When elements reach the surface, the gas they contain is released into the atmosphere. Additionally, the top layer of the water column can release gas through volatilization. However, the model does not account for any reverse flux from the atmosphere back into the water. Instead, it assumes that released gas rapidly disperses into the atmosphere, effectively removing it from the system.

2.3. Technical overview

Users can operate the model through either a graphical user interface (GUI) or a command line interface (CLI). The GUI is designed for ease of use, making it suitable for emergency responders or researchers conducting single simulations. The CLI is intended for institutional use, allowing integration into automated workflows or existing service platforms.

Installation instructions are included in the same repository [https://github.com/naturalsciences/SubSeaGasLeak]. The model is compatible with any platform supporting modern python 3 and able to install the required packages. The GUI needs PySide6, to support the Qt interface, but the model can run without it if only the CLI is used.

To execute a simulation, the model requires a set of input parameters. These parameters are specified in a file named XXXXX_request.json, where XXXXX corresponds to the unique identifier of the simulation. Optionally, an intermediate file named XXXXX_raw_request.json can be used during a preprocessing step. This raw input file is supplemented with additional information to generate the final XXXXX_request.json file, which is then read by the model.

The preprocessing phase enables the automatic retrieval of certain constant values, such as atmospheric composition (used to calculate the initial dissolved gas concentration, with 21278.25 Pa of oxygen and 80046.75 Pa of nitrogen) and water depth at the release location, based on available bathymetric data. This step can be skipped if a XXXXX_request.json is already present and a simulation is executed from the CLI.

After preprocessing, the simulation is initiated using the completed XXXXX_request.json file. The simulation proceeds for a duration defined by the user (refer to section 3). Alternatively, if a shorter time is sufficient, the model may stop automatically after four times the duration required for the first gas element to reach the surface. The simulation can also be interrupted manually at any point when using the GUI.

Upon completion, the raw output data are processed in the postprocessing phase to generate time series and spatial maps suitable for analysis and visualization. The full workflow is illustrated in the Figure 1.

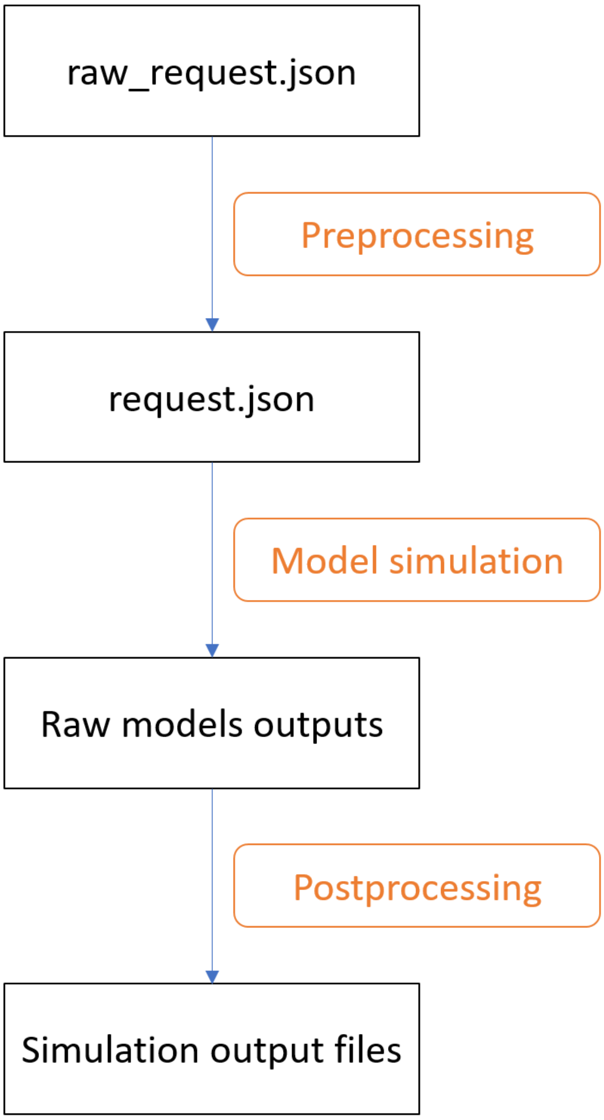

Figure 1: model workflow

In case the depth is provided relative to the seabed and not to the sea surface (only with CLI), the model will open the file “data/GEBCO_2024.nc”, from GEBCO Compilation Group (2024) GEBCO 2024 Grid (doi:10.5285/1c44ce99-0a0d-5f4f-e063-7086abc0ea0f). The file should be provided by the user/institution.

3. Inputs parameters

To run a simulation, the user must provide a set of input parameters. In the GUI, default values are pre-filled, with methane selected as the default chemical. Users are expected to complete or modify any parameters that differ from these defaults.

Once the required inputs are specified, the GUI generates a valid raw request file based on the selected parameters. This file is saved in the “requests” folder and can be used as a template for creating new input files when operating the model via the CLI.

In the next section, the Table 1 to Table 5 list all the parameters and what they are corresponding to.

3.1. Time and location

Table 1 : parameters for the time and location of the release

Name	Symbol	Units	Description
Start time	/	/	Time of the start of the simulation (only used in the netcdf output)
Maximum duration	/	s	Maximum time of the simulation (can be shorter if the simulation is stopped in the GUI or if 4 times the time needed for an element to reach the surface is shorter
Latitude	/	Degrees North	Release location (only used in the netcdf output)
Longitude	/	Degrees East	Release location (only used in the netcdf output)
Depth	H_w	m	Depth under the water surface. Can be set to “m above seabed” as units, it will then convert it to “m below sea surface” using an already installed bathymetry

3.2. Environment

Table 2 : parameters for the environment

Name	Symbol	Units	Description
Wind speed	u_{wind}	m s^{-1}	Wind speed
Temperature	T	°C	Temperature of the water (assumed uniform)
Water viscosity	μ_w	Pa s	Water dynamic viscosity
Water density	ρ_w	kg m^{-3}	Water density
Current speed	$\overrightarrow{u_w}$	m s^{-1}	Water speed (assumed uniform)
Vertical turbulent diffusivity	K_z	m^2 s	Vertical turbulent diffusivity (assumed uniform)

Horizontal turbulent diffusivity	K_{xy}	m^2 s	Horizontal turbulent diffusivity (assumed uniform)
Water clean	/	/	If the water « clean » ? (not salty)

3.3. Chemical properties

Table 3 : parameters for the environment

Name	Symbol	Units	Description
Component name	/	/	Name of the chemical
Molar mass	MW_{HNS}	g mol^{-1}	Molar mass of the HNS
Critical temperature	T_{crit}	K	Critical temperature of the HNS
Henry constant	H_{HNS}	mol m^{-3} Pa^{-1}	Henry constant of the chemical
Molar volume*	v_l	m^3 mol^{-1}	Molar volume of the HNS
Air diffusivity*	D_c	m^2 s^{-1}	Air diffusivity of the HNS

The air diffusivity and molar volume parameters can be set to the value "-1." When this value is used, the model will estimate realistic values based on the other provided parameters. While this makes it optional to explicitly define these parameters, it is recommended to supply accurate values whenever possible to improve the reliability of the simulation results.

3.4. Release Parameters

Table 4 : parameters for the release

Name	Symbol	Units	Description
Breach area	A	m^2	Breach area
Jet characteristic height	H_J	m	Height of the transition from a jet of gas to bubble at the terminal velocity
Average bubble diameter	μ_b	m	Average diameter of the bubble
Total mass	M	kg	Total mass of the HNS in the tank/pipeline
Flow rate	Q	kg s^{-1}	Flow rate of HNS at the jet basis
HNS density*	ρ_{HNS}	kg m^3	Density of the HNS in the tank/pipeline
Hole height*	H_B	m	Height of the hole relative to the bottom of the tank (only simple/double breach)
Pipeline pressure*	P_{pip}	Pa	Pressure inside of the pipeline

The flow rate can be estimated in the GUI, for a simple breach, a double breach or a hole in a pipeline. The parameters marked with "*" are discarded by the model once the flow rate is estimated and will not be present in the raw request file.

3.5. Advanced Parameters

Table 5 : advanced parameters

Name	Symbol	Units	Description
Max shape change	/	[]	How much a particle can flatten near the surface before being assumed to be fully in the atmosphere
Number timestep release	n_{tr}	[]	How many timestep between two particles releases
Number of layer	/	[]	Number of water layers
Bubble std	σ_b	m	Standard deviation of the bubble size
Output grid X	/	[]	Number of cell on the x axis for the map
Output grid Y	/	[]	Number of cell on the y axis for the map
Aliasing factor	/	[]	Super sampling factor for the antialiasing of the map

4. Model output

When a simulation is started, the model creates a folder in which it puts all the simulation results, in “results/XXXXX” with XXXXX being the id of the simulation. A zip file with the simulations outputs is also created in the output folder.

4.1. Simulation outputs

In the results/XXXXX/timeseries directory, the model generates four timeseries. A fictional example is provided in this section to illustrate the analysis and interpretation of those outputs.

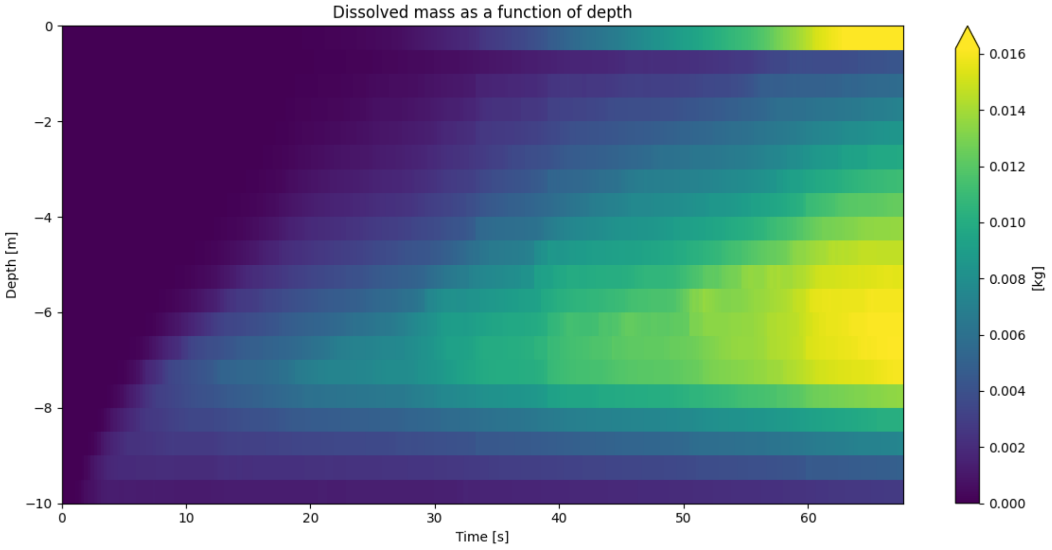

Figure 2 : Dissolved mass as a function of time. The x axis is the time (in seconds) since the start of the simulation), and the y axis is the depth of the layer. The color is represent the mass in the given layer of water at the given time

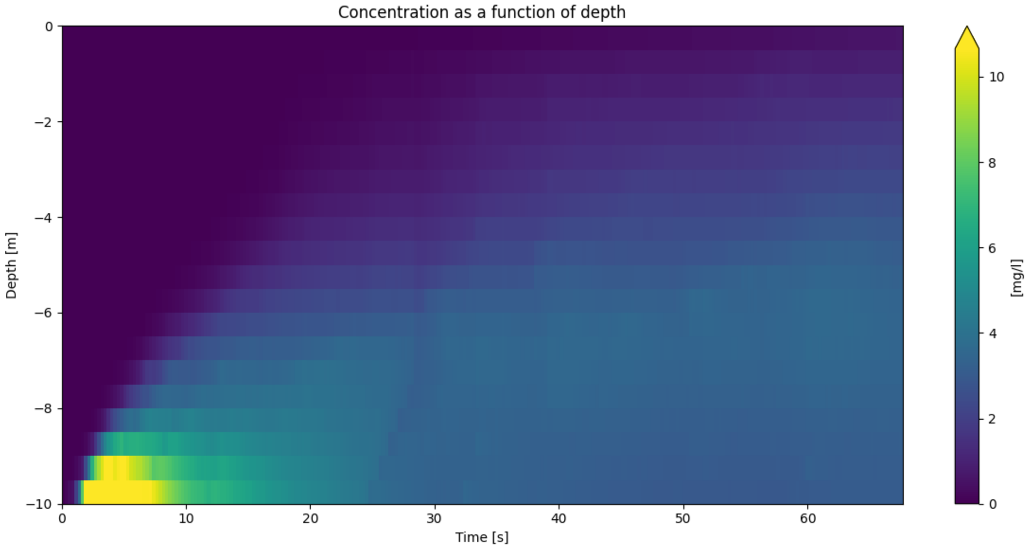

Figure 3 : Concentration in the water layers as a function of time. The x axis is the time (in seconds) since the start of the simulation), and the y axis is the depth of the layer. The color represent the concentration in the given layer of water at the given time

Figure 2 and Figure 3 provide a spatial representation of the plume behavior throughout the entire water column. These visualizations show that the concentration of dissolved gas is relatively uniform with depth, though slightly higher near the bottom than near the surface. Notably, most of the mass is concentrated in the middle of the water column.
The initially elevated concentration near the bottom at the start of the simulation is due to the very small size of the first layer when the first element enters it. This effect can be considered a numerical artifact. A similar artifact occurs at the top layer, which appears to contain a disproportionately large amount of mass. As plume elements reach the surface, their volume increases, causing the top layer to expand. While vertical diffusion between layers tends to equalize concentrations, the larger volume of the top layer means it retains more dissolved gas overall. The top layer for the mass and the first 10% of the simulation for the concentration can therefore be saturated in their color on the maps.

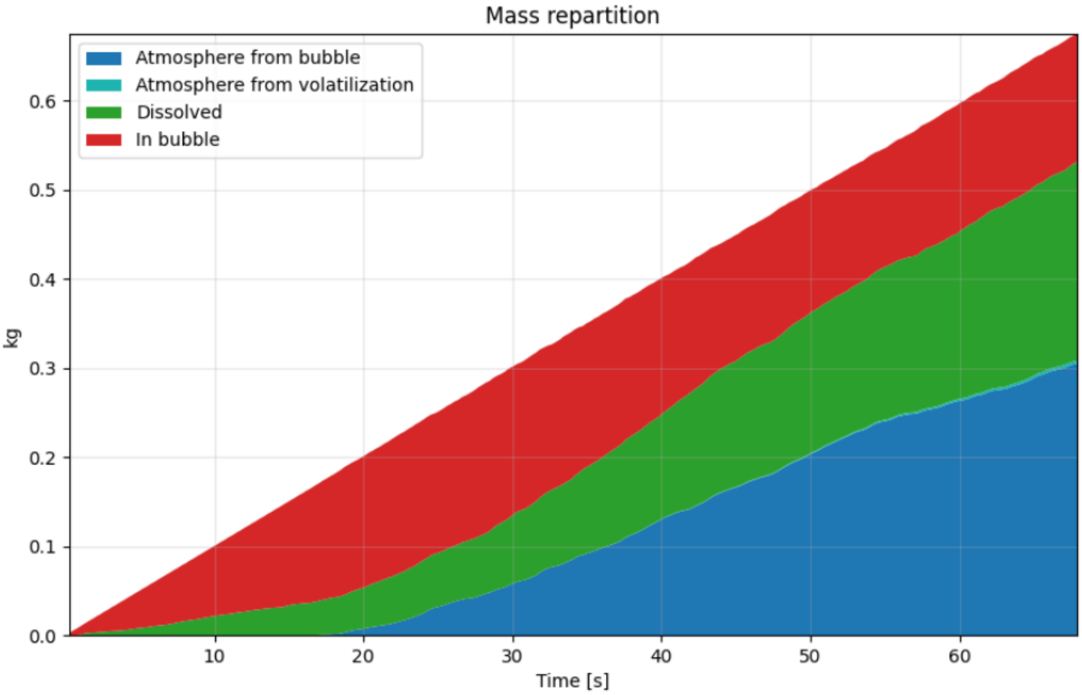

Figure 4 : mass balance as a function of time. Red is the mass in bubble, green is the mass dissolved, light blue is the mass volatilized from the water column and dark blue is the mass of gas that reached the surface due to the bubble

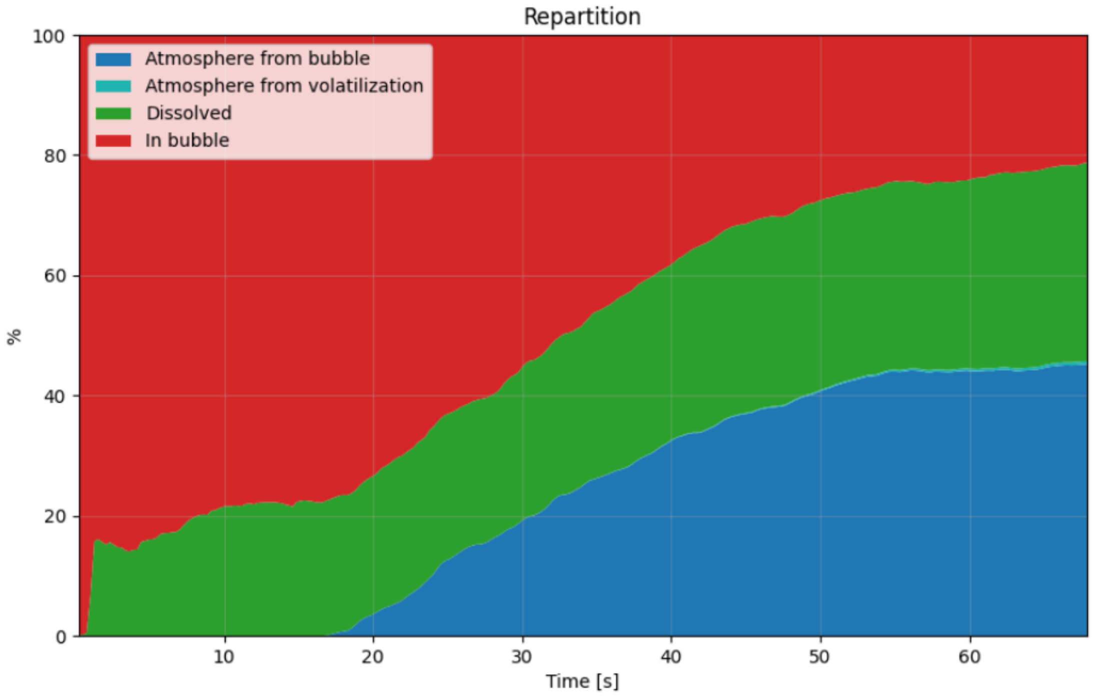

Figure 5 : mass repartition as a function of time. Red is the mass in bubble divided by the total mass, green is the mass divided by the total mass dissolved, light blue is the mass volatilized from the water column divided by the total mass and dark blue is the mass of gas that reached the surface due to the bubble divided by the total mass too

Figure 4 and Figure 5 illustrate the total mass balance over time. As expected, the total mass increases linearly, since the gas release rate at the source is constant throughout the simulation.

Initially, the mass contained in the bubbles increases, but it eventually reaches a steady state. This occurs because, after a certain period, the rate at which gas dissolves into the water and reaches the surface equals the rate at which it is being released. In contrast, the mass in the atmosphere continues to grow, as bubbles continually reach the surface and release gas.

The mass dissolved in the water also increases over time. This is due to advection: as dissolved gas is transported by water currents, local concentrations decrease, allowing additional gas to dissolve. Over the long term, this process leads to an equilibrium concentration in the water column. Meanwhile, some of the dissolved gas escapes to the atmosphere through volatilization at the water surface.

Eventually, the ratio of evaporated to dissolved mass stabilizes, indicating a partitioning equilibrium between the water column and the atmosphere for this particular release scenario. The relative mass contained in the bubble phase gradually decreases, not because the absolute mass of bubble changes, but because the atmospheric and dissolved masses continue to increase, reducing the bubble phase's proportion of the total.

4.2. Raw and advanced outputs

4.2.1. Maps

To visualize the volatilization process spatially, the model generates a NetCDF file named results/XXXXX/XXXXX_vola.nc. This file contains both spatial and temporal data related to the release of chemicals from the top water layer into the atmosphere.

All data in this file are organized on a common spatial grid, which covers the entire area reached by both the water layers and the rising particles. The output distinguishes between volatilization originating from surface-reaching particles and from the top water layer, while also providing their combined effect.

Specifically, the file includes:

- The mass of chemical volatilized during the last simulation timestep;
- The volatilization rate at the last timestep;
- The total volatilized mass over the entire simulation.

Each of these outputs is available separately for surface particles, the top water layer, or both combined.

4.2.2. Raw outputs

The model produces several output files that are essential for postprocessing. However, these files may also be valuable on their own for advanced users, and they are described below.

A JSON metadata file stores the depth of each water layer. A corresponding CSV file records the vertical positions of the layer boundaries at each timestep. Note that only layers reached by a Lagrangian element are included. This file also contains data on the quantity of dissolved gas in each layer, as well as the amount of gas that reached the surface during the current timestep (only for the surface layer).

Another JSON file provides detailed information about the Lagrangian elements (cylinders), including their positions, dimensions (radius and height), the quantity of gas in bubble form, the number of bubbles, and whether the element is in the jet or advection phase.

A final JSON file logs each instance when a Lagrangian particle reaches the surface. It records the amount of gas released, the particle’s radius, and its x and y coordinates at the time of surfacing.

5. Model equations

5.1. Initial condition: estimation of the flow rate

The model needs the flow rate of gas leaving the source. It can either be provided if know or be computed in the GUI using the following equations.

The pressure is estimated as function of the depth:

$$P = P_{atm} + \rho_w g H_w \tag{1}$$

P : pressure at the depth [Pa]
P_{atm} : atmospheric pressure [Pa]
g : earth acceleration constant [m/s²]
H_w : water height above, or depth of the release [m]

The flow rate can be estimated as follow:

$$Q = \frac{AU}{\rho_{HNS}} \tag{2}$$

U : velocity of the fluid [m/s]
A : Area of the breach [m²]

$$\rho_g = \frac{P \cdot MW_g / 1000}{RT}$$

MW_g: average molar weight of the gas in the bubble [g/mol]
ρ_g : Density of the gas at the output [kg/m³]
R: Perfect gaz constant 8.314 [m³·Pa/(K·mol)]
T : Temperature of the water [K]

5.1.1. Double breach

It is assumed that the hole by which the water is entering the tank is larger than the hole by which the chemical is leaving the hull.

$$U = 0.703 \sqrt{2 g H_B \frac{\rho_w - \rho_{HNS}}{\rho_w}} \tag{3}$$

5.1.2. Simple breach

It is assumed that the water must enter by the same hole as the gas leaving. It reduces the area available to 35%, and is accounted for in the velocity:

$$U = 0.246\sqrt{2gH_B\frac{\rho_w - \rho_{HNS}}{\rho_w}} \tag{4}$$

H_B : Height of the hole relative to the bottom of the tank [m]

5.1.3. Pipeline rupture

Using the Bernoulli equation:

$$P_{pip} = P + \frac{1}{2}\rho_{HNS}U^2 \tag{5}$$

P_{pip} : Pressure inside the pipeline [Pa]

$$U = \sqrt{\frac{2}{\rho_{HNS}}(P_{pip} - P)} \tag{6}$$

To estimate the density of the HNS outside of the pipeline, the perfect gas law is used:

$$\frac{P}{RT} = \frac{n}{V} \tag{7}$$

$$\frac{P}{RT} = \frac{n}{V} = \frac{1}{MW_{HNS}/1000}\frac{m}{V} = \frac{\rho_{HNS}}{MW_{HNS}/1000} \tag{8}$$

$$U = \sqrt{2\frac{RT}{P \times MW_{HNS}/1000}(P_{pip} - P)} \tag{9}$$

MW_{HNS} : Molar weight of the HNS [g/mol]

5.2. Initial conditions

The timestep of the model is computed to have a uniform initial size of the element.

$$\Delta t = \frac{\sqrt{\frac{A}{\pi}} \cdot x}{U \cdot n_{tr}} \tag{10}$$

Δt : model timestep [s]
n_{tr} : How many timestep between two particles releases []
x : Ratio of the height on the radius of the element at the start []. 0.5 means that the element has a radius equals to two times its height at the source.

The gas is modelled as a succession of Lagrangian particles released after one another. The particle i is attributed a mass of gas m_{gi}, initially:

$$m_{gi} = Q\rho_g n_{tr}\Delta t \tag{11}$$

m_{gi} : Mass of gas in the particle (initially pure HNS) [kg]

Q : Leakage flow rate [m³/s]

The particle is then attributed a cylindrical volume of height h_i [m] and radius b_i [m] in which all the gas is located. Initially this volume is enclosing only gas, but more and more water will be enclosed in the volume as it increases in size and the gas dissolve. This water is not represented by the particle, but it is the volume of water the bubble affected to this particle are in. The initial height is given based on the gas exit velocity by the following equation:

$$h_i = U n_{tr} \Delta t \tag{12}$$

h_i : Height of the cylinder [m]

Using perfect gas law, the occupied volume by the gas is:

$$V_{gi} = \frac{\frac{m_{gi}}{MW_{HNS}/1000} R T_i}{P_i} \tag{13}$$

V_{gi}: volume of gas [m³]

The initial radius is then given by:

$$b_i = \sqrt{\frac{V_{gi}}{h_i \pi}} \tag{14}$$

b_i : Radius of the cylinder [m]
From the height and the radius, a ratio can be computed as follows:

$$g_i = \frac{b_i}{h_i} \tag{15}$$

g_i : ratio of the radius to the height [] (stays constant for the entire rise of the particle in the water column, until it reaches close to the surface)
The gas is assumed to be inside bubbles of diameter d_i. This diameter is given randomly to each particle, with a probability given by this equation (lognormal distribution):

$$f(d_i) = \frac{1}{d_i \sigma_b \sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{\ln(d_i) - \mu_b}{\sigma_b}\right)^2} \tag{16}$$

d_i : Bubble diameter for the particle i [m]
σ_b : Standard deviation of the bubble size [m]
μ_b : Average diameter of the bubble [m]

The number of bubbles N_i in the bubble is defined as follow:

$$N_i = \frac{V_{gi}}{\frac{4}{3}\pi\left(\frac{d_i}{2}\right)^3} \tag{17}$$

And the number of moles in a bubble is defined as:

$$n_i = \frac{1000 \times \rho \times \frac{4}{3}\pi\left(\frac{d_i}{2}\right)^3}{MW_{HNS}/1000} \tag{18}$$

n_i : number of moles of gas in a single bubble [mol]

5.3. Particle simulation

The particle simulation is divided in three phases for each particle:

- Movement
- Increase of particle size
- Dissolution

Initially only containing gas, the particle size will increase, this represents the amount of water incorporated between the bubble, and the particle size then represents the extent of the spreading of bubbles in the water. The model can simulate several gas j, but at the start only the HNS from the release is present in the element, the other gases are dissolved in the layers.

5.3.1. Movement

The particle move is advected of the current and the particle slip velocity as follows:

$$\overrightarrow{P_{\imath(t+\Delta t)}} = \overrightarrow{P_{\imath(t)}} + \left(\overrightarrow{V_w} + \vec{\boldsymbol{k}}\, w_{si}\right)\Delta t \tag{19}$$

$\overrightarrow{P_{\imath(t)}}$: Position of the particle at the time t [m]
$\vec{\boldsymbol{k}}$: unitary vertical vector []
w_{si} : slip velocity of the bubble [m/s] (terminal velocity)

If the vertical distance between the source and the particle is less than H_J, the movement will instead follow these equations:

$$P_{i(t+\Delta t)x} = P_{i(t)x} + V_{wx}\Delta t \tag{20}$$

$$P_{i(t+\Delta t)y} = P_{i(t)y} + V_{wy}\Delta t \tag{21}$$

$$P_{i(t+\Delta t)z} = P_{i(t)z} + \left(\left(V_{wx} + \ w_{si}\right)\frac{H_w - P_{i(t)z}}{H_j} + U\left(1 - \frac{H_w - P_{i(t)z}}{H_j}\right)\right)\Delta t \tag{22}$$

Co-funded by
the European Union

The horizontal movement stays the same, the vertical velocity is linearly interpolated between the terminal vertical velocity of the bubble and the current and the velocity of the jet along the characteristic length H_J of the jet.

5.3.2. **Bubble rising velocity** (Clift, Grace, and Weber 1978)

Bubble volume estimation

The volume is computed from the content of bubble for each particle class, it is assumed they are spherical:

$$V_i = \frac{n_i R T_i}{P_i} \tag{23}$$

V_i : volume of the bubble [m³]

Bubble area estimation

The area of the bubble is computed from the volume:

$$A_i = 4\pi \sqrt[3]{\frac{3V_i}{4\pi}}^{2} \tag{24}$$

A_i: area [m²] of the bubble

Bubble radius

The radius of the bubble is computed from the volume:

$$r_i = \sqrt[3]{\frac{3V_i}{4\pi}} \tag{25}$$

r_i: radius [m]

Selection of the regime

To assess the velocity, the interfacial tension is needed, it is estimated from ("Water-Gas Interfacial Tension - an Overview | ScienceDirect Topics," n.d.), it has been validated on hydrocarbon.

$$\sigma_{hwj} = 111(\rho_w - \rho_j)^{1.024} \left(\frac{T}{T_{crit(j)}}\right)^{0.3125} \tag{26}$$

ρ_j: density of chemical j [kg·m^{-3}]
ρ_w : water density [kg·m^{-3}]
$T_{crit(j)}$: critical temperature of product j [K]

The interfacial tension is then estimated for the entire bubble as the weighted average of the one of each of the products inside of it at the timestep.

Eötvös and Morton are then computed (the absolute value is used):

$$Eo_i = \frac{g\left(\rho_w - \rho_g\right){d_i}^2}{\sigma_i} \qquad (27)$$

Eo_i: Eötvös number []
g: 9.81 [m·s^{-2}]
σ_i: interfacial tension of product [N·m^{-1}]
d_i: bubble diameter [m] (from the radius at the current timestep)

$$M_i = \frac{g\left(\rho_w - \rho_g\right)\mu_w}{\rho_w^2 {\sigma_i}^3} \qquad (28)$$

M_i: Morton number []
μ_w: water viscosity [Pa·s]

Rigid sphere

If the diameter is less than 1 mm, the bubble is considered spherical and rigid. The bubble velocity then depends on the diameter, the Reynolds number, and a drag coefficient. This requires resolution by iteration, taking a starting velocity of 1 m/s.

$$Re = \frac{w_{si}\rho_w d_i}{\mu_w} \qquad (29)$$

Re_i: Reynolds number []
Reynolds smaller than 1 :

$$w_{si} = \frac{g d_i^{2(\rho_w - \rho_g)}}{18\ \mu_w} \qquad (30)$$

Reynolds between 750 and 350000 :

$$w_{si} = 1.73\sqrt{\frac{g d_i\left(\rho_w - \rho_g\right)}{\rho_w}} \qquad (31)$$

Otherwise, the speed is computed from the drag coefficient:

$$w_{si} = \sqrt{\frac{4 g d_i\left(\rho_w - \rho_g\right)}{3\rho_w C_{Di}}} \qquad (32)$$

C_D: drag coefficient []
The drag coefficient is estimated from one of these equations:
Reynolds under 20 :

$$C_{Di} = \frac{24}{Re_i}\left(1 + 0.1315\ {Re_i}^{0.82 - 0.05\log_{10} Re_i}\right) \qquad (33)$$

Reynolds under 260 :

$$C_{Di} = \frac{24}{Re_i}\left(1 + 0.1935\ {Re_i}^{0.6305}\right) \qquad (34)$$

Reynolds under 1500 :

$$C_{Di} = 10^{1.6435 - 1.1242\ \log_{10} Re_i + 0.1558\ (\log_{10} Re_i)^2} \qquad (35)$$

Reynolds under 4·10^5 :

$$C_{Di} = 29.78 - 5.3\log_{10} Re_i \tag{36}$$

Reynolds under 10^6 :

$$C_{Di} = 0.1\log_{10} Re_i - 0.49 \tag{37}$$

Reynolds above 10^6 :

$$C_{Di} = 0.19 - \frac{800000}{Re_i} \tag{38}$$

Ellipsoïd

If the bubble is between 1 and 15 mm in diameter, the Eötvös number is below 40 and the Morton number is below 0.001, its velocity is calculated using the following equations:

$$H_i = \frac{4}{3} Eo_i {M_i}^{-0.149} \left(\frac{\mu_w}{0.009}\right)^{-0.14} \tag{39}$$

H_i smaller than 59.3:

$$J_i = 3.42{H_i}^{0.441} \tag{40}$$

H_i between 59.3 and 2 :

$$J_i = 0.94{H_i}^{0.757} \tag{41}$$

If H_i is smaller than 2, the bubble is considered « spherical cap » as described in the next section. Otherwise:

$$w_{si} = \frac{\mu_w}{d_i \rho_g} {M_i}^{-0.149}(J_i - 0.857) \tag{42}$$

« Spherical cap »

If the bubble is too big to be a sphere and does not have the requirement to be an ellipsoid, it follows the spherical cap regime:

$$w_{si} = 0.711\sqrt{\frac{g(\rho_w - \rho_g)d_i}{\rho_w}} \tag{43}$$

5.3.3. Increase of particle size

Jet phase

The particle will then incorporate some water between the bubble, increasing its size. The total volume of the particle is given as

$$V_{Ti} = b_i^2 \pi h_i \tag{44}$$

V_{Ti} : volume of the particle [m³]
This volume increases as follows:

$$V_{Ti(t)} = V_{Ti(t-1)} + Q_e \Delta t \tag{45}$$

Q_e : flow rate of water incorporated in the Lagrangian particle [m³/s]
A new radius and height can be computed, as follows:

$$h_i = \sqrt[3]{\frac{V_{Ti(t)}}{\pi g_i^2}} \tag{46}$$

$$b_i = g_i h_i \tag{47}$$

The flow rate of water is then incorporated as:

$$Q_e = Q_s + Q_v \tag{48}$$

Q_s : flow of water added to the element due to shear induce entrainment between the jet and water [m³/s]
Q_v : flow of water added to the element due to the advection of current [m³/s]

$$Q_s = 2\pi b_h h_k \alpha\, w_{si} \tag{49}$$

$$\alpha = \sqrt{2}\,\frac{0.057 + \dfrac{0.554 \sin \varphi}{F^2}}{1 + 5\dfrac{\overrightarrow{V_w}}{w_{si}}} \tag{50}$$

$$F = E\,\frac{w_{si}}{\sqrt{g\left(\dfrac{\Delta\rho}{\rho_w}\right) b_k}} \tag{51}$$

E : equals 2

$$\begin{cases} Q_{vx} = \rho_w |u_w| \left[\pi b_k \Delta b_k |\cos\theta\cos\phi| + 2b\Delta s\sqrt{1-\cos^2\theta\cos^2\phi} + \dfrac{\pi {b_k}^2}{2}|\Delta(\cos\theta\cos\phi)|\right] \\ Q_{vy} = \rho_w |v_w| \left[\pi b_k \Delta b_k |\sin\theta\cos\phi| + 2b\Delta s\sqrt{1-\sin^2\theta\cos^2\phi} + \dfrac{\pi {b_k}^2}{2}|\Delta(\sin\theta\cos\phi)|\right] \\ Q_{vz} = \rho_w |w_w| \left[\pi b_k \Delta b_k |\sin\phi| + 2b\Delta s|\cos\phi| + \dfrac{\pi b^2}{2}|\Delta(\sin\phi)|\right] \end{cases} \tag{52}$$

u_w, v_w, w_w : the ambient velocity $\overrightarrow{V_w}$ components [m/s]
θ_k and ϕ_k are angle between V_a' and w_{si}

Advection phase

When the element is only rising due to the current and the bubble buoyancy, the increase in size of the element is driven by the turbulent diffusivity as follows:

$$h_{i(t+\Delta t)} = h_{i(t)} + \sqrt{2\frac{K_z}{t_{pi}}\Delta t} \qquad (53)$$

t_{pi} : time since the element has change from the jet phase to the advection phase [s]

$$b_{i(t+\Delta t)} = \sqrt{b_{i(t)}^2 + \frac{4K_{XY}\Delta t}{\pi}} \qquad (54)$$

5.3.4. Transfer between bubble and water (Legrand et al. 2017)

All the j chemicals can be transferred between the water and the bubble.
« Le Bas » critical molar volume estimation :

- Organic

$$v_l = 4.9807 \times (MW_j)^{0.6963} \qquad (55)$$

- Inorganic

$$v_l = 2.8047 \times (MW_j)^{0.651} \qquad (56)$$

v_{lj} : critique molar volume [cm³·mol⁻¹]

$$D_{cj} = \frac{13.26 \times 10^{-5}}{\mu^{1.14} v_{lj}^{0.589}} \qquad (57)$$

D_c : diffusion coefficient [cm²·s⁻¹]
The transfer per bubble for a given layer is defined as :

$$\frac{dn_{jik}}{dt} = K_j A_i (C_{sj} - C_{kj}) \qquad (58)$$

K_j: transfer coefficient [m·s⁻¹]
C_{kj} : concentration of chemical j in the layer k [mol/m³]
$\frac{dn_{jik}}{dt}$: dissolution rate per bubble [mol·s⁻¹] (if smaller than 0, the product will go in the bubble)
C_{sj}: solubility of the product [mol/m³], computation as:

$$C_{sj} = PX_{ji}H \qquad (59)$$

X_{ji} : Molar fraction of j []
H_j : Henry constant of j [mol·m⁻³·Pa⁻¹]

$$\begin{cases} K = 1.13\sqrt{\dfrac{S_{di}}{0.45+0.2d}}D_{cj}^{a}, d_i < 0.5cm \\ K = 6.5D_{cj}^{a}, 0.5 < d_i \leq 1.3cm \\ K = 6.94{d_i}^{-1/4}D_{cj}^{a}, d_i > 1.3cm \end{cases} \tag{60}$$

a : diffusion exponent, between $1/2$ (bubble « clean ») and $2/3$ (bubble « dirty »)

In the case the bubble is in more than one layer of water, a transfer rate is then estimated for all the layers impacted, and each of them receive an amount:

$$\frac{dn_{Tjik}}{dt} = \frac{dn_{jik}}{dt} \times N_i \times \frac{l_{ik}}{h_i} \tag{61}$$

n_{Tjik} : total number of moles of j for the fraction of particle i in the layer k [mol]
l_i : height of the particle i included in the layer k [m]
For each layer in the column including some of the particle:

$$n_{jk(t)} = n_{jk(t-1)} + n_{Tjik}\Delta t \tag{62}$$

n_{jk} : number of moles of j in the k layer [mol]
Then, for mass conservation on the particle part:

$$n_{ij(t)} = n_{ij(t-1)} - \frac{\sum_k n_{Tjik}}{N_i}\Delta t \tag{63}$$

n_{ij} : number of moles of j in a bubble of the particle i [mol]

$$n_i = \sum_j n_{ij} \tag{64}$$

5.3.5. Behavior at the water surface

When the top of particle reach the surface of the water ($P_{iz} + \frac{h_i}{2} > 0$), h_i is decreased and P_{iz} adapted to still stay at the mass center:

$$\begin{gathered} h_i' = \frac{h_i}{2} - P_{iz} \\ P_{iz}' = -\frac{h_i'}{2} \end{gathered} \tag{65}$$

All the bubbles in the upper part are then gone in the atmosphere:

$$N_i' = N_i \times \left(1 - \frac{h_i'}{h_i}\right) \tag{66}$$

And the volume of gas that has leaved is then accounted for:

$$V'_{Ti} = V_{Ti} - \left((N_i - N'_i) \times V_i\right) \tag{67}$$

From there, the new radius of the particle can be computed, such as in equation 14. Once the particle is fully outside of the water, it is removed from the simulation.

5.4. Water simulation

These processes are executed before the particles dissolution.

5.4.1. Layer boxes

The water column is divided into many layer k. A box is attributed to each layer, composed of 4 points at the bottom of the layer, and 4 other points at the vertical of the 4 first points. The coordinates are : $x_{0k}, x_{1k}, y_{0k}, y_{1k}, z_{0k}, z_{1k}$. z_{0k} and z_{1k} are respectively the bottom and the top values of the layer k, and stays constant for the entire simulation. $x_{0k}, x_{1k}, y_{0k}, y_{1k}$ are initially undefined. Once at least one particle has reached the layer k, these values are updated as follow:

$$\begin{aligned} x_{0k(t)} &= min\left(x_{0k(t-1)} + u_w\Delta t,\ min(\forall P_{ix} - b_i)\right) \\ y_{0k(t)} &= min\left(y_{0k(t-1)} + v_w\Delta t, min(\forall\ \ P_{iy} - b_i)\right) \\ x_{1k(t)} &= max\left(x_{1k(t-1)} + u_w\Delta t,\ max(\forall P_{ix} + b_{i)})\right) \\ y_{1k(t)} &= max\left(y_{1k(t-1)} + v_w\Delta t, max(\forall P_{iy} + b_i)\right) \end{aligned} \tag{68}$$

Only the particles at the layer depth are considered. The goal of this is to make the volume drift horizontally with the current and increase in size to always include all the particles at their depth.

$$l_{ik} = \left| clamp\left(\frac{z_{1k} - P_{iz} - \frac{h_i}{2}}{z_{1k} - z_{0k}}\right) - clamp\left(\frac{z_{1k} - P_{iz} + \frac{h_i}{2}}{z_{1k} - z_{0k}}\right)\right| \times (z_{1k} - z_{0k}) \tag{69}$$

And $clamp(x) = \begin{cases} 0 \text{ if } x \ \leq 0 \\ x \text{ if } 0 \ < \ x \ < \ 1 \\ 1 \text{ if } x \ \geq 1 \end{cases}$

5.4.2. Estimation of the concentration

To estimate the concentration of compound in the water column the boxes in each layer are used:

$$C_{kj} = \frac{n_{jk}}{(x_{1k} - x_{0k}) \times (y_{1k} - y_{0k}) \times (z_{1k} - z_{0k})} \tag{70}$$

The dissolved gas already present in the seawater has a concentration that is kept constant.

5.4.3. Transfer between layers

If a layer has a different concentration in chemical compared to another layer, some exchange will occur due to the vertical diffusion.

$$n_{kj(t+\Delta t)} = n_{kj(t)} - A_{k,k+1} K_z \frac{C_{kj} - C_{k+1j}}{z_{1k} - z_{0k}} \Delta t \tag{71}$$

5.4.4. Volatilization (Lyman, Reehl, and Rosenblatt 1990)

Volatilization is the process for the transfer of the pollutant from the dissolved fraction to the evaporated one, at the surface of the water. Only the top water layer can transfer to the atmosphere.

H: Henry law constant [atm m³/mol]
P_{vp}: vapor pressure of the compound [atm]
S: solubility [mol m^{-3}]
If $\frac{1}{H_j} < 0.03$, volatilization is ignored.
H' : nondimensional Henry constant:

$$H_j' = \frac{1}{RTH_j} \tag{72}$$

Compute the liquid phase exchange coefficient
If M < 65 (g/mol)

$$k_l = 20\sqrt{\frac{44}{MW_j}} \tag{73}$$

k_l: liquid phase exchange coefficient [cm h^{-1}]
Else (approximative), if windspeed < 3 m/s:

$$k_l = 2.5$$

if windspeed < 6 m/s

$$k_l = 10$$

if windspeed < 10 m/s

$$k_l = 23$$

if windspeed > 10 m/s

$$k_l = 50$$

Compute the gas phase exchange coefficient
If MW_j < 65:

$$k_g = 3000\sqrt{\frac{18}{MW_j}} \tag{74}$$

k_g: gas phase exchange coefficient [cm h^{-1}]
If the molar mass is greater than 65:

$$k_g = 1137.5(V_{wind} + V_{curr})\sqrt{\frac{18}{MW_j}} \tag{75}$$

V_{wind}: wind speed [m s^{-1}]
V_{curr}: current speed [m s^{-1}]

Compute the overall liquid phase mass transfer coefficient

$$K_{Lj} = \frac{H'\, k_g\, k_l}{H'\, k_g + k_l} \tag{76}$$

K_{Lj}: mass transfer coefficient [cm hr^{-1}]

Compute the flux

With the following equation, assuming the concentration of chemicals in the atmosphere is negligible.

$$N_j = K_{Lj} C_{lj} \tag{77}$$

l: Index of the top layer []
N_j: flux [mol cm^{-2} h^{-1}]

$$n_{kj(t+\Delta t)} = n_{kj(t)} - N_j(x_{1k} - x_{0k}) \times (y_{1k} - y_{0k})\frac{3600}{10000}$$

6. Conclusion

A new model has been developed to simulate the ascent of gas from underwater sources. It is capable of handling a wide range of chemical substances, providing valuable support to emergency responders in determining the most appropriate course of action during HNS release incidents.

The model simulates the behaviour of gas as it rises through the water column, from the point of release to the water surface, including gas transfer processes between the water and the atmosphere. This includes both dissolution into the water and volatilization into the air, capturing key mechanisms involved in gas dispersion.

The model is publicly available on GitHub under the European Union Public License (EUPL), allowing users to freely download, use, and further develop the tool.

7. References

Clift, R., John R. Grace, and Martin E. Weber. 1978. *Bubbles, Drops, and Particles*. New York: Academic Press.

Legrand, Sébastien, Florence Poncet, Laurent Aprin, Valérie Parthenay, Eric Donnay, Gabriel Carvalho, Sophie Chataing-Pariaud, et al. 2017. "Modelling Drift, Behaviour and Fate of HNS Maritime Pollution, HNS-MS Final Report, Part II." Royal Belgian Institute of Natural Sciences; CEDRE; ARMINES, Ecole des Mines d'Alès; Alyotech France; Belgian FPS Health, food chain safety and environment.

Lyman, J.L., W.F. Reehl, and D.A. Rosenblatt. 1990. *Handbook of Chemical Property Estimation Methods*. Whashington D.C.: Americain Chemical Society.

"Water-Gas Interfacial Tension - an Overview | ScienceDirect Topics." n.d. Accessed August 31, 2023. https://www.sciencedirect.com/topics/engineering/water-gas-interfacial-tension.