Promote financial instruments for liability on environment (LIFE PROFILE)

Action B.1: Environmental damage risk assessment for key-category activities as ranked in action A1

Deliverable B.1. Environmental risk assessment methodology and implementation for each examined activity category

PROmote Financial Instruments for Liabilty on Environment

Athens, October 2024

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Abbreviations

ELD	Environmental Liability Directive
EU	European Union
GIS	Geographical Information System
GRIFFIN	Griffin Environmental Consulting
HSE	Health and Safety Executive
IMPEL	European Union Network for the Implementation and Enforcement of Environmental Law
IRAM	Integrated Risk Assessment Method
IUCN	International Union for Conservation of Nature and Natural Resources
MEE	Ministry of Environment and Energy
METDC	Ministry of the Ecological Transition and the Demographic Challenge
NACE	Nomenclature of Economic Activities
NCSR	National Centre of Scientific Research
NOA	National Observatory of Athens
NTUA	National Technical University of Athens
PD	Presidential Decree
PNEC	Predicted No-Effect Concentration
UHER	Panteion University

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Executive Summary

The deliverable entitled "Environmental risk assessment methodology and implementation for each examined activity category" presents the risk assessment framework, which is developed to assist the prevention and the remediation of environmental damage. The developed framework is in line with the European Directive 35/2004/EC, which calls the EU Member States to incorporate in their legislation the Directive's provisions that render each operator whose activity can cause or threaten to cause environmental damage in protected species and natural habitats as environmentally liable. The aim of the framework is to support all stakeholders, namely, regulators, operators, and insurers, to assess the environmental risk that may be caused by potential accidents during the operation of the activities selected in Deliverable A1.3 of the LIFE Profile project. However, the framework is potentially applicable not only for these selected key-activities but for every activity while it can be incorporated in each EU Member State.

The proposed risk assessment framework considers environmental impairments as the consequences that the initiating events can cause on specific natural resources and regarding biodiversity on habitats. Therefore, the risk assessment framework follows a resource-oriented approach while from the biodiversity perspective it follows a habitat-oriented approach. As a result of the adoption of the aforementioned approaches, three models are developed or identified, each of which is associated with certain type of natural resource and habitat, as well. These models are: (i) the model for surface soil (ii) the model for soil together with groundwater, and (iii) the two models for surface water, i.e. lakes and rivers.

Testing process results illustrate the robustness of the developed methodology in various key-activities and under various conditions. In particular, the analysis of the fire accident that occurred in a recycling factory in Aspropyrgos in the region of Attica in June 2015 indicates that the results of the developed Gaussian air dispersion model, which is part of the surface soil model, do not diverge significantly bearing in mind the limitations of Gaussian dispersion models, since the pollutant concentration presented in post-accident reports is similar to the surface soil model's results. Meanwhile, the consequences on both the habitat and natural resources, although presented in numerical values in the developed surface soil model, resulted to the same conclusions comparing to the conclusions of the post-accident reports especially regarding the significant concentration of heavy metals in the examined area, which is a 4km-radius-area around the fire location.

The second case study, which examines the extrusion process of aluminium, including activities like hot or cold rolling, is analysed for its potential environmental risks. Given the lack of real accident data in the Ministry of Environment and Energy databases, theoretical scenarios are developed to evaluate the impact on soil and groundwater, rivers, and lakes using the proposed risk assessment models. The analysis focused on the potential release of sulphuric acid, a significant auxiliary material used in surface treatment, which could severely affect the environment in the event of a leak. The testing process highlighted the high risk of contamination through underground transportation networks and nearby rivers, particularly during normal operations or due to waste treatment failures. Additionally,

a hypothetical scenario involving a tanker spill is introduced to assess the risk of lake contamination. The results of these scenarios are then compared against the environmental thresholds for sulphuric acid, demonstrating the framework's effectiveness in estimating contamination risks under various conditions for a radius of 2 km around the key-activity.

In conclusion, this report introduces a robust risk assessment framework that aligns with European Directive 2004/35/EC, helping Greece as well as every EU Member State to prevent and remediate potential environmental damage. Designed to support regulators, operators, and insurers, the framework applies to various industrial activities and can be adaptable across the EU. It incorporates models for assessing impacts on surface soil, soil and groundwater, and surface water, and was validated through both real-world and theoretical scenarios. The framework effectively simulates environmental risks, providing a tool for supporting the evaluation of potential impacts on natural resources and habitats.

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1. Introduction

1.1. Purpose of the Deliverable

The purpose of Action B.1 of the program LIFE PROFILE 19 GIE/GR/001127 is the development of a framework that will assess the risk to the environment, and especially on the biodiversity, resulting from potential accidents during the operation of the ten key-category activities, which were selected in Deliverable A.1.3. The developed framework will enable both practitioners and regulators to evaluate each facility that belongs to the group of the selected activities based on the potential environmental damage they can cause. Meanwhile, by providing Action B.2 with the required data for the economic evaluation of the environmental damage, the ultimate goal of the developed framework is to support all the relevant with the environmental protection stakeholders (refer to Action A.3 – Deliverable 3.2) to assess the environmental risk of the examined facility, and as a result inform them in order to receive all the appropriate measures to avoid or mitigate potential impairment of the environment.

1.2. Implementation phases/steps

Action B.1, and correspondingly Deliverable B.1, was implemented by the research team of the School of Mechanical Engineering of the National Technical University of Athens (NTUA), in collaboration with the Ministry of Environment and Energy (MEE/COIEL), University Research Institute of Urban Environment and Human Resources, Panteion University (UHER) and Griffin Environmental Consulting LP (GRIFFIN). The leader for the implementation of Action is NTUA. The final development of the methodology was achieved with the collective contribution of all partners, considering all their critical inputs during the implementation process of the Action.

The steps followed for the implementation of Action B.1 were the following:

Step 1: Method selection

As far as the probabilities are concerned, based on the outcome of Action A.1.2, the proposed framework is developed by considering the event tree technique as the appropriate tool for identifying the probabilities of each examined environmental system after the initiating event.

Step 2: Determination of Baseline conditions - Criteria selection

The record of the initial conditions before an environmental accident is of primary importance for the proper assessment of the subsequent impacts. A set of crucial parameters-criteria is determined concerning the under-examination activity to be used as a baseline. Inputs from Deliverables A.1.2 and A.1.3 have also been considered for the criteria selection process.

Step 3: Development of the Scenarios sets.

In this phase, a list of the initiating events is defined in accordance with the standardization of critical accidents in national legislations and the methodologies currently being used (e.g., database of Spanish

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Methodology SIRMA, IRAM's checklist, etc.). Based on the list of initiating events, the event trees will create multiple paths of scenarios to estimate the detailed scenario sets.

Step 4: Consequences estimation

The developed framework provides estimates for environmental risk on both surface and underground water, soil, and air (in case surface soil and biodiversity is affected, since ELD excludes air from its scope). Therefore, multiple techniques are incorporated for modelling all the natural resources, namely a Gaussian model for estimating the effect of air toxicity on soil and biodiversity, three-dimensional approaches for estimating underground soil pollution, surface water pollution and groundwater pollution. During this phase of Action B1, several workshops among the collaborative partners MEE/COIEL, UEHR and Griffin as well as meetings with biodiversity experts in the seminar organized by Prof. Parmakelis at the Ministry of Energy and Environment June 2024 took place (for more details see Deliverable B.2).

Step 5: Testing process

The aim of this step is to assess the robustness of the developed methodology based on real case studies, where existed. Initially, in order to test the framework, and particularly the surface soil model, the analysis of the fire accident that occurred in a recycling factory in Aspropyrgos in the region of Attica in June 2015, is performed based on the reports provided by the MEE/COIEL. The results do not diverge significantly bearing in mind the limitations of Gaussian dispersion models, since the pollutant concentrations presented in post-accident reports are similar to the surface soil model's results. Meanwhile, the consequences on both the habitat and natural resources, although presented in numerical values in the developed surface soil model resulted to the same conclusions comparing to the conclusions of the post-accident reports especially regarding the significant concentration of heavy metals in the examined area around the fire location. Given the lack of real accident data in the Ministry of Environment and Energy databases, theoretical scenarios are developed to evaluate the impact on soil and groundwater, rivers, and lakes using the proposed risk assessment models. The results highlighted the high risk of contamination through underground transportation networks and nearby rivers, particularly during normal operations or due to waste treatment failures.

1.3. Structure of the Deliverable

The current Deliverable is structured in 5 Sections, and 1 Appendix as follows:

Section 1: Section 1 presents the scope of the Deliverable, the stages followed for its implementation and its structure.

Section 2: Sections 2 describes, briefly, the developed risk assessment framework.

Section 3: Section 3 analyses in depth the developed risk assessment framework.

Section 4: Section 4 applies the models included in the developed risk assessment framework in various case studies in order to test their validity and applicability.

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<u>Section 5</u>: Section 5 includes conclusions and limitations for the use of the developed method.

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2. Risk Assessment Framework – Overview

In this section an overview of the developed risk assessment framework is presented prior to proceeding to the detailed description of its models and its function. In brief, the flowchart of the developed framework consists of five (5) distinct phases following a sequential process as it is depicted in Figure 1.

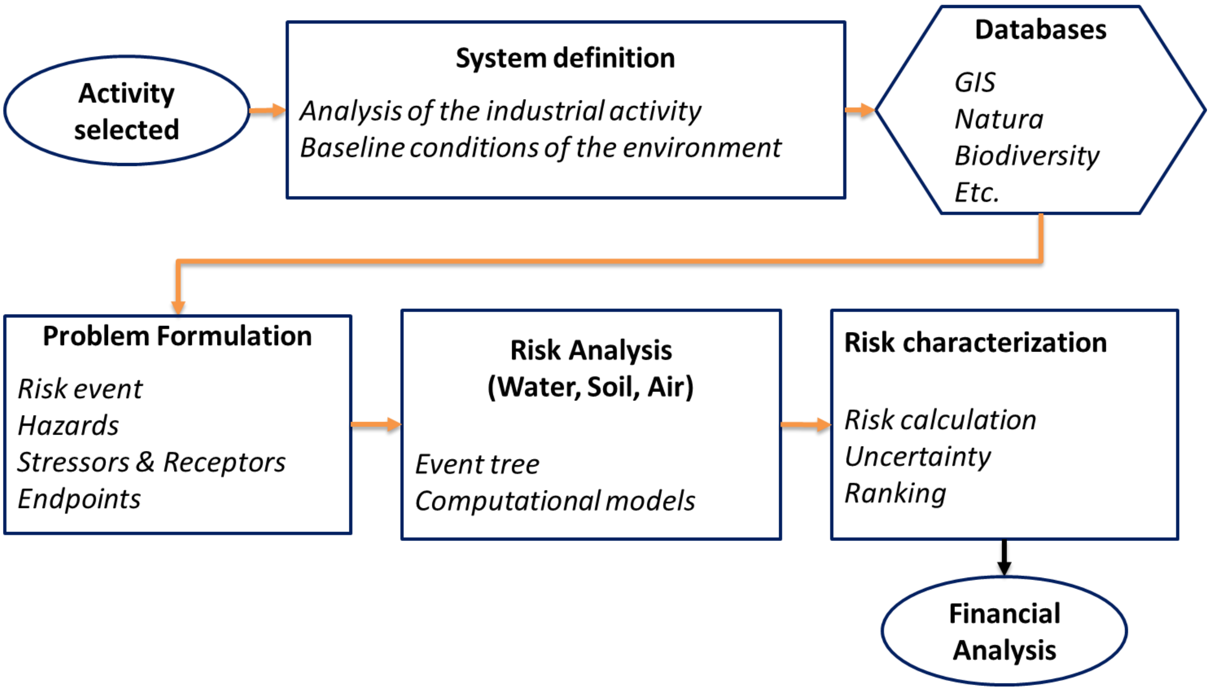

Figure 1: *Flowchart of the developed risk assessment framework*

Initially, the first phase is the selection of the examined activity. Bearing in mind that based on Deliverable A.1.3 of the LIFE PROFILE project, ten (10) activities were selected since these were considered as key-category activities based on the combination of their criticality in causing potential accidental events and their significant role their sectors possess for the Greek economy (PROFILE, 2022c). Therefore, the framework is designed to embed certain databases regarding accidental events and chemical substances for each of these key-activities. However, due to its generic structure, it should be mentioned that the developed risk assessment framework is designed to address potential accidents regardless of the type of the industrial activity is selected.

The second phase of the framework deals with the definition of the examined system. The examined system is divided into two major parts, namely, the industrial activity and the environment. Firstly, the developed framework focuses on the analysis of the examined industrial activity. In detail, the legislation under which the activity must conform with is identified, the operation parameters of the activity as well as the safety measures/barriers are recorded, which will be used in the subsequent event tree analysis (e.g. tanks, boilers, shelters, warning systems, human parameters, surveillance

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systems, etc.). Afterwards, the baseline conditions of the environment are identified and recorded since the launch of the Directive 35/2004/EC introduced the need of considering the baseline conditions (EC, 2004). To this respect, the condition of the environment prior to accident are estimated by taking into account the concentration of the examined chemical substance in both habitats and natural resources in order to assist the risk calculation in the next phases of the framework.

Subsequently, the ecological risk assessment process is followed. With this respect, specific databases associated with the developed framework are used. Initially, a Geographic Information System (GIS) will support the identification of the location of the examined accident in the region as well as the calculation of the affected area. These results will assist the economic evaluation that will be conducted in Deliverable B2.2 of the LIFE Profile project (PROFILE, 2024). Furthermore, databases containing Natura sites within the European Union (Natura, 2000), land uses through the Corine database, and Biodiversity information (IUCN, 2023) are also associated with the framework, although the results of the calculation process regarding these issues is also conducted in Deliverable B2.2 of the LIFE Profile project (PROFILE, 2024).

Regarding the ecological risk assessment process that is part of the developed risk assessment framework, its first step is the problem formulation. In this step, the detailed description of the examined event is conducted, namely, its type (e.g. fire, leakage, rupture, etc.), the chemical substance or the stressor included, the natural resource and habitat or receptors being affected. A significant point that is defined in this stage is the endpoint of the analysis since this is strongly related with the consequences part (see section 4.3). In general, the endpoint is considered as the end of the examined accidental or initiating event. Therefore, the consequences of the event at the time the accidental event ends are calculated. This approach stems primarily from the need of regulative authorities as well as the rest stakeholders to be aware of the direct consequences an initiating event causes on the environment. However, it should be mentioned that this approach does not restrict the capability of the framework to analyse the consequences in any time frame. For instance, in case the pollution of soil due to air is estimated from another event that can be examined by the model considering as the initiating event the surface soil pollution and aiming to estimate how this event affects both soil and underground water, as well.

Having conducted the problem formulation, risk analysis is performed. This phase is separated in two parts, the hazard and consequence analysis parts. As far as the hazard analysis part is concerned, it deals with both, the probabilities or frequencies, in case an ex-post analysis of an accident is examined, and the event tree analysis, which is incorporated in the developed framework. A detailed analysis on the event tree analysis is presented in section 4.3. Regarding the consequences estimation part, due to different modelling requirements of each natural resource and habitat, three different models are developed. The first model estimates the environmental consequences in surface soil due to air pollution, the second model estimates environmental consequences in soil and underground water, the third model estimates the environmental consequences in lakes, and the fourth model in rivers. Each of the aforementioned models works in different time frames and incorporates different modelling techniques and assumptions. A detailed analysis on the event tree analysis is presented in section 4.3. All the models follow a single-stressor approach since environmental consequences are

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considered as the concentration of the chemical pollutant in both the examined area or else habitat and the volume of the natural resource, water or soil, affected by the pollutant in the examined area.

At last, risk characterization phase is followed. In this phase, the risk calculation is conducted to assist the ranking of the scenarios being developed in the event tree analysis. In addition, a weighting process is performed to identify the criticality of the examined system's parameters. In the end, the uncertainty associated with the environmental risk is estimated and depicted.

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3. Key Activity Characteristics

The documentation of the key characteristics of the industrial facilities is critical for assessing the environmental impact of potential future accidents, as they inform the accident scenarios and their probability of occurrence. This chapter will outline what this documentation should entail.

3.1. Industrial Facility Details

First, the type of the industrial activity, it's NACE code and a detailed operating plan of the unit shall be reported. In addition, a production process flow diagram would be useful for the later stages of identifying the possible accident scenarios. Next, the following details of the industrial facility need to be included for a comprehensive documentation of its operations:

1. List of Raw Materials
2. Quantities of Raw Materials required
3. Auxiliary Materials - Additives
4. Main Product
5. Secondary Product
6. Production Capacity
7. Operation Time (i.e. how old is the facility and the related equipment)
8. Surface Area of the Site
9. Installed Nominal Power (kW)
10. Number of Employees
11. Description of Buildings and Other Facilities
12. Description and Quantities of Equipment
13. Types, Quantities and Capacities of Storage Tanks
14. Expected Quantities of Waste from the production process
15. Waste Management Processes
16. e-Waste (i.e. discarded electrical equipment) Management
17. Liquid Waste from the industrial production process
18. Rainwater Distribution
19. Distribution of Wastewater from the Facility Personnel
20. Available Prevention and Remediation Techniques

In addition to the details of the facility's operations, its location, and the baseline condition of its surrounding environment are of paramount importance.

3.2. Industrial Facility Location & Existing Environmental Condition

This section addresses the required documentation of the existing environmental conditions of the area where the industrial facility is located. For this, the exact location (i.e. coordinates) of the facility is needed. This will determine the resources under risk, the probability of occurrence of floods and earthquakes and the general existing environmental situation.

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Resources under risk entail the flora and fauna of the area, the forest land, the soil, air, surface and underground water. It is, therefore, crucial to record the distance from protected areas (e.g. Natura 2000 areas or other protected areas), from forest land, as well as the land use of adjacent areas.

In order to assess the environmental impact of an accident in the premises of the industrial facility, the existing environmental situation of the area needs to be evaluated. For this, the following details of the area, where the industrial facility is located, need to be documented:

1. Climatic and Bioclimatic Characteristics
2. Morphological and Landscape Characteristics
3. Geological, Tectonic and Soil Characteristics
4. Surface Water Bodies
5. Groundwater Bodies
6. Current Condition of the Natural environment; Flora and Fauna
7. National System of Protected Areas
8. Forests and Woodlands
9. Existing Sources of Pollution or other Pressures on the Environment
10. Exploitation of Natural Resources
11. Assessment and Evaluation of the Existing Soil, Water and Air Quality in the Area based on available data

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4. Developed Method

4.1. Development of the scenarios sets

4.1.1. Introduction

The purpose of the Directive 2004/35/EC is to establish a framework of environmental liability based on the polluter pays principle and the precautionary principle, as well (EC, 2004). As far as the precautionary principle is concerned, it urges those who may be legally liable against any environmental damage to take measures in response to the potential accidental events due to their operations (EC, 2004, p. 3). With a view to fulfil the aforementioned goal, the first step of the proposed risk assessment framework is to develop a method in order to facilitate the framework with a reliable tool dealing with the construction and estimation of all the possible scenarios that can evolve after the emergence of an initiating event.

The ultimate goal of this method is to support both practitioners and regulators in evaluating all the potential initiating events that any industrial facility belonging to the group of ten (10) key-category activities selected in Deliverable A.1.3 of the LIFE PROFILE project can cause (PROFILE, 2022c). As a result, it enhances the ability of the proposed framework to inform them in order to examine whether the appropriate measures to mitigate or avoid, if possible, potential impairment of the environment caused by the examined initiating event(s) have been taken or not. Meanwhile, having the ability to adjust to the specific requirements each Member State imposed in its regulation, the proposed risk assessment framework can be applied by each Member State responding thus to the lack of a commonly accepted method on this issue within the European Union (EC, 2021).

4.1.2. Scenario development

The first and foremost step prior to the development of the scenarios sets of the proposed method is the introduction of scenario. Since the aim of the proposed framework is the assessment of the risks and the corresponding damages each selected key-category activity can cause to the environment due to potential accidents during their operation, it is of utmost importance the identification of the “risk events” or “accidental events” or “initiating events”. For the rest of the document the term “initiating event” is used.

An “initiating event” is defined as the first significant deviation from the normal situation of a system (e.g., gas leak or spark of fire, etc.) and which may possibly cause unwanted consequences on the environment (e.g., soil pollution, biodiversity loss, etc.) of the examined system itself as well as on the surrounding area. An initiating event is characterized by the release of chemical substances. Therefore, it can be associated with more than one chemical substance. However, the emergence of an initiating event may lead to many different consequences (Rausand & Hoyland, 2004). The reason for this issue is that most of systems are designed to receive safety measures, the so-called “barriers” that are implemented to reduce or eliminate, if possible, the occurrence or/and consequences of an initiating event (DOE, 1990). As a result, the probability as well as the level of the resulted consequences that an examined event will lead to depends on whether these safety measures will function effectively or not. Meanwhile, consequences can also be affected by additional events, the so-called “risk factors”

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that may arise during the progress of the initiating event (e.g. change of the wind direction after the leakage of a substance, human engagement, etc.).

Therefore, using the term "scenario" a certain path consisted of the initiating event and a number of safety measures and risk factors is considered. Scenario is employed to estimate this path's probability together with the magnitude of the consequences caused until a specific endpoint imposed by the analyst or the regulation is reached. In parallel, the identification of the potential sources of danger is necessary to describe the cause-and-effect relationships between safety measures and the event progression (Rausand & Hoyland, 2004). Hence, development of the scenarios sets leads to a complete set of scenarios, which identify all the potential propagation paths following the occurrence of an initiating event.

4.1.3. Initiating events

As mentioned above, the crucial point of a scenario is the definition of the initiating event. Based on the results provided regarding the existing environmental risk assessment methods in Deliverables A.1.1 and A.1.2 of the LIFE PROFILE project (PROFILE, 2022a,b) and the key activities selected in Deliverable A.1.3 of the LIFE PROFILE project, the list of the initiating events is defined (PROFILE, 2022c).

In addition to the aforementioned Actions, the list is also developed in accordance with the standardization of the critical accidents highlighted in many national databases (PROFILE, 2022a). Initially, the British Health, Safety and Environment (HSE) database is a comprehensive guide on failure rates and event data for use within risk assessments. It provides established failure rates for various items and equipment used in the chemical and process industries, such as vessels, pipelines, and mechanical components (HSE, 2019). Additionally, the Flemish database provides guidelines and failure frequencies for various types of installations and safety systems to be used in the preparation of safety reports for Seveso companies (Flemish Government, 2009).

Furthermore, the methodologies currently being used by the Member States (for those States that have developed such methodologies as it was mentioned in Deliverable A.1.2 of the LIFE PROFILE project) were also reviewed (PROFILE, 2022b). In particular, the database of the Spanish Methodology SIRMA is reviewed (METDC, 2019). The Spanish methodology SIRMA (Sistema de Información de Responsabilidad Medioambiental) is a comprehensive tool designed to assist operators in managing environmental risks and fulfilling obligations under Spain's environmental liability legislation. It encompasses the ARM (Environmental Risk Analysis), IDM (Environmental Damage Index), and MORA (Economic Evaluation of Damages) modules. Operators can identify high-risk elements, estimate environmental damage, and calculate financial guarantees required by law. SIRMA aids in risk management decisions, such as equipment changes or substance substitutions to reduce risks, and provides a framework for estimating the cost of primary, compensatory, and complementary remediation measures for environmental damages.

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The methodologies for the regulation of the inspection frequencies and the methodologies for the calculation of the financial provision cost have different aims, but they both assess risk as the product of effect and probability (risk = effect * probability). However, each method defines and estimates effect and probability differently, highlighting a lack of agreement on a standardized estimation process. In the IMPEL methodology, effect is indicated by impact criteria, while probability is determined by operator performance criteria. The Spanish methodology uses the Environmental Damage Index to represent effect, with probability based on a combination of event trees selected by the operator in the ARM tool. The Irish methodology employs a straightforward risk matrix that considers Likelihood (probability) and Consequence (effect) (PROFILE, 2022b).

The complete list of the initiating events is presented in Appendix 1. It includes, for each event, its description, the type of failure, and the associated probability of occurrence.

It should be noted that the initiating events presented in Appendix 1 are related with the key-categories, therefore, initiating events that do not appear in the selected key-categories are intentionally not included in the final list.

4.1.4. Event tree analysis

Having completed the first branch of the development of the scenarios sets, namely the list of initiating events, each of which requires its own analysis, the identification of specific safety measures and risk factors is carried out prior to proceeding to the estimation of the scenarios sets. To this respect, the event tree analysis is employed.

Event tree analysis is an inductive procedure used to study the effect of an initiating event on an examined system by illustrating all possible outcomes resulting from the initiating event. The choice of this method to incorporate on the risk assessment framework is based on its inductive reasoning that allows the display of all intervening event possibilities and their individual tracks to each possible outcome. In doing so, a complete description of each accident process is possible (Khakzad et al., 2011).

Event tree analysis is based on the initiating event, because the effect of an initiating event on the system and the environment depends on what might happen next and the sequence of occurrence. Therefore, it is important to identify all the possible scenarios along with their occurrence probabilities and their consequences. To do so, a six-step process is followed consists of:

1. The selection of the initiating event, existed in the database (IE_Ej) or inserted (IE_Ij)
2. The identification of the safety measures that are designed to deal with the selected event,
3. The identification of the potential sequences,
4. The determination of the probabilities of occurrence of all safety measures and risk factors,
5. The calculation of the probabilities of each branch, and
6. The calculation of the consequences of each branch.

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After completing the construction of the event tree, the branch probabilities can be estimated (refer to step 4 above) as the intersection of the probabilities of all safety measures and risk factors along a branch. In addition to the probabilities calculation, the consequence for each branch is the other part of the event tree that is also estimated (refer to step 6 above). Commonly, consequences are expressed in different units depending on the type of the examined event. For instance, it is possible to define the consequences of an outcome as pollutant concentration per square/cubic meter of soil or as volume of polluted water, etc. Details on this issue are presented in section 4.3.

At the end of the analysis each branch's outcome is characterised by its own risk. Therefore, based on the specificities of each scenario, the risk mitigation can be conducted either by reducing the occurrence probability through system or component changes or else by reducing the potential consequences through system or component changes to the scenarios, as well.

4.1.5. Design of the method

Bearing in mind the background of the approach employed for the development of the scenarios sets, a brief overview of how the method will work within the software tool is presented.

Initially, the selection of the initiating event, from the list presented in Appendix 1 or insertion of a new, should be conducted. In doing so, the type of the first significant failure of the examined system is recorded while the amount of the toxic substance released in the environment together with its associated probability of occurrence is estimated. It should be noted that apart from the predefined initiating events included in Appendix 1, the method enables the user to create their own initiating events. Subsequently, the introduction of barriers and additional events, if existed, should be inserted for the development of the tree. To this respect, the method is designed based on a two-level taxonomy of safety measures and risk factors. The first level consists of seven categories, which are inserted in the method. The seventh category deals with the process described above at the first step of the process. These categories are:

1. Human factor
2. Facilities
3. Infrastructure
4. Regulation
5. Environmental conditions
6. Chemical substance
7. Initiating event

During the construction of the tree, a dialogue window (Table 1) will open, and the user should fill the required information. In brief, Level I will be selected based on the predefined list. Subsequently, the title of level II barrier/event should be given along with a small description regarding its function. After that, the probability is required. It should be noted that there is not predefined that safety

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measures/risk factors are independent events. Thus, probabilities may be conditional. At last, the numerical value of the barrier/event needed for the consequences calculation should be inserted. The value parameter indicates the reduction percentage of a barrier on the release rate or the specific numeric value in case a model parameter is filling.

***Table 1**: Dialogue window*

A/A	Fields
1	<Level 1>
2	<Title>
3	<Description>
4	<Probability>
5	<Value>

For a few indicators used by the models in section 4.3, the relevant boxes have been already developed and inserted in the method in order to enable users filling the required information without missing important indicators needed in the models of the next section. This is conducted through embedded drop-down lists along with default values. Nevertheless, the method is designed to allow users to freely insert and design as many safety measures/risk factors associated with the chemical substance as they consider they need for the construction of their own event tree without any restriction. Another important aspect of the method is the fact that since values are inserted in this stage, developed models presented in the section 5 can use the values inserted in the trees to calculate automatically the consequences of the initiating event. In case these values are missing, models will require the information needed opening relevant windows prior to proceeding to the calculation section.

In the end of this section an example of an event tree developed for a polyurethane facility is depicted in Figure 2.

This type of facility falls into the sixth key-category as selected in a Deliverable A1.1.4. The initiating event in this case is an instantaneous leakage in the storage tank of the chemical volatile substance Di-Chloro-Methane (CH2CL2) due to its rupture, which is used as a solvent during the production process of polyurethane in a typical polyurethane facility in Greece (Environmental Consequences Study, 2019). This initiating event is not recorded in the relevant database. Therefore, the user has to design it by filling all the relevant values, as mentioned above. The elements of the event tree along with their associated probabilities are presented in Table 2. It should be noted that in this case probabilities of Table 2 are considered independent.

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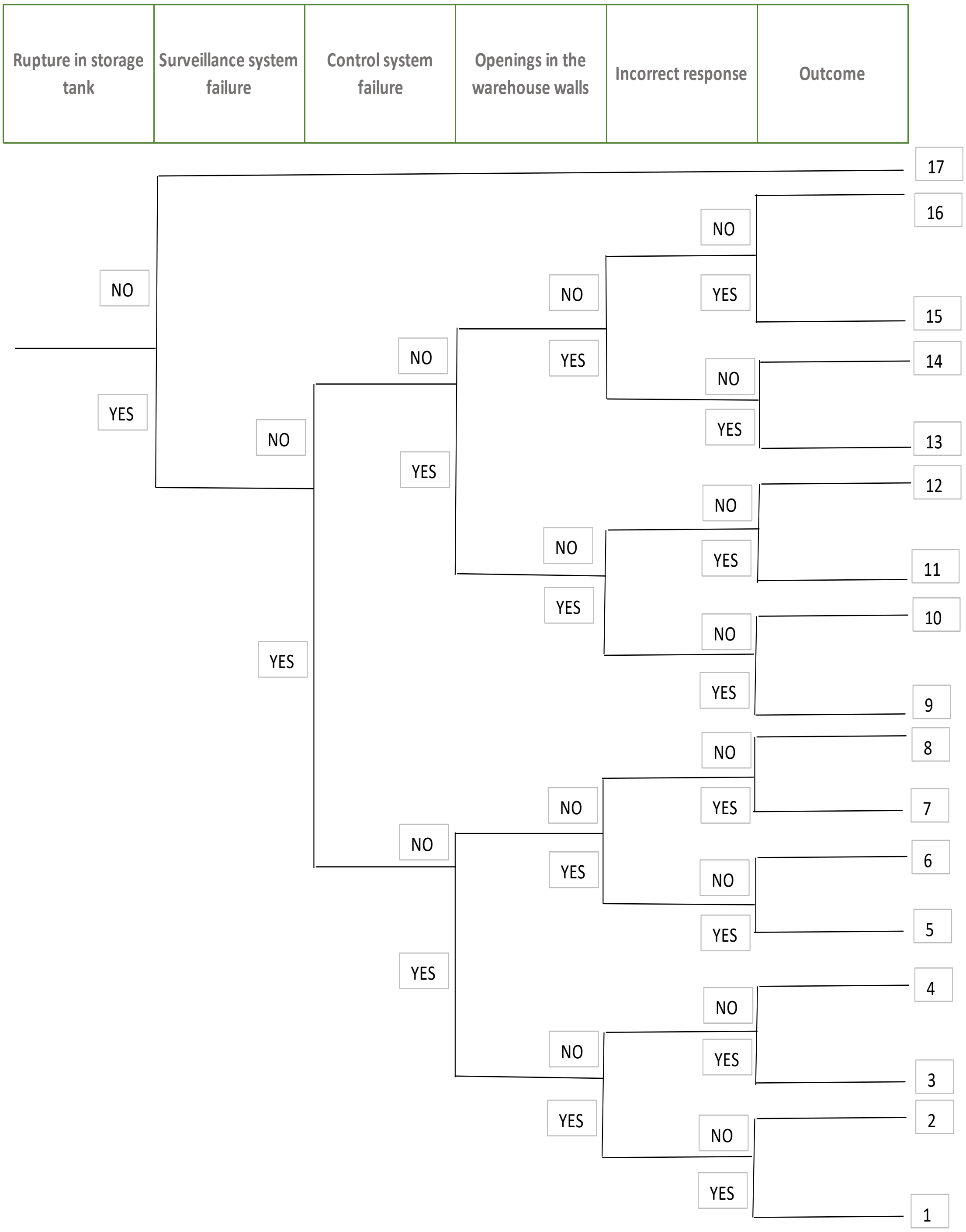

***Figure 2**: Event tree for a polyurethane facility*

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__Table 2:__ Example of event tree developed for a polyurethane facility: probabilities.

	Initiating Event Rupture in storage tank	**Facilities** Surveillance system failure	**Facilities** Control system failure	**Infrastructure** Openings in the Warehouse walls	**Human factor** Incorrect response
YES	0.035%	0.0057%	0.00008%	0.0000096%	0.000006%
NO	99.965%	99.9943%	99.99992%	99.9999904%	99.999994%
Value (reduction factor)	-	50%	50%	100%	60%

This kind of initiating events are associated with the surface soil contamination method. However, at this point, the presented example aims to provide a quick overview on how the developed method can operate. Thus, only some basic details of the developed scenarios are provided. The method regarding the contamination of surface soil is presented in detail in Section 4.4. Therefore, the scenario depicted in Figure 2 and Table 2 as well as the analysis presented in Table 3 are designed to calculate the consequences up to the point of the mass of the chemical released in the air instead of providing the concentration of Di-Chloro-Methane per square meters in a three-kilometre-area around the examined facility, which is the ultimate goal in such events.

Table 3 shows that Scenario S1 (light orange) includes the highest release of the examined substance but the lowest probability of occurrence while Scenario S12 (orange) has the highest probability of occurrence but zero release. Scenario S17 (bold letters) depicts the probability to avoid the rupture. Regarding the risk level, it is depicted that Scenario S14 (light blue) has the highest risk.

Scenarios' probabilities are estimated following Equation 1:

$$P(Sj \text{ I } IE) = f*P(SM/RF1 \cap ... \cap SM/RFi) = f*P(SM/RF1)*...*P(SM/RFi \text{ I } SM/RF1 \cap ... \cap SM/RFi\text{-}1) \quad (1)$$

where:

P(): Probability
Sj: Scenario j
IE: Initiating event
f: Probability of the initiating event
SM/RF: Safety measures/Risk factors within scenario Sj

$$Q' = Q * \Pi(Value\ SMj) \quad (2)$$

Instantaneous leakage is calculated according to Equation 2 by multiplying the initial release rate Q with the reduction factors (Value) that users insert next to the selected Safety measures.

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Table 3: *Scenario analysis from the event tree of Figure 4*

Scenario	Probability	Q' Instantaneous leakage (kg)	Risk Probability x Instantaneous leakage	Ranking
S1	9.19E-29	10.0	9.19E-28	8
S2	1.53E-21	8.0	1.22E-20	5
S3	9.58E-22	0.0	0.0	9
S4	1.60E-14	0.0	0.0	9
S5	1.15E-22	5.0	5.75E-22	6
S6	1.91E-15	2.5	4.79E-15	2
S7	1.20E-15	0.0	0.0	9
S8	1.99E-08	0.0	0.0	9
S9	1.61E-24	7.0	1.13E-23	7
S10	2.69E-17	4.0	1.07E-16	3
S11	2.10E-11	0.0	0.0	9
S12	3.50E-04	0.0	0.0	9
S13	2.02E-18	3.0	6.06E-18	4
S14	3.36E-11	1.5	5.04E-11	1
S15	1.68E-17	0.0	0.0	9
S16	2.80E-10	0.0	0.0	9
S17	**9.99E-01**	**0.0**	**0.0**	

4.1.6. Weights of the event tree elements

An important feature of the developed method is its focus on the weighting of each element of the event tree, namely the barriers and the additional events, some of which can work as the parameters of the models. The relevant importance of each criterion is estimated by exploiting the results of the examined initiating event. The estimation process follows Equation's 3 approach. In brief, the weight is the rate of the sum of the consequences of those scenarios of the event tree that cause environmental damage, and for which the examined element is taking part ("YES" choice), to the sum of the consequences of those scenarios of the event tree that cause environmental damage. In the end, the closer the weight to one, the higher the importance of the examined element.

$$W(SM/RFj) = \sum(Sz) / \sum M(SM/RFj) * P(SM/RFj)(Si) \quad (3)$$

where:

W(): Weight (0, …, 1]
SM/RFj: Element j
P(SM/RFj): Probability of the Element j

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M(SM/RFj): Release Mitigation factor of the Element j

The results of the weighting process of the event tree in Figure 2 are illustrated in Table 4. The results show that openings in walls is the most significant element (Weight=1) since the dysfunction of this barrier causes the dispersion of Di-Chloro-Methane in the air.

Table 4: *Weights of the event tree elements of the polyurethane facility*

	Initiating Event Rupture in storage tank	Facilities Surveillance system failure	Facilities Control system failure	Infrastructure Openings in the Warehouse walls	Human factor Incorrect response
Weight		0.622	0.707	1.000	0.610

4.2. Consequences estimation

The proposed risk assessment framework considers environmental impairments as the consequences that the initiating events can cause on specific natural resources and with regard to biodiversity on habitats. Therefore, the risk assessment framework follows a resource-oriented approach while from the biodiversity perspective it follows a habitat-oriented approach. As a result of the adoption of the aforementioned approaches, four models are developed, each of which is associated with certain type of natural resources and habitat, as well. These models are:

1. The model for surface soil (see Section 4.4),
2. The model for soil together with underground water (see Section 4.5 & 4.6),
3. The model for surface water -rivers (see Section 4.7).
4. The model for surface water -lakes (see Section 4.7).

Furthermore, each model is also related to specific initiating events. For instance, fire events need an air dispersion model to estimate the consequences the plume causes on surface soil. Hence, the modelling approach being adopted stems from the need to estimate the consequences on different types of habitat and natural resources that require very different modelling techniques.

4.3. Baseline Conditions

Consequences estimation for each of aforementioned models requires a starting point for the respective analysis. This starting point is named as baseline conditions. Baseline conditions depict the existing condition of the environment in which the consequences of an initiating event are to be added. Since each model focuses on different natural resources/habitat, each model entails different baseline conditions. The following Table 5 illustrates the baseline conditions required as an input for each model.

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Table 5: Baseline Conditions for each model

Model	Baseline Condition
Surface Soil Model	Average Pollutant Concentration of the examined substance (**Ch**) on the ground (**Bj**)
Soil Model*	Average Pollutant Concentration of the examined substance (**Ch**) in the soil (**Bj**)
Groundwater Model*	Average Pollutant Concentration of the examined substance (**Ch**) in the groundwater (**Bj**)
Lake Model	Average Pollutant Concentration of the examined substance (**Ch**) in the lake (**Bj**)
River Model	Average Pollutant Concentration of the examined substance (**Ch**) in the river (**Bj**)

*Soil and groundwater are part of the same model

It should be noted that if users do not insert any number in the specific field, the default value of baseline conditions will be zero.

4.4. Surface soil model

The present section illustrates the surface soil model developed to estimate the consequences of those initiating events that have an impact on surface soil, which functions both as natural resource and habitat. The seven criteria used to assist decision-making process on the structure of the following approach are listed in Table 6 and are explained in the description of the model's steps in Figure 3.

In general, the release of a volatile chemical substance due to accidents or fires can pose a serious threat to the environmental life. Such events can have adverse effects far from the point of release. In order to estimate the consequences of such initiating events, air dispersion models are used to estimate the hazard zones associated with plumes. In brief, air dispersion models are used to predict how the concentration of a pollutant released in the air varies per time and location. Although ELD excludes air from its scope, in case the toxic air impacts on soil causing pollution and thus impacts on biodiversity, it falls in its scope (EC, 2004).

Therefore, the developed risk assessment framework incorporates an air dispersion model in its surface soil model focusing on the effect of pollutants on surface soil. However, due to the aforementioned scope, the air dispersion model restricts on the estimation of the ground level concentration of the pollutant per time and location.

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Table 6: *Criteria selection for soil surface model*

	Criterion	Answers for Surface Soil Model
1	Group of chemical substances	Used for Volatile chemical substances
2	Type of accidents	Used for Fire events and Releases
3	Natural resource	Soil
4	Habitat	Surface soil
5	Stressor	Pollutants dispersed through air
6	Outcome	Pollutant concentration on ground
7	Supports economic evaluation of D.B2	Estimates Volume of polluted soil and Treat zones

By being part of the risk assessment framework, the ultimate goals of the surface soil model is to enable both practitioners and regulators to estimate:

1. The dose of the pollutant that the affected area received at the end of the accident,
2. The parameters that have significant impact on the environmental damage, and
3. The distribution together with a ranking of the scenarios set of the initiating event based on their risk outcome.

The developed air dispersion model is a Gaussian dispersion model intended to be used with vapour clouds that do not significantly affect the ambient air flow and are not affected by gravity. Thus, the chemical substances being used are considered passive pollutants.

In brief, the Gaussian model predicts that the concentration distribution of a steady-state release of neutrally buoyant gas will approach a Gaussian distribution with increasing down-wind distance. The parameters characterizing the distribution are based on well-known empirical measurements. Increasing averaging times of the measurements also tend to drive the distribution to a Gaussian shape, as well as widen the spatial distribution. However, it should be mentioned that the actual concentration distribution from a release can vary significantly from Gaussian at any single instant in time (Palazzi et al., 1982).

Furthermore, the model considers instantaneous release, which is modelled as a single steady-state release giving rise to a single cloud. A continuous release is modelled as a sequence of single steady-state releases giving thus rise to a sequence of single clouds. The structure of the developed surface soil model follows a sequential process consisted of five basic steps. Figure 3 illustrates the basic steps of the model.

STEP 1: Identification of the initiating event's characteristics

The first step of the process (**STEP 1**) deals with the parameters of the initiating event required for the consequences estimation. These parameters are:

1. The release rate of the chemical substance, Q(t),
2. The toxicity threshold(s) of the volatile chemical substance released, T,

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3. Baseline condition regarding the examined volatile chemical substance, B,
4. The height of the release from the ground of the chemical substance, h, and
5. The wind speed at the height of the release, u.

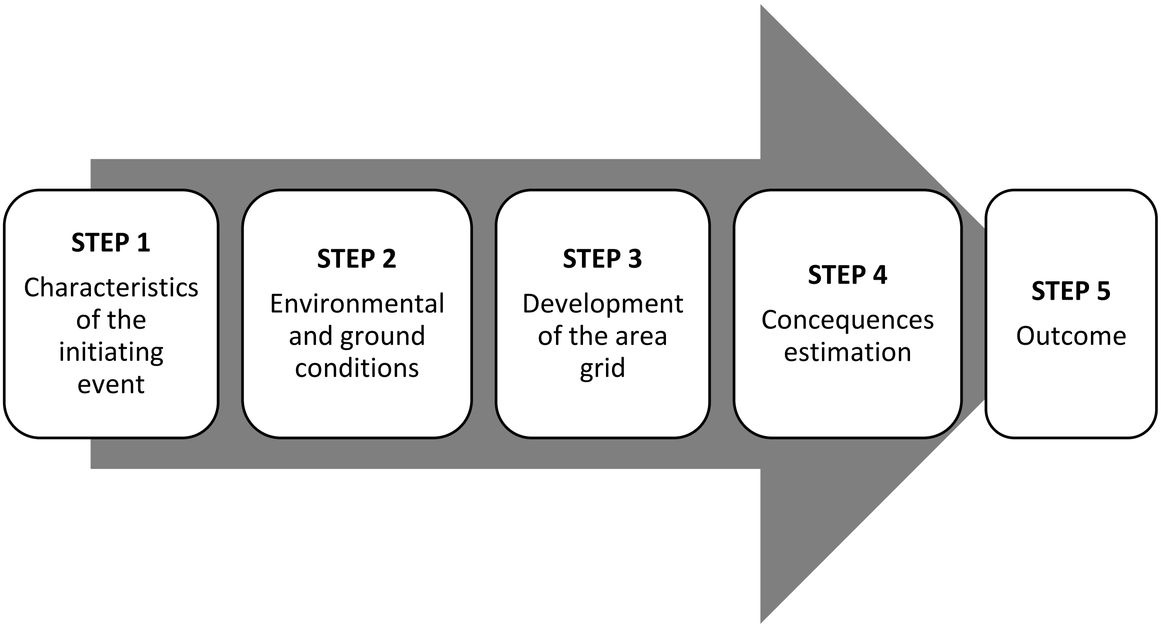

Figure 3: *Flowchart of the process of the surface soil model*

STEP 2: Identification of Environmental conditions (Air and Ground)

The second step of the process (**STEP 2**) deals with both the identification of the environmental conditions, namely the air and the ground conditions existing in the examined area. It should be noted that the model is designed to estimate the pollution of the surface soil within area radius of 4 km around the location of the accident. In particular, the radius is derived as a result of the discussions amongst the project team of the National Technical University with the teams of the Ministry of Environment and Energy, the Griffin Environmental Consulting LP, and the Hellenic Association of Insurance Companies. This radius is selected since it is in line with the Greek regulative requirements regarding the scope of the assessment of industrial accidents in Greece (PD, 2009).

In detail, air conditions include both the stability categories and wind conditions. Stability class varies among six classes, namely A to F, with regard to the wind conditions and solar and cloud conditions. Table 7 provides the relevant information. Wind conditions, namely wind speed, wind direction and wind frequencies during the accident are also required.

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Ground conditions include the definition of the type of the ground, urban or rural or both since it is related to roughness of the ground (see Table 8).

It should be mentioned that parameters of both **STEP 2** and **3** are inserted during the scenario development phase of the risk assessment framework (refer to section 4.2.5).

Table 7: *Solar Insolation and stability class categories*

Wind Speed	Part of the Day: PD Day			Part of the Day: PD Night	
At 10m (m/s)	Solar Isolation (SI)			Cloud cover (CC)	
	Strong	Moderate	Slight	≥50%	<50%
<2	A	A	B	E	F
[2-3)	A	B	C	E	F
[3-5)	B	B	C	D	E
[5-6)	C	C	D	D	D
≥6	C	D	D	D	D

STEP 3: Development of the area grid

The third step of the process (**STEP 3**) deals with the development of an area grid. As mentioned before, the examined area is a zone of 4 km radius around the location of the accident. The wind direction defines the central line, i.e. the x axis, which is the position in the downwind direction. For each point of the central line/x axis, the points on y axis, which is the position in horizontal crosswind direction are estimated for the range of [- $3\sigma_y, + 3\sigma_y$] (see Equation 5). However, x should be greater than 100m since below this threshold the estimation is not considered accurate. This area grid will be inserted in the Geographical Information System of the software tool.

STEP 4: Ground level concentration calculation of the pollutant per time and location

The fourth step of the process (**STEP 4**) focuses on the consequences estimation. In particular, for each point (x, y) of the grid, the model estimates the average 10-minute ground level concentration of the pollutant. The estimation is conducted according to Equation 4.

A time-dependent release, as here for 600s, is modeled as a series of 600 finite-duration steady-state releases each giving rise to a cloud that does not interact with the other clouds. The ground level concentration at a point in space and time is found by summing the contributions from each cloud.

Ground level concentration for instantaneous release of chemical substance (Bergeles, 2003):

$$C(x, y, t) = \frac{Q}{2^{\frac{1}{2}}\Pi^{\frac{3}{2}}(\sigma_\chi \sigma_y \sigma_z)} * e^{-\frac{(x-ut)^2}{2\sigma_\chi{}^2}} * e^{-\frac{y^2}{2\sigma_y{}^2}} * e^{-\frac{h^2}{2\sigma_z{}^2}} \quad (4)$$

where:

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C: Ground level concentration (μg/m^3)

Q: Instantaneous release (μg/s)

u: average 10-min wind speed at the height of the release (m/s)

t: time (s)

h: height of the release (m)

x: position in downwind direction (m)

y: position in horizontal crosswind direction (m)

The concentration distribution described above is a Gaussian distribution parameterized by three empirical dispersion parameters, σ_χ, σ_y and σ_z (Palazzi et al., 1982). These are the standard deviations of the Gaussian distribution and are calculated based on Equations 5, 6, and 7.

$$\sigma_\chi = s_{x_1} * x^{s_{x2}} \tag{5}$$

$$\sigma_y = \frac{s_{y_1} * x}{\sqrt{(1+s_{y_2} * x)}} \tag{6}$$

$$\sigma_z = s_{z_1} * x * \left(1 + s_{z_2} * x\right)^{s_{z3}} \tag{7}$$

The dispersion parameters depend upon the stability class of the environment based on Table 7.

Table 8: *Values for the coefficients used to estimate the dispersion parameters, σ_χ, σ_y, σ_z (Palazzi et al., 1982)*

		Stability Class					
Roughness (R)	**Coefficient**	**A**	**B**	**C**	**D**	**E**	**F**
Both	S_{x1}	0.02	0.02	0.02	0.04	0.17	0.17
	S_{x2}	1.22	1.22	1.22	1.14	0.97	0.97
	S_{y1}	0.22	0.16	0.11	0.08	0.06	0.04
	S_{y2}	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
Rural	S_{z1}	0.2	0.12	0.08	0.06	0.03	0.016
	S_{z2}	0	0	0.0002	0.0015	0.0003	0.0003
	S_{z3}	0	0	-0.5	-0.5	-1	-1
Urban	S_{z1}	0.24	0.24	0.20	0.14	0.08	0.08
	S_{z2}	0.001	0.001	0	0.0003	0.0015	0.0015
	S_{z3}	0.5	0.5	0	-0.5	-0.5	-0.5

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At this point, it should be mentioned the empirical Equation 8 used in order to calculate the wind speed in case the speed is known for a height up to 20m (Bergeles, 2003).

$$u = u_0*(h/h_0)^a \quad (8)$$

where:

u: wind speed (m/s)

h: height (m)

a: dimensionless factor: 0.2 for A,B Stability Class; 0.17 for C, D Stability Class; 0.13 for E, F Stability Class

Subsequently, the hourly ground level concentration (C_{hr}) is estimated for each point of the grid based on the following empirical Equation 9 developed by Pasquill (Pasquill, 1973).

$$C_{hr} = 0.72*C(x,y,t) \quad (9)$$

In addition, the total dose of each grid point is estimated by multiplying the hours and the hourly ground level concentration. In the end of the process, the dose or else the percentage of ground level concentration that surface soil receives from air is estimated. This task considers that the calculation up to this point estimated the ground level concentration as μg of the substance per m^3 of air. X percent of the estimated dose falls in the ground. Due to the fact that factor X can vary amongst different chemical substances, ground and environmental conditions, it is decided to receive its value by the user based on the specific attributes each case possesses. Hence, the final outcome is the μg of the substance per m^2 of surface soil in each point of the grid.

STEP 5: Outcome

Finally, in the last step of the process (**STEP 5**) the results of the air dispersion model calculations are depicted through the use of threat or contour zones/polygons. Threat zones represent the area within which the ground level concentration of the substance exceeds the level of concern being imposed by the thresholds. The concentration of the pollutant is a function of both location and time. In order to generate a threat zone, the model calculates the imposed concentration as a function of time for all points in the examined space. In case no threshold is imposed, it is considered that the affordable concentration of the examined chemical substance is zero.

The aforementioned outcome is added to the baseline conditions of the ground that were inserted in a previous step of framework. It is considered that the examined area is uniformly distributed to the imposed baseline. Again, in case no baseline is imposed, it is considered that the concentration of the examined chemical substance is zero on the surface ground prior to the accident.

As a result of this step, the areas that include specific concentrations are calculated, as shown in Figure 4. An important feature of Figure 4 that should be noted is that dotted lines around the E1, E2, E3 areas indicate that each area does not have strict boundaries with its surroundings but there is always an intermediate area characterized by its own biodiversity as analyzed in detail in Deliverable B.2. In the end, an average ground concentration of the whole area is estimated, which depicts the consequence

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factor. This factor is multiplied by the probability of this specific scenario (see Risk column of Table 4) in order to provide the risk of the scenario needed for the scenario ranking (see last column of Table 4). In addition, the model can create diagrams that depict the concentration level in selected locations of the examined area per time (see Figure 5). As far as the estimation of the impairment of the natural resource, in this case soil, is concerned, since the pollutant falls on the surface soil, it is assumed that the affected soil extends up to one meter depth. Therefore, the volume of soil affected is calculated by multiplying the area estimated with the depth (d).

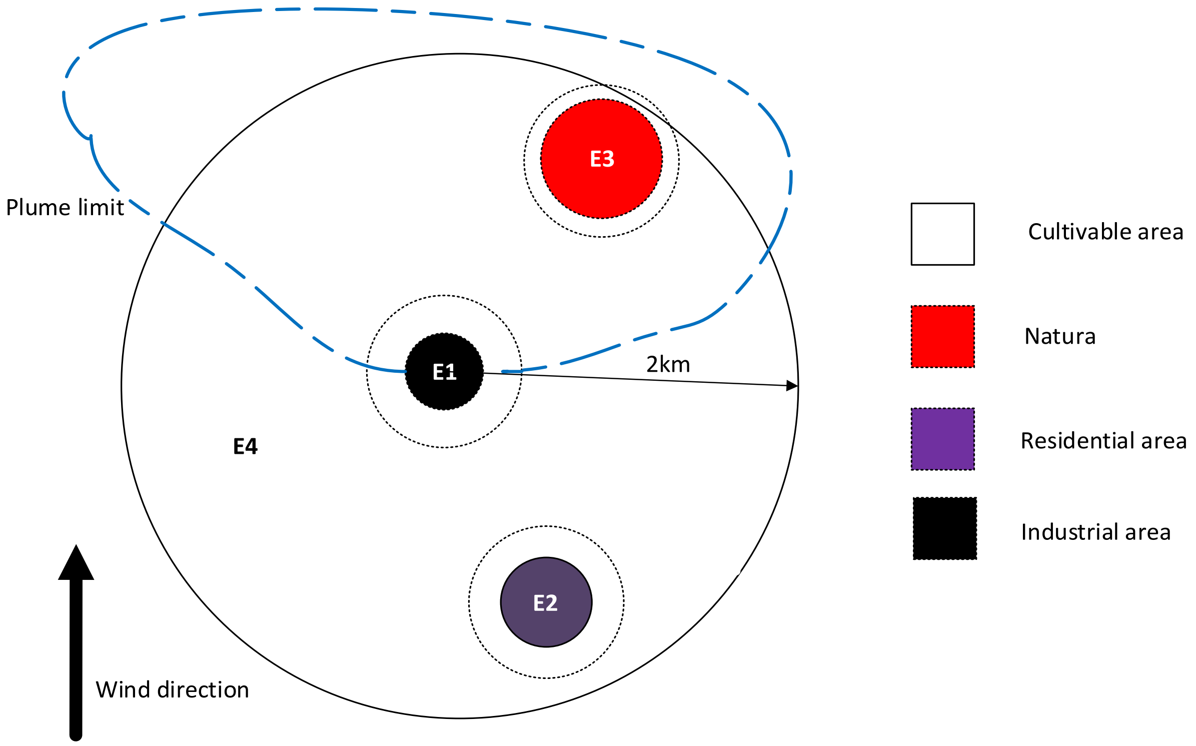

Figure 4: *Indicative case (the impact of pollution on specific areas is examined in Deliverable B2)*

$\Sigma V_{Soil} = \Sigma(A_i*1)$ (10)

where:

V: volume of soil (m^3)

A_i: Area i with pollutant concentration (m^2)

Following the indicative case of the polyurethane facility analyzed in section 4.2, a part of the total results is illustrated in Figure 5 in order to give a brief overview of the outcome derived by the air dispersion model. More detailed analysis is presented in the testing process of the model in section 5.1.

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The scenario considered by the model is scenario S1 of Table 4, which although ranked 8th, it is the worst-case scenario regarding the consequences part of the initiating event. Since there is no threshold imposed by the Greek legislation on this substance for the surface soil and biodiversity, it is considered zero.

The height of the release is 2m, stability class is C, and wind speed is 6m /s with direction from North while the roughness of the ground is urban.

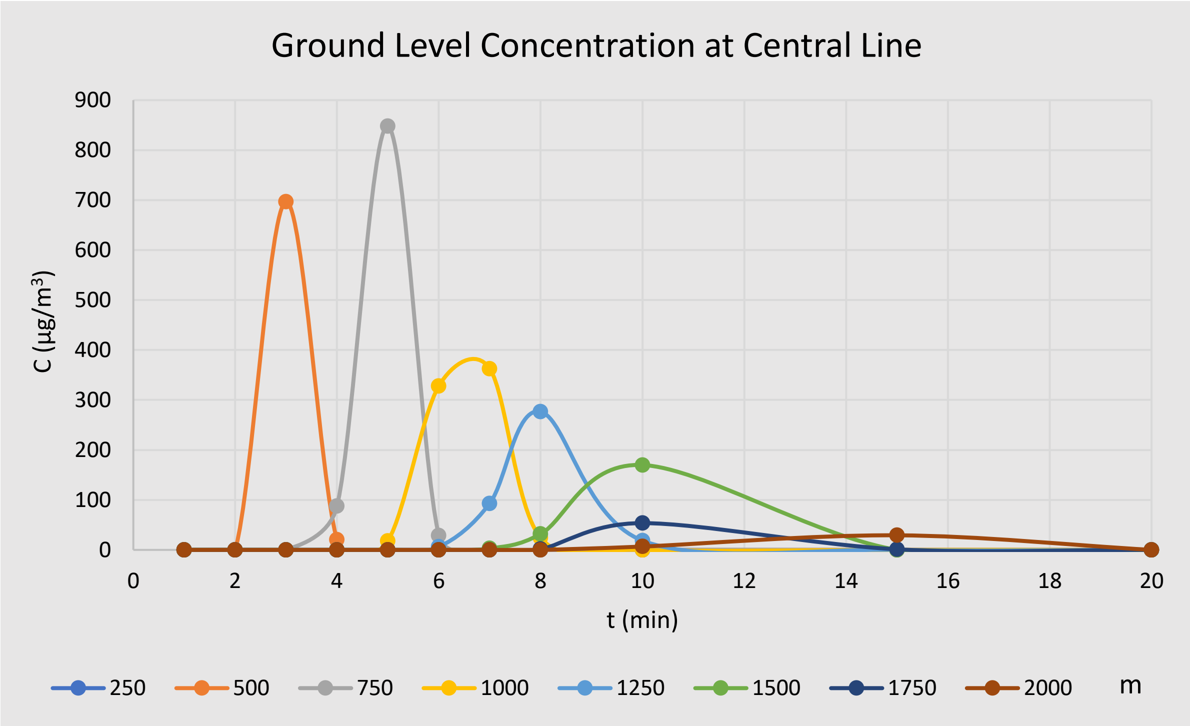

Figure 5: *Indicative case (the impact of pollution on specific areas is examined in Deliverable B2)*

Figure 5 depicts that on the x axis/central line up to a distance of 1,500m receives high doses of Di-Chloro-Methane for about 10 minutes after the release of the substance. In particular, concentration at 250m is not visible in the above figure since it is very low due to the high speed of wind that pushes the plume in longer distances. The concentration of the substance that falls in the ground is assumed to be at 10%. Hence, for instance, at distance 750m from the point of release, the surface soil receives approximately 85μg of Di-Chloro-Methane per m^2.

4.5. Soil

The study of the interaction between pollutants and soil requires systematic mapping of each phase and its components. For this reason, it is important to use indicators to distinguish between the gaseous ($_a$), the aqueous ($_w$), the solid ($_s$) and, in the general case, the non-aqueous liquid phase ($_n$). The ratio of soil phases is given by the soil mechanical characteristics of the soil, such as porosity (n), the dry density of the soil (ρ_d) and the degree of saturation for the water (S_w).

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Table 9. Criteria selection for soil model

	Criterion	Answers for Surface Soil Model
1	Group of chemical substances	Liquid chemical substances
2	Type of accidents	Used for leakage events and Releases
3	Natural resource	Soil
4	Habitat	Soil
5	Stressor	Liquid chemical substance
6	Outcome	Polluted volume of soil
7	Supports economic evaluation of D.B2	Estimates Volume of polluted soil and Treat zones

The calculation process for soil contamination considers the following soil characteristics:

Porosity (n) = $\frac{soil\ pore\ volume}{soil\ sample\ volume}$

Values of the soil porosity parameter can be either measured directly or estimated from the following table (Table 9).

Dry soil density (ρ_d) = $\frac{mass\ of\ solid\ soil}{volume\ of\ soil\ sample}$ and

Degree of saturation for the water (S_w)= $\frac{volume\ of\ water\ in\ soil\ pores}{volume\ of\ soil\ pores}$

In the case of an organic contaminant not mixed with water, it should also be known whether there is a non-aqueous liquid phase in the subsurface, the amount of which can be calculated by the

Degree of saturation for the non-aqueous phase (Sn) = $\frac{volume\ of\ non\!-\!aqueous\ phase\ in\ the\ soil\ pores}{volume\ of\ soil\ pores}$

and the density (ρ) of the non-aqueous phase contaminant (Kavadas, 2013).

The present study requires the calculation of the volume of contaminated soil, for which there is no standard methodology in the literature for calculating contamination spread from potential leakage of contaminants; the prevailing approach is accurate sampling, which is only meaningful after-the-event. After meetings and discussions with academic experts in this field, it was proposed to adopt the empirical rule of the absorption of a part of the contaminant by the soil based on its porosity.

It is estimated that, a quantity of the contaminant, equal to 10% * n, will be adsorbed to by soil grains, thus leading to the calculation of the volume of contaminated soil based on both the surface area and the depth of the affected area. It is assumed that the contaminant will spread exactly below the whole surface spill area due to gravity.

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Table 10: Range of values of Porosity (n) (Kavadas, 2013)

	n(%)
Unconsolidated deposits	
Gravel	25-40
Sand	25-50
Silt	35-50
Clay	40-70
Rocks	
Fractured basalt	5-50
Karst limestone	5 -50
Sandstone	5-30
Limestone, dolomite	0-20
Shale	0-10
Fractured crystalline rock	0-10
Dense crystalline rock	0-5

4.6. Groundwater

The term groundwater is usually reserved for the subsurface water that occurs beneath the water table in soils and geologic formations that are fully saturated.

Table 11: Criteria selection for groundwater model

	Criterion	Answers for Surface Soil Model
1	Group of chemical substances	Liquid chemical substances
2	Type of accidents	Used for leakage events and Releases
3	Natural resource	Groundwater
4	Habitat	Groundwater
5	Stressor	Liquid chemical substance
6	Outcome	Polluted volume of groundwater
7	Supports economic evaluation of D.B2	Estimates Volume of polluted groundwater and Treat zones

The basic processes for the spread of conservative contaminants in space are Advection, Dispersion and Diffusion. Advection is the process by which moving water carries soluble contaminants. The term diffusion is used for the spreading of the contaminant in stagnant water, while the term dispersion is used for moving water. In the case of active substances, there are physical and chemical processes (adsorption, ion exchange, chemical reactions, etc.), which cause a retardation of the movement of the contaminant, so that it does not move as predicted by its transport rate. The above processes may occur simultaneously in the porous medium ((Freeze & Cherry, 1979); (Kavadas, 2013)).

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The basic law of flow is Darcy's law, and when it is put together with an equation of continuity that describes the conservation of fluid mass during flow through a porous medium, a partial differential equation of flow is the result (Freeze & Cherry, 1979) (Kavadas, 2013).

During advection, the contaminant is guided by the hydraulic gradient through Darcy's law: v = K $(-\nabla h)$, where v is the apparent groundwater velocity (i.e. flow rate per unit area) which is often referred to as Darcy velocity, K is the hydraulic conductivity (dimensions: m/sec, values depicted in Fig. 6), and ∇h is the slope of the hydraulic load function (h).

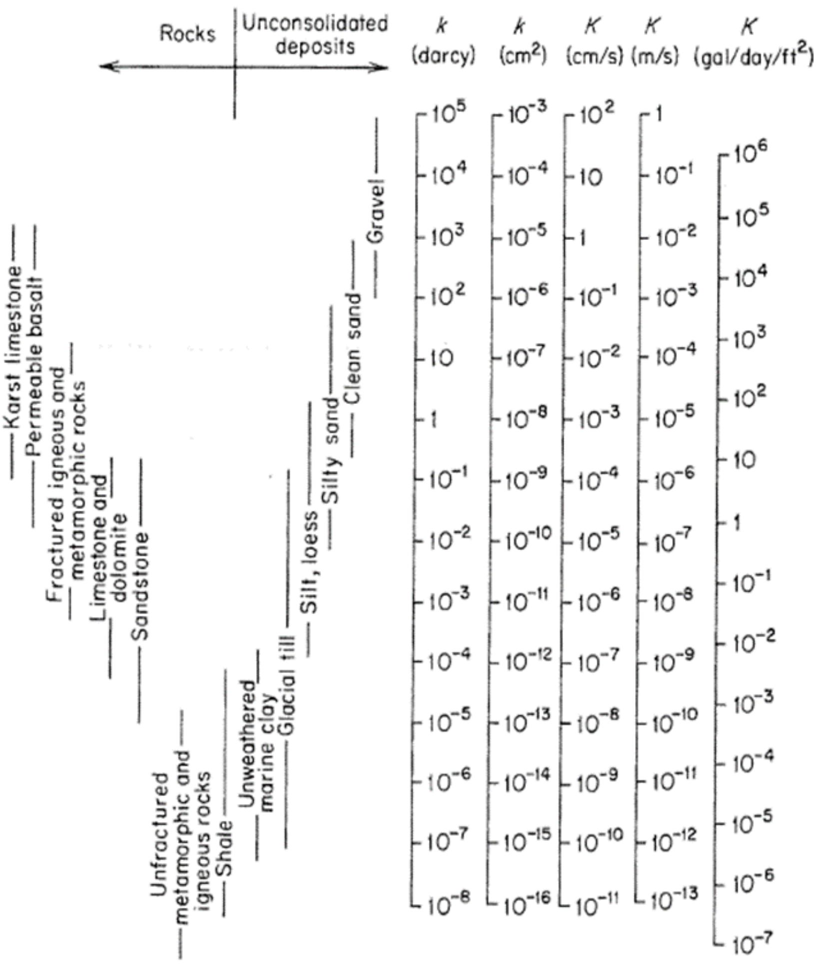

***Figure 6**: Ranges of values of Hydraulic Conductivity (K) and permeability (k) (adopted from Kavadas, 2013)*

The transport of contaminants due to diffusion and dispersion is usually described in a uniform way, through Fick's law, which expresses that the mass $d\dot{m}''$ of the pollutant passing through (due to diffusion and dispersion) per unit time through an elementary surface dS (with direction vector n) is

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proportional to the slope of concentration of the pollutant (∇c): $d\dot{m}'' = (-\nabla c) \cdot n(D_2 + D_3) \cdot n \cdot dS$, where n is the active porosity of the soil, D_2 is the diffusion coefficient and D_3 is the dispersion coefficient. Often a single coefficient is used in the above relationship, the hydrodynamic dispersion coefficient, $D = D_2 + D_3$. The diffusion coefficient (D_2) of pollutants in water is of the range of $10^{-9}m^2/sec$. The dispersion coefficient (D_3) depends on the speed of the groundwater velocity ((Freeze & Cherry, 1979); (Kavadas, 2013)).

The one-dimensional contaminant transfer (only along x-axis) is described by the following equations, taking, also, into consideration the additional assumption that the velocity of the ground water is practically constant.

1st Case: Conservative contaminant, i.e., a contaminant that does not absorb soil grains or degrade (break down):

$$D\frac{\vartheta^2 c}{\vartheta x^2} - \bar{v}\frac{\vartheta c}{\vartheta x} = \frac{\vartheta c}{\vartheta t} \quad (11)$$

2nd Case: Non-conservative contaminant, that adsorbs to the soil grains but does not degrade (decompose):

$$\frac{D}{R_d}\frac{\vartheta^2 c}{\vartheta x^2} - \frac{\bar{v}}{R_d}\frac{\vartheta c}{\vartheta x} = \frac{\vartheta c}{\vartheta t} \quad (12)$$

Where lag coefficient $R_d = 1 + \frac{\rho_d K_p}{n}$ and ρ_d is the (dry) density of the soil and K_p a separation coefficient. The lag coefficient is used to calculate the degradation of the pollutant load through absorption of the pollutant on the soil grain surface.

3rd Case: Non-conservative contaminant, that adsorbs to soil grains and breaks down:

$$\frac{D}{R_d}\frac{\vartheta^2 c}{\vartheta x^2} - \frac{\bar{v}}{R_d}\frac{\vartheta c}{\vartheta x} - \lambda c = \frac{\vartheta c}{\vartheta t} \quad (13)$$

where λ is the linear degradation factor used to describe the mass reduction of the contaminant due to biochemical reactions whose rate of progression is proportional to the mass of the contaminant. $\lambda = ln2/T$, where T = half-life (time required to reduce the concentration from c to c/2).

In three dimensions the velocity v is a vector with components v_x, v_y, and v_z. In the case of three-dimensional transport of a conservative contaminant and one-dimensional flow, the equation of motion is:

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$$D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial xy^2} + D_z \frac{\partial^2 c}{\partial z^2} - \overline{v_x} \frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} \quad (14)$$

Where $\bar{v} = \frac{v}{n} = \frac{(K \cdot i)}{n}$ is the mean linear velocity of groundwater and i is the hydraulic gradient at each position.

For a point source (x = y = z = 0) emitting at the time t = 0, pollutant mass M (= $V_o C_o$), the equation for the concentration of the contaminant is:

$$C(x, y, z, t) = \frac{M}{8 \cdot n \cdot (\pi \cdot t)^{3/2} \sqrt{D_x D_y D_z}} \exp\left(-\frac{X^2}{4D_x t} - \frac{Y^2}{4D_y t} - \frac{Z^2}{4D_z t} \right) \quad (15)$$

Where X = x - $\overline{v_x} t$, Y = y, Z = z, $D_x = a_L \overline{v_x} + D_e$, $D_y = D_z = a_T \overline{v_x} + D_e$

a_L is the coefficient of longitudinal dispersivity ($\alpha_L = 0.1\ x$)

a_T is the coefficient of transverse dispersivity ($\alpha_T = \left(\frac{1}{20} to \frac{1}{5}\right) \alpha_L$

For the current type of research, where a sudden accident creates a case of contaminant leakage, equation 15 has been adopted for the calculations (Freeze & Cherry, 1979; Kavadas, 2013).

The simulation has been developed using an algorithm written in python programming language developed in-house by the NTUA research team:

Underground water Algorithm structure

Initially, the pollutant dispersion measurement time is defined in t days, as well as the scale of the contamination field dimensions in meters. This procedure creates a 3D Cartesian system with length [-edge, edge] in its dimension.

The following data must then be entered to start the process of calculating the contaminated volume of groundwater:

***Table 12**: Input Data in Underground Water Algorithm*

M	The mass of the pollutant
K	The hydraulic conductivity
i	The hydraulic gradient
n	The porosity
D_2	The diffusion coefficient

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ω	ω = 0.01 – 0.5 (for clay ω ~ n)
t	The time of measurement in days after the first moment of contact of the pollutant with the groundwater
PL	The permissible limit of the pollutant

The groundwater pollutant concentration function C (x, y, z, t) is then defined. The latter is called by the code repeatedly for each point of the field, and with an appropriate condition it is checked if the value of the concentration of the pollutant is greater than or equal to its allowed limit PL. If the above condition applies, the point is recorded on three different dimensions X, Y, Z.

To display the contaminated volume in the 3D system, the results from the X, Y, Z planes are combined, giving the actual shape of this volume.

Due to the high volume of required computations, the assumption that the volume is enclosed in a rectangular parallelepiped was used. Its dimensions are the maximum differences of the values of the X, Y, and Z planes respectively. Therefore, the final volume of contaminated groundwater is assumed to be equal to the volume of the rectangular parallelepiped that encloses it.

The Flowchart below (Figure 7) expresses the aforementioned procedure in a more representative way:

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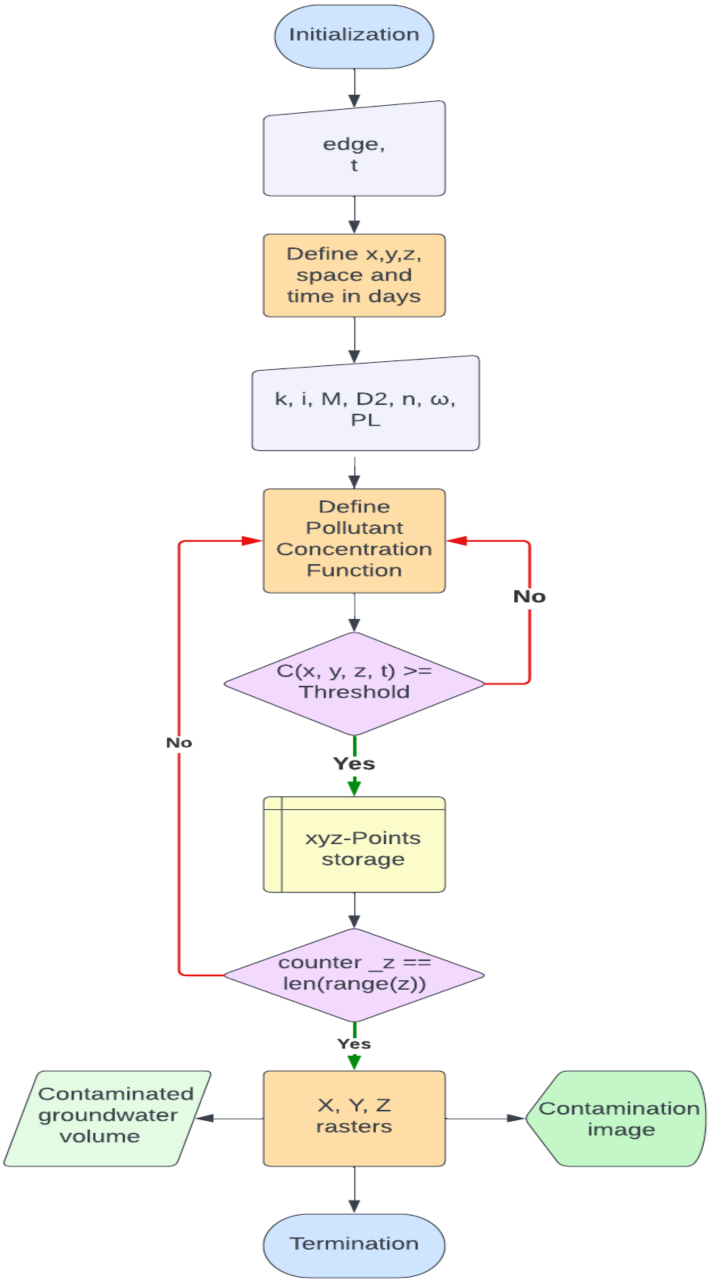

***Figure 7**: Algorithm Flowchart for groundwater contamination*

4.7. Surface water

A contaminant or polluting substance is any soluble (hydrophilic e.g. inorganic salts) or insoluble (hydrophobic, e.g. hydrocarbons, PCBs, solvents, etc.) substance in water, which, when introduced into

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the environment due to human activities, causes adverse environmental effects. In general, there are two major categories of contaminants: conservative or reactive. Conservative ones are those that do not react with the soil and/or the neighboring underground layers or do not undergo biological or radioactive degradation. When the pollutant is active, it reacts by resulting in a reduction in its mass and its velocity, causing the contamination to slow down. Furthermore, a contaminant might be in solid or liquid form. In the case of leakage of a liquid contaminant, it may be either in the pure phase or in the form of a solution, which may then either be transported as such or mixed with water. In the case of a solid contaminant leakage, it can be either dissolved in an organic substance or in an aqueous solution (Voudouris, 2006).

When contaminants leave an enclosure space where they are stored, they move through the partially saturated zone (vadose zone). Some of the contaminants are retained at the surface of the soil grains either by geochemical absorption or by mechanical retention through capillary forces, and the remainder eventually reaches the surface water compartments. During their movement, contaminants are subject to a variety of mechanical, chemical and biological processes that result in the expansion of pollution, the dilution of pollutants and the gradual degradation (attenuation) of the pollutant load. This section presents the mathematical simulation of the transport of pollutants in soils and aquifers (Kavadas, 2013).

Table 13. *Criteria selection for surface water models*

	Criterion	Answers for Surface Soil Model
1	Group of chemical substances	Liquid chemical substances
2	Type of accidents	Used for leakage events and Releases
3	Natural resource	Lakes and Rivers
4	Habitat	Lakes and Rivers
5	Stressor	Liquid chemical substance
6	Outcome	Polluted volume of surface water compartments
7	Supports economic evaluation of D.B2	Estimates Volume of polluted surface water compartents and Treat zones

The subsection of surface water includes the independent study of contaminant leakage into lakes and rivers:

4.7.1. Rivers

This subsection describes river hydraulics and advective-dispersive transport of substances dissolved or suspended in the water column. It is used as a one-dimensional description, which means that all variables are averaged over the river cross section and the depth of the sediment is not resolved. One-dimensional river hydraulics can be described by a set of two partial differential equations representing a mass and a momentum balance. The two most important approximations to these so-called St. Venant equations, the kinematic and diffusive wave approximations are implemented to describe river hydraulics. The equations for river hydraulics are coupled with advection-diffusion equations to

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describe transport of substances dissolved or suspended in the water (Reichert, 1998; Grigoropoulou & Papadopoulou, 2021).

For the case of a river section, three types of components of a conservation law must be distinguished: The first component concerns the conservation of water volume within the river (water is approximated to be incompressible). The second component of equation describes substances transported with the water flow along the river. The last component of equation describes substances settled to the bottom or sorbed to surfaces of the riverbed.

The one-dimensional fluxes of the substances with one-dimensional densities as described by equation are given as follows:

$$\hat{j} = \begin{pmatrix} Q \\ QC_i - AE\frac{\vartheta C_i}{\vartheta x} \\ 0 \end{pmatrix} \qquad (16)$$

Where Q the discharge of a substance/contaminant into the river, C_i the concentration of substance/contaminant, A the cross-sectional area and E is the coefficient of longitudinal dispersion.

The dispersion coefficient E, determines the spread of pollutant/tracer/substances in the river, and according to Fischer et al (1979) it can be estimated as:

$$E = c_F \frac{w^2 (\frac{Q}{A})^2}{u^* d} \qquad (17)$$

Where $c_F = 0{,}011$ is a dimensionless coefficient

w is the width of the river (L)

u^* is shear velocity, $u^* = \sqrt{\tau_o/\rho} \approx \sqrt{gdS_f}(LT^{-1})$, τ_o is the down shear point

d = w/A, the river depth (average- d_{mean})

Calculation of river hydraulics requires the formulation of the cross-sectionally averaged friction force as an empirical function of averaged flow properties. Usually, instead of the friction force, the non-dimensional friction slope, S_f, is used: $S_f = \frac{1}{K_{st}^2}\left(\frac{P}{A}\right)^{4/3}\frac{Q^2}{A^2}$, K_{st} = 25^1/3/s is the coefficient of friction according to Strickler, and P is length of wetted perimeter (Reichert, 1998).

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4.7.2. Lakes

This subsection describes the stratification of the water column, vertical mixing and advection of substances dissolved or suspended in the water column, sedimentation and resuspension of particles, exchange of dissolved substances between water column and pore water of the top sediment layer, advective and diffusive exchange between an arbitrary number of sediment layers, and transformation processes in the water column as well as in the sediment layers. A one-dimensional description is used that averages all variables over horizontal cross sections. This limits the applicability of this compartment to situations in which the dimensions of the lake, the stratification and the time scales of the investigated processes make a horizontally averaged description reasonable (Reichert, 1998; Grigoropoulou & Papadopoulou, 2021).

The lake equations consist of a combination of a conventional advection-diffusion equation for the water column with a sediment model describing an arbitrary number of sediment layers, and with a k-ϵ turbulence model that has been extended by a simple model of energy storage in seiche motion in the lake basin. In order to formulate the one-dimensional conservation laws:

$$\frac{\vartheta \hat{\rho}}{\vartheta t} + \frac{\vartheta \hat{\jmath}}{\vartheta z} = \hat{r} \qquad (18)$$

compartment-specific expressions for the one-dimensional density, $\hat{\rho}$ (amount of conserved quantity per unit compartment length), for the one-dimensional flux, $\hat{\jmath}$ (amount of the conserved quantity transported per unit time), and for the one-dimensional source term, $\hat{r}$ (amount produced per unit compartment length and per unit time), must be derived.

In order to formulate the lake equations, eight types of components of a conservation law must be distinguished. The first component describes the conservation of the water volume (water is approximated to be incompressible). The one-dimensional density of water volume (volume per unit of depth) is given by the cross-sectional area, A, of the lake. The second component describes a horizontal water flow induced by the surface shear of the wind. This component is used in mixing models to calculate the production of turbulent kinetic energy by shear forces of wind induced water flow. The third component describes turbulent kinetic energy. The one-dimensional density of turbulent kinetic energy is given as the product of the cross-sectional area of the lake, A, the density of water, ρ, and the turbulent kinetic energy, k (turbulent kinetic energy per unit mass of water). The fourth component is an equation for the dissipation, ϵ, of turbulent kinetic energy. This quantity together with k can be used to estimate the coefficient of turbulent diffusion, K_z, of substances dissolved or suspended in the water column. The fifth and sixth components describe dissolved and suspended substances in the water column of the lake. Both one-dimensional densities are given as the product of the cross-sectional area of lake A, and the horizontally averaged volumetric concentration of the substance. The last two components describe the concentrations of dissolved substances and of particles in the pore volume of sediment layers of the lake. (Reichert, 1998)

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The variables A, U, k and ϵ are named as Cross-Sectional Area, Horizontal Velocity, Turbulent Kinetic Energy and Dissipation. The variable `Diffusion' is used to specify the coefficient of turbulent diffusion, K_z. The coefficient of turbulent diffusion can be parameterized as a simple function of space (z) and time (t). The parameters of such a function can be estimated using measured data of temperature or substances without or with known transformation processes. An alternative can be to parameterize the coefficient of vertical turbulent diffusion using the stability or Brunt Vaisalla frequency, N^2:

$$K_z = \begin{cases} \min\left(K_{z,max}, \frac{\alpha}{(N^2)^b}\right) & for\ N^2 > 0 \\ K_{z,max} & for\ N^2 \leq 0 \end{cases} \qquad (19)$$

The stability or Brunt Vaisalla frequency, N^2 is: $N^2 = -\frac{g}{\rho}\frac{\vartheta\rho}{\vartheta z}$

In the case of a freshwater lake, the following formula can be used to approximate the density of the lake water:

$$\rho = 999.84298\frac{kg}{m^3} + 10^{-3}\ kg/m^3 \cdot (65.4891℃^{-1}T - 8.56272℃^{-2}T^2 + 0.059383℃^{-3}T^3)$$

The parameters α and b of expression (19) can be estimated using several temperature profiles of the lake. An additional option is to use the turbulence sub model to estimate the coefficient of vertical turbulent diffusion (α = 13, b = 0.35) (Reichert, 1998).

4.7.3. Simulation program for river and lake contamination

The simulation model for surface waters has been implemented in Python programming language developed in-house by the NTUA research team. The methodological approach was based on principles aligned with the freely available simulation program AQUASIM for the simulation of river and lake contamination. AQUASIM is written in the standardized object-oriented programming language C++. The AQUASIM software is designed to study and simulate water bodies systems on a laboratory or pilot scale, as well as for the study of natural systems (lakes, rivers). The performance of a simulation is equivalent to the numerical integration of a system of equations with time.

The NTUA-developed models share the main assumptions and limitations with AQUASIM:

Lakes:

- A one-dimensional description is used that averages all variables over horizontal cross sections. This limits the applicability of this compartment to situations in which the dimensions of the lake, the stratification and the time scales of the investigated processes make a horizontally averaged description reasonable. The current version of the lake compartment

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has no connections to advective or diffusive links, so that it can only be used to describe a single lake with given inputs and processes.
- It is assumed that the contaminant is uniformly distributed from 0 to 1 cm depth within the lake, providing reasonable initial conditions (aligned with the assumptions of the Aquasim program).
- The Aquasim simulation for the lake compartments cannot simulate the dispersion of a pollutant for more than 100 days; hence, this limitation has been adopted in the NTUA models as the maximum reasonable time horizon for analysis.

Rivers:

- The length of the river cannot exceed the hypothetical radius of the circle (2 km), around the point of the accident.
- The width and the depth of the river stay constant along its length.

5. Testing Process

This section refers to the methodology assessment process step. In the updated description of B1 in the midterm report, it was mentioned that 'past accidents that fall into the list of the selected activities will be used as case studies, and for which relevant data can be provided to the research team'. The aim of this step is to assess the robustness of the developed methodology in various key activities and under various conditions. It was also mentioned that case studies of past accidents had been identified by partner COEIL/MEE (i.e. fire accident in recycling factory in Aspropyrgos and underground water polluted by Chromium (Cr) in Aluminum factory in Greece). After receiving the available data, it became clear that the second case (underground water polluted by hexavalent Cr) was not suitable for use, since in reality it involved widespread contamination over a long time period from unknown sources; this case was not linked to any specific industrial accident or activity, but rather hypothesized that it may have been an impact form aluminum production processes. In this respect, and since the second case was unsuitable for use for the purposes of this deliverable, it was replaced by a fictitious accident in the aluminum production process, due to lack of any other industrial accident with sufficient data available.

5.1. Case study 1: Surface soil model

In this section, the surface soil model for estimating the environmental risk on surface soil is tested. In brief, a real case of a fire accident in a recycling facility that belongs to the 1st key-category selected in Deliverable A1.3, namely, installations for the recovery of materials from non-hazardous mixed recyclable waste by mechanical and/or manual waste sorting, in Aspropyrgos, Attica region, is examined. The testing process follows a sequential process consisting of five distinct steps according to the structure of the developed risk assessment framework (refer to section 2) and the surface soil model (refer to section 4.4).

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5.1.1. Model selection and Initiating event design

Since the consequences that the initiating events can cause on natural resources and with regard to biodiversity on habitats varies (refer to section 4.3), the definition of these two parameters, which are: the initiating event and the model, prior to the scenarios development and consequences estimation is of utmost importance.

The examined case deals with a fire accident in a recycling facility. Due to fire, atmospheric pollutants/particulate matters and toxic substances hazardous to human health and the environment were released, exceeding the limits according to the measurements made immediately after the fire, as documented by the relevant reports (NOA, 2015). These substances are airborne and settle on the surface soil causing damage to soil and water.

The burning of stored waste and in particular plastics causes environmental damage or is a threat to cause environmental damage to soil. It produces dioxins, furans, which are airborne and settle in soil as well as polycyclic aromatic hydrocarbons and other hazardous chemical compounds. Moreover, ash from the burning of waste is likely to contain heavy metals.

Because the details from the post-accident reports do not provide the information required regarding the spark of the fire in order to select an initiating event from the provided in Appendix 1, the required details of the initiating event should be defined by the user. For details regarding the requirements see section 4.2.5. As an initiating event is considered a fire event and the chemical volatile substance that is examined for the purposes of illustration of this work is the PM_{10} released from the fire since the post-accident reports provide the details needed for the relevant calculations by the model. Figure 8 indicates the percentage of maximum emission rate of PM_{10} released from fire during the event. Release rate of 100% is considered as 0.12 Kg/s (NOA, 2015). Furthermore, Greek legislation categorizes PM_{10} as a toxic substance although it provides certain thresholds only for human health and not for biodiversity, calling operators to implement effective safety measures in order to mitigate its impact on the environment (PD, 2009).

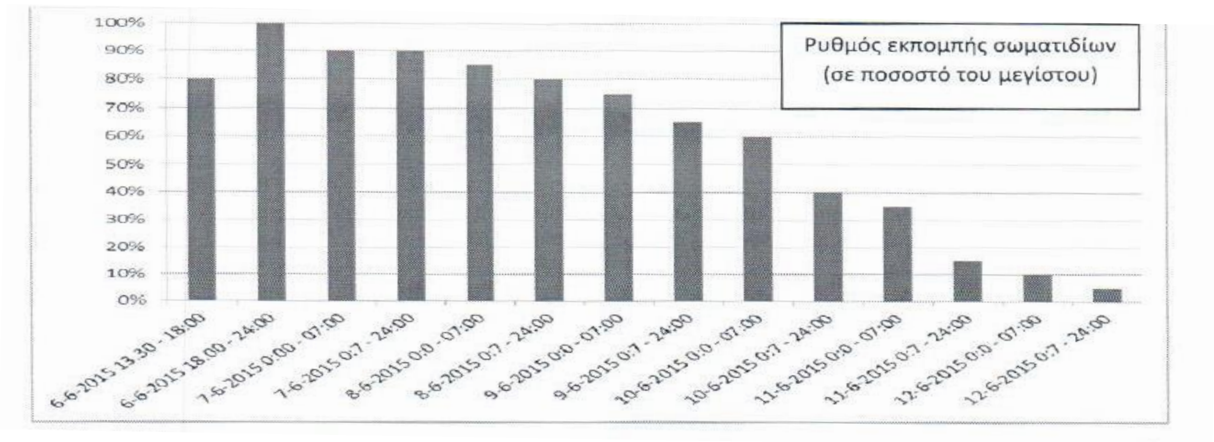

***Figure 8**: Emission rate of PM10 from fire (source: NOA, 2015)*

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5.1.2. Industry's characteristics

The second step of the process focuses on the identification of the industry's characteristics. The examined facility deals with the recycling of metallic and non-metallic non-hazardous solid waste-sorting (mechanical and manual sorting), cutting, baling, trading of recyclable non-hazardous solid waste (wastepaper, plastic, wood, metal, broken glass, etc.). According to the Greek categorization its NACE code is 3832 based on the relevant list in Deliverable A.1.3 of LIFE PROFILE project (PROFILE, 2022c).

Initially, the compliance of the industry with the obligations imposed by law is examined (see Table 14). This type of industry falls into the provisions of the IED law regarding emissions (IED, 2019), the environmental protection law regarding the insurance legislation that imposes compulsory insurance (PD, 2009). However, the only clue that existed from the reports is that the facility wasn't complying with the obligations of aforementioned provisions at the time of the accident without further details (NOA, 2015; NCSR, 2015). Moreover, it hasn't been identified how the fire sparked. It should be mentioned that in the end of the event a total destruction of the facility's warehouses was recorded while 140,000.00 m^3 of burnt wastes deposit in the area.

***Table 14**: Law compliance*

Legislation requirements	Compliance
IED	√
SEVESO	-
Compulsory insurance	√
Relevant Presidential Decrees	√
…	…

As far as the level of safety of the industry is concerned, Table 15 illustrates whether the facility met the criteria listed in the framework for initiating events that are associated with the surface soil model.

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Table 15: Characteristics of the industry for these type of initiating events

Risk factors (RF) / Safety measures (SM)	Compliance
Volatile substance (RF)	-
Flammable substance (RF)	√
Heat source (RF)	√
Detection system (S)	N/A
Alarm system (S)	N/A
Electric circuit (RF/S)	N/A
Human engagement (RF/S)	N/A
Scada system (S)	N/A
Manual system (S)	N/A
Automatic system (S)	N/A
Protective zone (S)	N/A
Storage tank (RF)	√
…	…

The aim of this list is to compare whether the mentioned safety measures/barriers are taken into account in the forthcoming event tree analysis enabling operators and auditors to evaluate the level of preparedness of the examined industry.

5.1.3. Baseline conditions

Having completed the description of the initiating event and the industry's characteristics, the subsequent step prior to the development of the scenarios' sets is the identification of the baseline conditions of the environment of the examined area, in this case the surface soil within a radius of 4km around the location of the fire event.

To this respect, data was retrieved from a report conducted for the whole region, which encircles the examined area, focused on mapping the environmental impact (NCSR, 2019). In brief, the report illustrates the concentration of heavy metals, polycyclic aromatic hydrocarbons, furans and toxins in the soil of the region that includes the examined area.

Therefore, after calculating the concentration of PM_{10} and based on the details of the post-accident report that analyses the content of PM_{10} in heavy metals, toxins, etc., risk assessment process focuses on the estimation of the concentration of an indicative heavy metal, which is nickel (Ni), in order to pinpoint also the effectiveness of the developed model possesses in proving the user with results capable of assisting further analyses.

Regarding PM_{10}, there are no thresholds regarding PM_{10} imposed on surface soil. However, the reports indicate the percentage of heavy metals on PM_{10} emitted by the fire as well as the concentration of

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heavy metals soil in this area. To this respect, the toxicity threshold is considered zero, T_{PM10}=0μg/m^2. However, for the illustration purposes of this deliverable instead of the default value, four thresholds are imposed, namely 1, 5, 40 and 1,000 μg/m^2 (see Figure 10). Moreover, reports also indicate that for the examined area 50 μg/m^3 is the daily average concentration, which is the baseline value B_{PM10}=50μg/m^3. As far as the baseline conditions regarding Ni is concerned, reports indicate that although there is no threshold above which soil is considered toxic for fauna and flora, T_{Ni}=0μg/m^2, the average ground concentration for the examined area is 10μg/m^3 thus B_{Ni}=10μg/m^3 (NCSR, 2019). Also in this case, four thresholds are imposed, namely 12, 60, 480 and 12000 μg/m^2 each one receives different color (see Figure 10).

5.1.4. Scenarios' sets development

The fourth step of the process is the development of the event tree in order to identify all the potential propagation paths following the occurrence of the examined initiating event.

Since there are many scenarios that should be analysed in order to estimate the environmental damage caused by the initiating event, which is calculation intensive, only an indicative scenario is analysed for the illustration purposes of this deliverable. Its characteristics are indicated in Table 16. It should be mentioned that an ex-post analysis is conducted. However, the developed risk assessment framework can also operate in this case by addressing the relevant probabilities. Therefore, the probabilities needed for the development of the scenarios' sets are the frequencies referred to the post-accident reports.

***Table 16**: Input Table*

A/A	Initiating Event	P	Environmental Stability	P	Wind Direction	P	Wind Speed	P	Release rate	P	Substance	P	Baseline	P	Outcome
S1	Fire/Release of PM10	1	D	0.4	N	0.2	7.2 m/s	0.5	0.12 kg/s	1	PM10	1	50μg/m3	1	R(S1)
S2			...	...	...	...	...	...	...	...	...	...	...	...	
S3															
S4															
S5															
...															Σ(S1+S2+...)

Scenario S1 relates to the 4% of the time of the duration of the accident, namely twelve hours. In other words, the conditions of the event are similar to the conditions of Scenario S1 (environmental, fire, ground) only for twelve hours. It is selected because it includes the part of the event that has the highest wind speed.

5.1.5. Results

For validation purposes, a comparison is conducted between the results of the air dispersion model with the actual results referred in the post-accident reports. This task is conducted since the reports did not provide any data or estimations regarding the pollution of soil apart from the hypothesis that pollution has occurred (NOA, 2019). The comparison shows that the estimations of the model are close to the actual and thus considered acceptable as shown on Figure 9. Concentration in 500m from the fire location has the similar value with the air dispersion model (300 to 350 μg/m^3.

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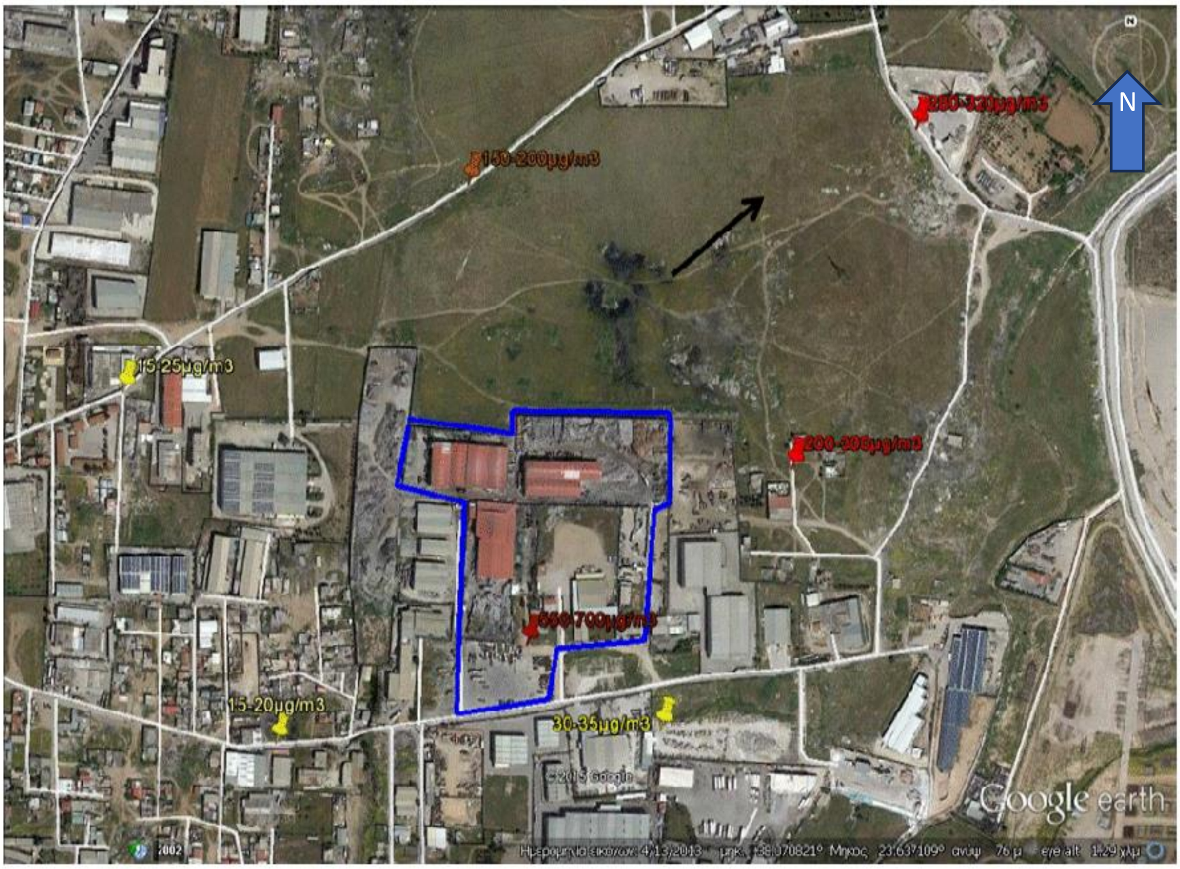

***Figure 9**: Ground level concentration in the area near the facility; Black arow depicts the wind direction (source: NCSR, 2015)*

The final step is the calculation process. To this respect, equations 4-7 of section 4.4 are employed. The results are depicted in Figure 10. Figure 10 illustrates four consecutive outcomes, namely, (i) the hourly average ground level concentration of PM_{10}, (ii) the hourly average ground level concentration of PM_{10} received by surface soil, (iii) the total ground level concentration of PM_{10} received by surface soil, namely the concentration received for twelve similar hours, and (iv) the total ground level concentration of Ni received by surface soil.

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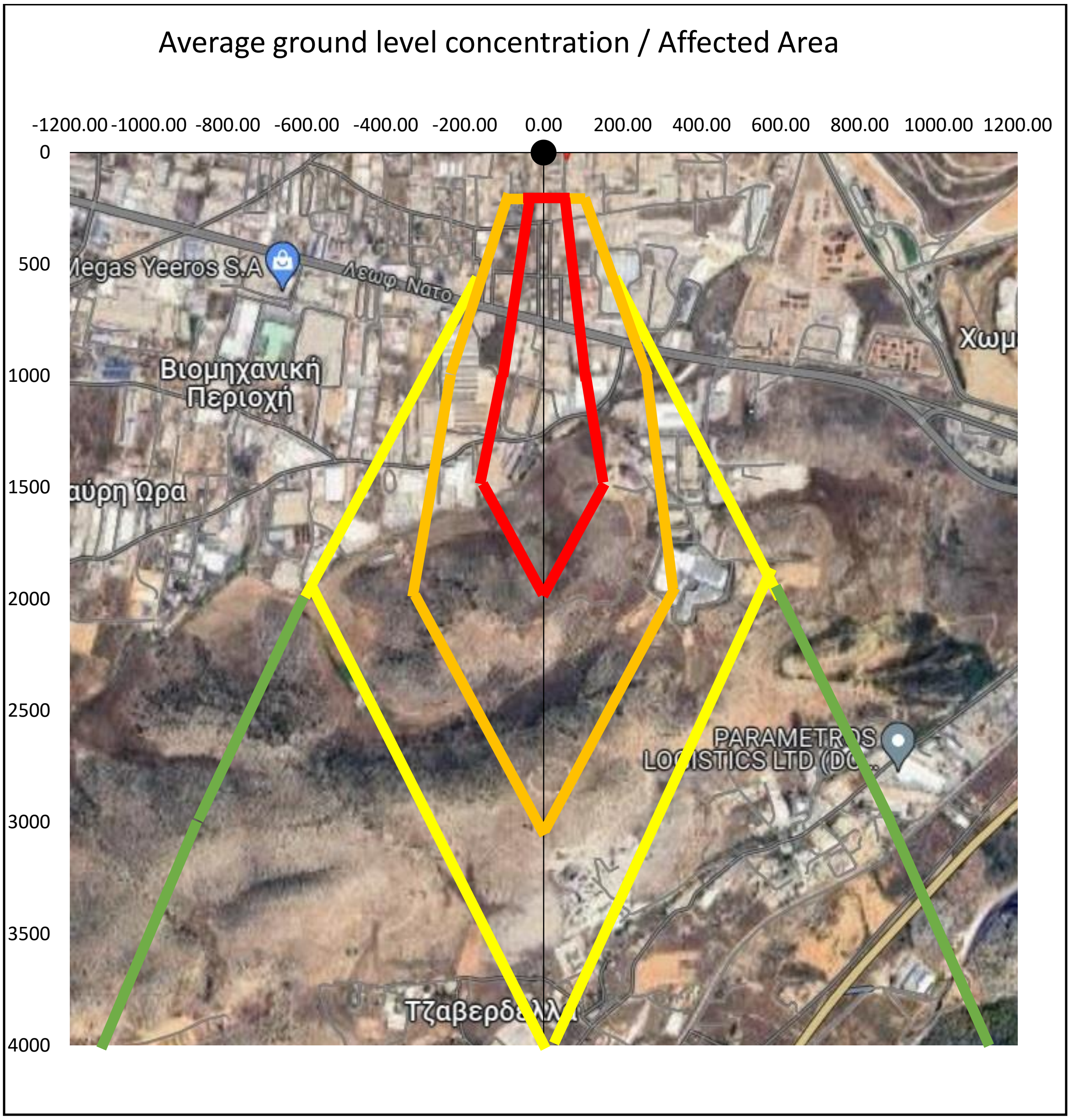

C (μg PM10/m3 Air)	C (μg PM10/m2 soil)	ΣC (μg PM10/m2 soil)	ΣC (μg Ni/m2 soil)
0 < Green < = 10	0 < Green < = 1	0 < Green < = 12	0 < Green < = 0.12
10 < Yellow < = 50	1 < Yellow < = 5	12 < Yellow < = 60	0.12 < Yellow < =0.60
50 < Orange < = 400	5 < Orange < = 40	60 < Orange < = 480	0.60 < Orange < = 4.80
400 < Red < = 10000	40 < Red < = 1000	480 < Red < = 12000	4.80 < Red < = 120.00

***Figure 10**: Color-coding system for the affected area without adding the baseline*

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It should be noted that by adding the baseline conditions on the above outcome the green area alters to yellow too. Hence the final outcome does not include any green area.

For each of the above case and for each zone the area is calculated. Subsequently, the average ground concentration is estimated. According to Equation 20, the risk of the scenario is estimated by multiplying the average ground concentration by the scenario's probability. Furthermore, the volume of the resource is also estimated considering the depth (d) to be 1m.

$$R(S1) = S1*[\Sigma(Ai*C_{avg})/\Sigma ai] \quad (20)$$

Table 17: *Risk Results for Figure 10*

Polygon (color)	Area (m^2)	Volume (m^3)	Concentration ($\mu gNi/m^2 soil$)	R(S1) (Eq. 20)
Red	$220*10^3$	$220*10^3$	87.00	3.46
Orange	$330*10^3$	$330*10^3$	3.20	
Yellow	$495*10^3$	$495*10^3$	0.42	
Green	$390*10^3$	$390*10^3$	0.05	

5.2. Case study 2: Soil, Underground water, River, and Lake contamination

In this section, the models of soil, underground water, river, and lake contamination for estimating the environmental risk on soil, underground water, and surface water are tested. The following activity is examined: Extrusion process of aluminium – Hot or cold rolling or other mechanical treatment of aluminium for the production of intermediate products (profiles, rods, tubes, etc.)

Extrusion is the process used to create objects of a fixed cross-sectional profile. The raw material from aluminium alloy cylinders ("billets") is preheated to 400 °C - 500 °C, then pressed in a horizontal hydraulic press and, depending on the matrix (mould) the various profile shapes are produced. They are cooled by air on the special cooling table, which transports them to the tensor. There, they are aligned and then transported lengthwise to the cutting machine for the desired lengths. They are automatically packed in special pallets which are transported to aging ovens (175 °C for 6 hours) for heat treatment (aging), in order to obtain mechanical properties. The scraps of the saw are cubed in a special press for remoulding in the melting foundry. The finished product (profiles) from the aging ovens after being wrapped and packaged is transported to the warehouse. Afterwards, is the process of anodizing. The term anodising of aluminium means the electrochemical formation of pure aluminium layer of surface aluminium oxide which contributes to an increase in the resistance of aluminium profiles against corrosion and mechanical stresses. The produced profiles are subjected to mechanical finishing on the brushes. After the profiles are attached to suitable bars, they are transported by cranes to the various chemical treatment baths where the cleaning and the neutralization are implemented, and in the main anodizing baths the profiles are electrolysed to obtain a protective layer on their surface. At the same time, the pores open to accept various colors in special

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baths. Then the pores are sealed again in special baths and finally they are hung from the bars and go to packaging and storage.

Raw and auxiliary substances used in the above process have been determined with the aid of the obtained data from the Environmental Impact Studies for industries in this category of activity. The raw material used in the activity under study is aluminium in billets (solid aluminium cylinders). This raw material is not classified as hazardous according to Regulation (EC) 1272/2008 (CLP) and therefore is excluded from further investigation as regards its potential to cause pollution of the subsoil and groundwater. This industry includes a range of auxiliary materials, some of which are classified as hazardous. It should be noted that chromium is no longer used in the production process, which is confirmed by the study of Environmental Impact Studies.

5.2.1. Theoretical Scenarios

In the key category activity of production process of aluminum there was no data on real accidents in the Ministry of Environment and Energy databases, therefore theoretical scenarios were created to utilize the models of soil, underground water, river and lake contamination. The testing process follows a sequential process consisting of five distinct steps according to the structure of the developed risk assessment framework and the aforementioned models.

5.2.2. Model selection and initiating events

It was observed that sulphuric acid has a significant high annual quantity consumption (approximately 22 kg sulphuric acid per ton raw material aluminum is needed), that can cause serious effects on soil and groundwater in the event of a release. Sulphuric acid is used as an auxiliary material in the production process and specifically in surface treatment. It is stored in stainless steel tanks, surrounded by a sealed spill containment basin of sufficient volume for contents in case of spillage. Its use and circulation are carried out through closed piping. Any residues from the production process are discharged to the wastewater treatment plant via closed pipelines. However, a potential source of sulphuric acid contamination is the underground transportation network of industrial waste, anodizing and pre-anodizing processes, as it is presented in the following flow chart (Figure 11). In this case, an accidental leakage of a high concentration of sulphuric acid from the pipe network is possible, leading to leak to the soil, that impacts the soil and, potentially, the underground water.

Furthermore, it was found that the majority of the installed industrial plants are located close to a river. During the normal operation of the plant, liquid waste from the electrostatic painting and anodizing line after treatment ends up into the nearby river. It was therefore considered appropriate to study additionally the possibility of a failure of the waste treatment plant for a short period of time with a possible leakage of HSO_4 into the adjacent river.

Because factories are usually not situated near lakes, and they do not discharge water from their industrial processes into them, an extra theoretical scenario has been introduced to test the model of lake contamination. As such, for this case, it is considered a hypothetical situation involving a leakage from a tanker truck's tank, which belongs to the aforementioned aluminium factory, that transfers HSO_4 in the industrial area. In this scenario, 500 litres of the substance spill onto concrete, eventually making its way to a nearby lake and causing contamination.

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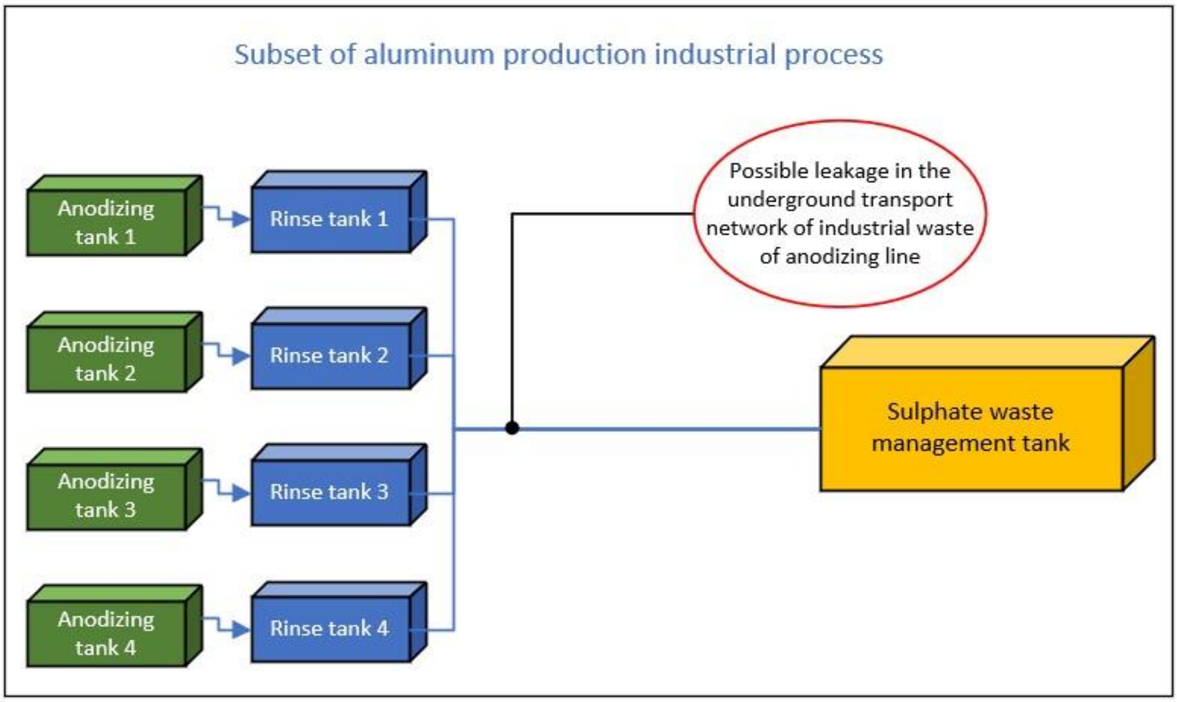

Figure 11: Flowchart of possible leakage of sulphuric acid

5.2.3. Industry's characteristics

The second step of the process focuses on the identification of the industry's characteristics. The examined facility deals with aluminum production. According to the Greek categorization its NACE code is 2442 based on the relevant list in Deliverable A.1.3 of LIFE PROFILE project (PROFILE, 2022c).

Initially, the compliance of the industry with the obligations imposed by law is examined (see Table 18). This type of industry falls into the provisions of the IED law regarding the emissions (IED, 2019), the environmental protection law regarding the insurance legislation that imposes compulsory insurance (PD, 2009). Moreover, it hasn't been identified how either the breach in the pipes network, the failure in the waste management system or the truck accident happened.

***Table 18**: Law compliance*

Legislation requirements	Compliance
SEVESO	-
Compulsory insurance	√
Relevant Presidential Decrees	√
…	…

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Table 19 illustrates whether the facility met the criteria listed in the framework for initiating events that are associated with the soil or groundwater or river or lake model.

***Table 19**: Characteristics of the industry for these type of initiating events*

Risk factors (RF) / Safety measures (SM)	Compliance
Volatile substance (R)	-
Flammable substance (R)	N/A
Heat source (R)	N/A
Detection system (S)	√
Alarm system (S)	√
Electric circuit (R/S)	N/A
Human engagement (R/S)	√
Scada system (S)	N/A
Manual system (S)	N/A
Automatic system (S)	N/A
Protective zone (S)	√
Storage tank (R)	N/A
…	…

5.2.4. Baseline conditions

Having completed the description of the initiating event and the industry's characteristics, the subsequent step prior to the development of the scenarios' sets is the identification of the baseline conditions of the environment of the examined area, in this case the soil, the underground water, the rivers, and the lakes within a radius of 2km around the location of the leakage event.

To this respect, due to the absence of data the models' results were compared with thresholds of the HSO4 when it is released in the environment.

Therefore, after calculating the concentration of HSO4, the risk assessment process focuses on the estimation of the concentration of HSO4 in the contaminated environmental bodies.

Regarding HSO4, it is assumed there are no thresholds regarding HSO4 imposed on any of the examined bodies. To this respect, the toxicity threshold is considered zero, B_{HSO4}=0 mg/m^3.

5.2.5. Scenarios' sets development

The characteristics of the developed event trees are indicated in the following two tables, for the two separate initiating events, the pipe leakage and the truck's tank accident. Furthermore, there are two extra tables naming each scenario separately. For each initiating event there were only 6 scenarios made, since this case study is a demonstration of how the whole methodology operates.

Breach in underground pipeline network releasing HSO4:

The probability of the event derives from the FlemishGov 2009 list

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__Table 20__: Input Table

A/A	Initiating Event	P	Volume (lt)	P	Substance	P	Manometer – Detection System	P	Alarm System	P	Human response	P	Baseline	Outcome
S1	Breach in underground pipeline network releasing HSO4	6.9E-8	200	1	HSO4	1	Works	0.99	Works	0.99	Fast	0.1	0	R(S1)
S2			201	1	HSO4	1	Works	0.99	Works	0.99	Fast	0.1	0	R(S2)
S3			300	1	HSO4	1	Works	0.99	Works	0.99	Fast	0.1	0	R(S3)

A/A: Scenario description

S1: Instant leakage of (200 lt) HSO4.

S2: Instant leakage of (201 lt) HSO4.

S3: Instant leakage of (300 lt) HSO4.

Failure of the waste treatment plant liquid waste from the electrostatic painting and anodizing line releasing HSO4:

The probability of the event was not in any of the lists, so it was placed manually.

__Table 21__: Input Table

A/A	Initiating Event	P	Release rate (mg/s)	p	Substance	P	Duration of Release (s)	Waste liquid PH sensor	P	Human response	P	Baseline	Outcome
S4	Failure of the waste treatment plant liquid waste from the electrostatic painting and anodizing line releasing HSO4	5.0E-5	10	1	HSO4	1	100	Works	0.99	Fast	0.1	0	R(S4)

A/A: Scenario description

S1: Progressive leakage (10 mg/s) of HSO4 which contaminates the river

Truck's tank breach followed by a subsequent leakage of HSO4:

The probability of the event come from the Purple book 2005 (Ale & Uijt, 2005).

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Table 22: Input Table

A/A	Initiating Event	P	Volume (lt)	p	Substance	P	Protective Zones around facility	P	Human response	P	Baseline	P	Outcome
S5	Instantaneous release of the complete inventory	5.0E-7	500	1	HSO4	1	Works	0.95	Fast	0.1	0	1	R(S5)

A/A: Scenario description

S5: Truck accident with (500 lt) HSO4 leakage that does reach the lake.

5.2.6. Calculations and Results

Sulphuric acid Leakage into the ground

It is assumed a leakage of sulphuric acid into the ground from a potential failure of the pipeline network. The case of a shallow groundwater table at 5m depth is considered. The examined soil is composed mainly of sandy clays, sands or gravels. In general, the formations of underground water system consist of deposits such as sands, gravels, silts, clays, sandy clays, etc. A value equal to 40% has been selected for the porosity of the soil, based on the described synthesis. The hydraulic gradient of the groundwater has been assumed 0.001 (almost horizontal inclination) and the hydraulic conductivity, K, has been assumed 10m/day (based on the range of values for sand and gravel) (Freeze & Cherry, 1979). Furthermore, according to Material Safety Data Sheet for sulphuric acid, the maximum allowable aquatic toxicity (acute) of the components of the mixture for aquatic life (EC50) is c_{max} = 100mg/lt.

1st Scenario: Leakage of 200 lt sulphuric acid

It is estimated that the leakage covers a surface area of $1m^2$. For every 1m of depth for the examined area of $1m^2$, a quantity of the pollutant, sulphuric acid, equal to 10% * n = 10% * 0.4 = $0.04m^3$ will be adsorbed by the soil grains.

Therefore, at a depth of 5m, $0.2m^3$ of soil will have been contaminated and the contaminant will not reach the water table.

2nd scenario: Soil & Groundwater contamination – Leakage of 201 lt sulphuric acid

This case describes the minimum additional amount of sulphuric acid needed to reach the groundwater aquifer and to examine its effect on groundwater. As calculated in the previous case $0,2m^3$ of soil has been contaminated and the volume of 1lt contaminant will end up in the water table (or M = 1.52 kg, as the density of sulphuric acid is $1.52gr/cm^3$).

Groundwater contamination:

The volume of the contaminated groundwater will be calculated, using the equations of Section 4.6.

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Mean velocity of groundwater $\bar{v} = \frac{K \cdot i}{n} = \frac{10 \cdot 0.001}{0.4} = 0.025m/d$

Hydrodynamic dispersion coefficient (the scale of 500m is initially used in place of X):

$D = D_{diffusion} + D_{dispersion} = \omega \cdot D_2 + \alpha_L \cdot \bar{v} = \omega \cdot D_2 + 0.1 \cdot X \cdot \bar{v} = 0.4 \cdot 10^{-9} \left(\frac{m^2}{s}\right) + 0.1 \cdot 500m \cdot 0.25 \left(\frac{m}{d}\right) = 3.5 \cdot 10^{-5} \left(\frac{m^2}{d}\right) + 12.5 \left(\frac{m^2}{d}\right) \approx 12.5 \left(\frac{m^2}{d}\right)$

$$C(x,y,z,t) = \frac{M}{8n(\pi t)^{3/2}\sqrt{D_x D_y D_z}} \exp\left(-\frac{X^2}{4D_x t} - \frac{Y^2}{4D_y t} - \frac{Z^2}{4D_z t}\right)$$

For the solution the time is kept constant e.g., for t = 10, 30, 60, 180 and 360:

***Table 23**: Contaminated groundwater (m³), 2nd possibility*

Time [days]	Contaminated groundwater (m^3)
10	2,736
30	9,720
60	22,464
90	**32,292**
180	67,048
360	105,222

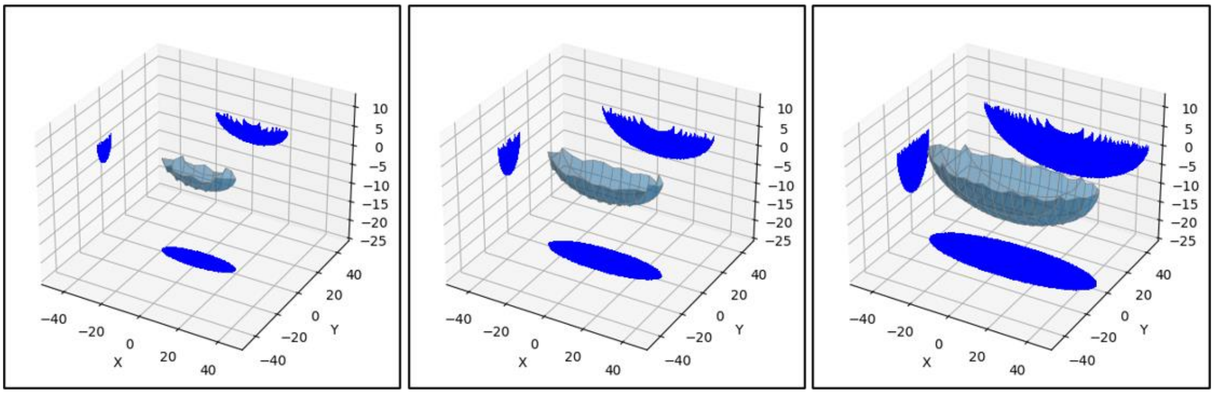

***Figure 12**: Leakage scenario of 1.5 kg of H_2SO_4 over 10, 30, and 90 days respectively, illustrating the expansion of the polluted groundwater area where pollutant concentration exceeds the toxicity threshold.*

3rd Possibility: Soil & Groundwater contamination – Leakage of 300 lt sulphuric acid

This case describes the maximum quantity of sulphuric acid that can leak based on the results of the event tree. As calculated in the previous case 0.2m³ of soil has been contaminated and the volume of

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100lt contaminant will end up in the water table (or M = 152 kg, as the density of sulphuric acid is 1.52gr/cm^3).

Groundwater contamination:

The volume of the contaminated groundwater will be calculated, using the equations of Section 4.6.

Mean velocity of groundwater $\bar{v} = \frac{K \cdot i}{n} = \frac{10 \cdot 0.001}{0.4} = 0.025 m/d$

Hydrodynamic dispersion coefficient (the scale of 500m is initially used in place of X):

D = $D_{diffusion}$ + $D_{dispersion}$ = $\omega \cdot D_2 + \alpha_L \cdot \bar{v} = \omega \cdot D_2 + 0.1 \cdot X \cdot \bar{v} = 0.4 \cdot 10^{-9} \left(\frac{m^2}{s}\right) + 0.1 \cdot 500m \cdot 0.25 \left(\frac{m}{d}\right) = 3.5 \cdot 10^{-5} \left(\frac{m^2}{d}\right) + 12.5 \left(\frac{m^2}{d}\right) \approx 12.5 \left(\frac{m^2}{d}\right)$

$$C(x, y, z, t) = \frac{M}{8n(\pi t)^{3/2}\sqrt{D_x D_y D_z}} \exp\left(-\frac{X^2}{4D_x t} - \frac{Y^2}{4D_y t} - \frac{Z^2}{4D_z t}\right)$$

For the solution the time is kept constant e.g., for t = 10, 30, 60, 90, 180 and 360 days:

***Table 24**: Contaminated groundwater (m3), 3rd possibility*

Time [days]	Contaminated groundwater (m^3)
10	5,040
30	24,000
60	57,024
90	**96,330**
180	242,528
360	558,348

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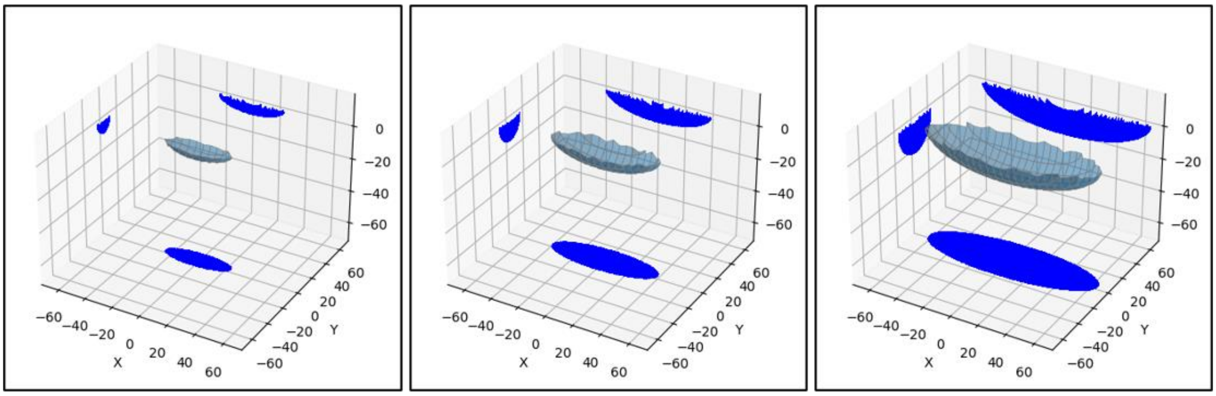

Figure 13: Leakage scenario of 150 kg of H_2SO_4 over 10, 30, and 90 days respectively, illustrating the expansion of the polluted groundwater area where pollutant concentration exceeds the toxicity threshold.

For the needs of this project the contamination of underground water bodies will be examined only for the 90 days period.

SO_4 leakage into the river

Assume a river of 2000 m length, with river discharge 2m^3/s. It is assumed that the contaminant influx increases from 0 to 10 mg/s during the first 100s, remains constant during 1 day and then decreases to zero within 4 days.

The algorithm developed by the NTUA team will be used for the simulation, following the below steps:

The 1st Step includes the definition of variables: The concentration, C (mg/m^3) of contaminant is a state variable.

The program variables are:

t	Time (s)
x	Space Coordinate along the river (m)
z0	Water Level Elevation (m)
A	Cross Sectional Area (m^2)
P	Perimeter Length (m)
Q	River discharge (m^3/s)
w	Surface width (m)
Sf	Friction Slope

The formula variables are:

wB	Riverbed width (10m)
S0	River Slope (=0.001)
Kst	Coefficient of friction Strickler (=25 m$^{1/3}$/s)
cF	Fischer coefficient (=0.011)

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Qin	Discharge of water (= $2m^3/s$)
zB	Riverbed elevation (= -S0 * x) (m) (bed elevation assuming zero elevation at x= 0 m)
dmax	Maximum water depth, as difference of water and bed elevations (= z0 – zB) (m)
dmean	Mean water depth (= A/w) (m), river depth is useful for the formulation of shear velocity and dispersion
ustar	Shear velocity (= sqrt(9.8 * dmean * Sf)) (m/s)

The real list variable is Fin = contaminant input flux (mg/s).

The 2nd Step includes the definition of river section compartment (Reichert, 1998):

A = dmax*wB (21)

P = wB+ 2* dmax (22)

Sf = 1/Kst^2*(P/A)^(4/3)*(Q/A)^2 (23)

Dispersion = cF*w^2*(Q/A)^2/ustar/dmean (24)

Furthermore, the following are, also, defined: Active variable C, Initial condition Qin for the variable Q and Input with a water inflow of Qin, and the Input flux Fin for variable C. In the 3rd Step the diagrams to be created are defined, 2 plots: 1st plot contaminant concentration vs time (Figure 14) and 2nd plot contaminant concentration vs space (Figure 15). The simulation process can be configured with any step size (here 20), which defines the time intervals between calculations, and a total of 500 steps.

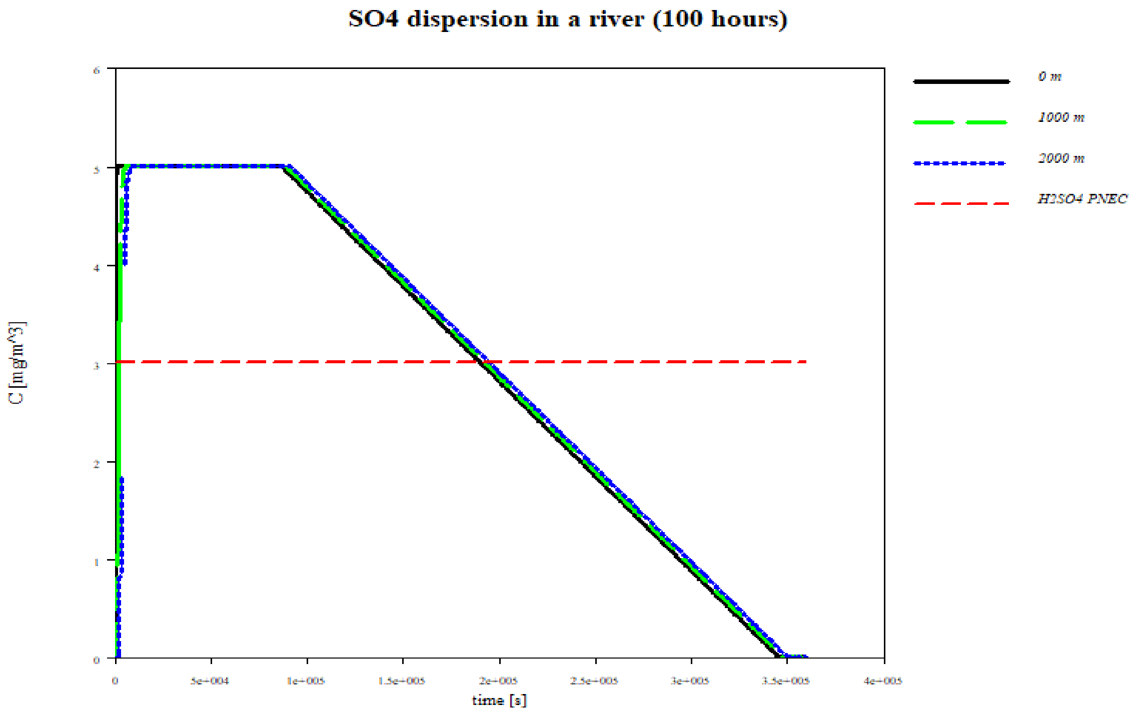

Figure 14: Contaminant concentration vs time for different distances from the leakage point

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According to Material Safety Data Sheet for sulphuric acid, the Predicted No-Effect Concentration (PNEC) for fresh water is 3mg/m^3. Based on this limit it was calculated that **9,000m^3** of water is contaminated.

Lake contamination:

In this specific instance, a leakage of 500 liters of HSO_4 solution (50% V/V)[1] (INTERCHIM, 2024) is assumed, equating to 250 liters of solute HSO_4 being discharged into the lake. We will assume that the contaminant is uniformly distributed from 0 to 1 cm depth within the lake, providing reasonable initial conditions. Another assumption is that the simulations take into account only a one-dimensional description of the lake, that averages all variables over horizontal cross sections (Reichert, 1998). Lastly, the designated threshold for the contaminant is set as the PNEC of HSO_4, with a value of 3 mg/m^3 (Roth, 2022).

The transfer of the solute into the lake is examined with consideration given to turbulent diffusion. For the purpose of this study, we will assume a lake depth of 30 meters, with linear interpolation providing the cross-sectional area (A) as follows:

***Table 25**: Cross-sectional area (A)*

Depth z (m)	Area A (m^2)
0	$1 * 10^7$
10	$8 * 10^6$
20	$5 * 10^6$
30	$1 * 10^5$

A vertical turbulent diffusion Kz is assumed with values as shown in table below (linear interpolation):

***Table 26**: Vertical turbulent diffusion Kz*

Depth (m)	Kz-value (m^2/day)
0	10
4.9	10
5.1	0.05
9.9	0.05
10.1	0.5
30	0.5

[1] Aluminum industries use solution of HSO_4 which has concertation 50% volume to volume

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Given the assumption that the lake's intersection surface remains constant within the depth range of 0 to 1 cm, which is determined to be 10^7 m^2 in the studied case, the volume for the initial conditions can be calculated using the following equation:

$$V_2 = A_{lake} * depth = 10^7 * 0.,01(m^3) \leftrightarrow \boldsymbol{V_2 = 10^5\, m^3} \quad (25)$$

To compute the dilution of the contaminant into the water, the dilution equation should be applied (eq. 26). Initially, given that 50% of the solution is pure HSO_4[1], the parameter M1 can be associated with the density. Additionally, the parameter V1 is equivalent to the leakage volume, whereas V2 has been previously calculated based on the assumptions made regarding the lake's intersection surface and depth distribution.

$$M_1 * V_1 = M_2 * V_2 \quad (26)$$

where

$M_1 = \rho = \frac{m}{V} = 1.8\left(\frac{g}{cm^3}\right) = 1.8 * 10^9(\frac{mg}{m^3})$

$V_1 = 0.25\, m^3$

$C_0 = M_2 = \frac{0.25*1.8*10^9}{10^5}\left(\frac{mg}{m^3}\right) = 4{,}500(\frac{mg}{m^3})$

The analytical equations for examining the dynamic diffusion of contamination into the lake are as follows (Reichert, 1998):

$$C = C_0 * \exp\left(-\frac{(z-z_o)^2}{2*\sigma^2}\right) \quad (27)$$

In which $z_o = 0\, m, and\ \sigma = 0.5$

Upon solving the equation, the depths at which the pollutant's concentration exceeds the threshold values can be determined. By combining these identified depths with linear interpolation, the surface area of the lake's intersections can be calculated. The following equation illustrates the linear interpolation methodology, where y represents the surface area and x corresponds to the depth:

$$\frac{y - y_0}{x - x_0} = \frac{y_1 - y_0}{x_1 - x_0} \quad (28)$$

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After calculating the surface area for each intersection, the lake is presumed to have a perfect circular shape for each horizontal section. Therefore, the following equation for the surface area of a circle can be utilized to calculate the radius:

$$A_{circle} = \pi * r^2 \leftrightarrow r = \sqrt{\frac{A_{circle}}{\pi}}$$

In the final Step the diagram to be created is defined for contaminant concentration vs space (Figure 15).

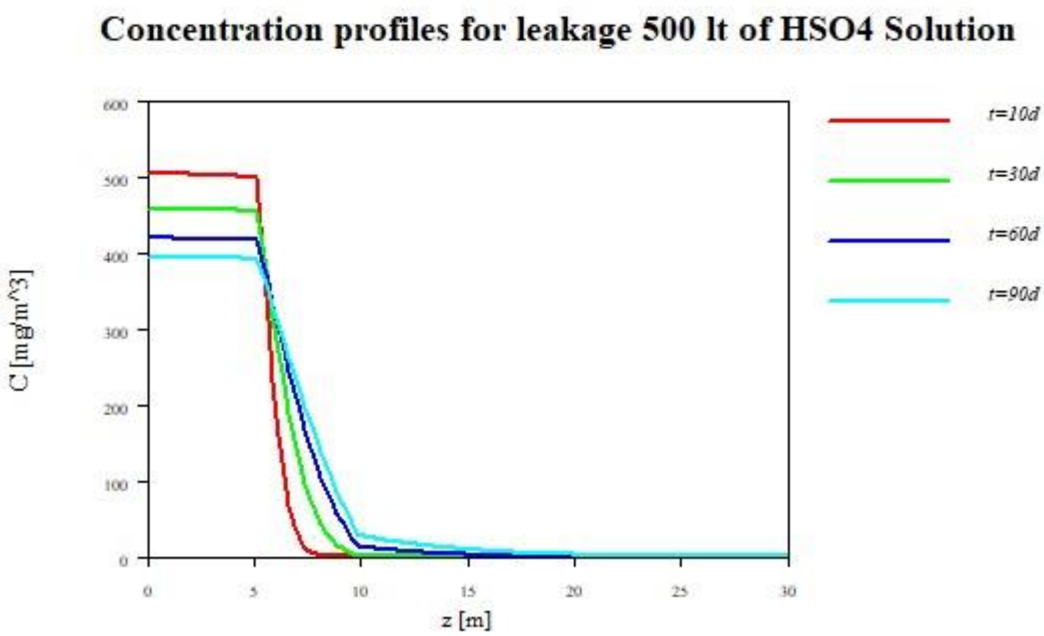

Figure 15: Contaminant concentration vs space for different time periods

To calculate the volume of the contaminated area, the shape of a cone is assumed to represent the volume of the lake. Considering that the contaminant has reached a specific depth within the lake, the following equation encapsulates the worst-case scenario of the volume that could be contaminated. Additionally, Figure 16 provides a visual representation of the shape of the contaminated volume.

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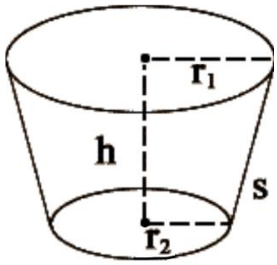

Figure 16: Cone shape of the contaminated volume of the lake, where r1 symbolizes the surface radius at z=0m, and r2 is the radius at the depth where the contamination has come to a halt.

$$V_{contaminated} = \frac{\pi}{3} * depth * (r_1^2 - r_2^2)$$

The results of the simulation indicated the following values:

Table 27: Lake's model simulation Results

Time (days)	Depth (m)	Surface (m²)	Radius (m)	Contaminated Volume (m³)
0	0	10000000	1784	-
10	7.875	8425000	1638	4120140
30	9.625	8075000	1603	6179070
60	14.63	6611000	1451	16504085
90	19.38	5186000	1285	31079915

This table illustrates the depth, surface area, radius, and contaminated volume over time as sulfuric acid leaks into a lake. The lake's surface area remains constant at the beginning (Time = 0), and the contaminated volume grows over time as the acid spreads through the water body.

- **Depth** (m): Refers to the vertical distance from the lake's surface to the maximum point where the contaminant has penetrated. It represents how deep the contamination has reached in the lake.
- **Radius** (m): Represents the distance from the center of the lake to the outer edge of the contaminated area, only for the surface of the lake (**r1**).
- **Surface** (m^2): The total area of the lake's surface that is exposed to contamination, calculated based on the surface radius **r1** (the cone-shaped contaminated volume).

For the needs of this project the contamination of the lake bodies will be examined only for the 90 days period.

Results Calculations

It should be noted that by having a zero baseline conditions in the examined area, the space where the pollutant's concentration is above the indicated threshold will be considered contaminated.

The risk of the scenario is estimated by the product of each scenario's probability with the fraction of the scenario's contaminated volume, divided by the highest measured ground volume from all the scenarios.

R(Si) = Si *(Vi/max(V))

Soil and Groundwater (For 90 days)

Table 28: *Risk Results for Soil*

Scenario	Area (m^2)	Volume (m^3)	Concentration - Threshold	Risk – R(Si)
S1	1	0.2	-	$6.76 * 10^{-9}$
S2	1	0.2	-	$6.76 * 10^{-9}$
S3	1	0.2	-	$6.76 * 10^{-9}$

Table 29: *Risk Results for Groundwater*

Scenario	Area (m^2)	Volume (m^3)	Concentration – Threshold (mg/lt)	Risk – R(Si)
S1	-	-	100	-
S2	-	32,292	100	$2.27 * 10^{-9}$
S3	-	96,330	100	$6.76 * 10^{-9}$

River

The contaminated area will be assumed to be the surface of the river inside the 2km radius around the initiating event, indicating a polygon.

Table 30: *Risk Results for River*

Scenario	Area (m^2)	Volume (m^3)	Concentration – Threshold (mg/m^3)	Risk – R(Si)
S4	20,000	9,000	3	$4.95*10^{-6}$

Lake (For 90 days)

The contaminated area will be assumed to be the surface of the lake inside the 2km radius around the initiating event, indicating a polygon.

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Table 31: *Risk Results for Lake*

Scenario	Area (m^2)	Volume (m^3)	Concentration – Threshold (mg/m^3)	Risk – R(Si)
S5	10,000,000	31,079,915	3	$4.75*10^{-8}$

6. Conclusion

In this report, the risk assessment framework, which is developed in order to assist the prevention and the remediation of environmental damage, is presented. The framework is in line with the European Directive 35/2004/EC, which calls the EU Member States to incorporate in their legislation the Directive's provisions that render environmentally liable each operator whose activity can cause or threaten to cause environmental damage in protected species and natural habitats. By incorporating the Directive in their national provisions, Member States have the obligation to develop appropriate frameworks in order to support all the relevant stakeholders to estimate potential adverse changes and impairments that activities can cause to the environment in a measurable way.

Serving the aforementioned goals, the aim of this deliverable is to develop a framework that will support all stakeholders, namely, regulators, operators, and insurers, to assess the environmental risk that may be caused by potential accidents during the operation of certain activities selected in Deliverable A1.3 of the LIFE Profile project. However, the framework is developed not only for the selected key activities but for every activity while it can be incorporated in each EU Member State.

To do so, five (5) main objectives have been addressed:

1. Definition of the baseline conditions (see section 4.3)

2. Definition of the risk events examined (see section 4.1.3)

3. Robustness under different conditions (see section 5)

4. Support the evaluation of environmental risk in monetary terms (refer to Deliverable B.2)

5. Be part of the software tool (refer to Action B.3)

The risk assessment framework is developed following a sequence of seven distinct steps in accordance with the sequences presented in the initially acceptable proposal and the mid-term report.

1. Method selection (three models based on the natural resources requirements, see sections 4.4, 4.5, 4.6 & 4.7)

2. Criteria selection (certain set for each model, see sections 5.1.1 & 5.2.1)

3. Weighting process (see section 4.1.6)

4. Scenarios sets development (see section 4.1)

5. Assessment process (see sections 4.1, 4.2, 4.3, 4.4, 4.5, 4.6 & 4.7)

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6. Testing process (see section 5)

The proposed risk assessment framework considers environmental impairments as the consequences that the initiating events can cause on specific natural resources and with regard to biodiversity on habitats. Therefore, the risk assessment framework follows a resource-oriented approach while from the biodiversity perspective it follows a habitat-oriented approach. As a result of the adoption of the aforementioned approaches, three models are developed, each of which is associated with certain type of natural resource and habitat, as well. These models are:

1. The model for surface soil (see Section 4.4),
2. The model for soil together with underground water (see Section 4.5 & 4.6), and
3. The model for surface water, i.e. lakes and rivers (see Section 4.7).

Testing process results illustrate the robustness of the developed methodology in various key-activities and under various conditions. In particular, the analysis of the fire accident occurred in a recycling factory in Aspropyrgos in June 2015 indicates that the results of the developed Gaussian air dispersion model, which is part of the soil surface model, do not diverge significantly bearing in mind the limitations of Gaussian dispersion models, since the pollutant concentration presented in post-accident reports are similar to the model's results. Meanwhile, the consequences on both the habitat and natural resources although presented in numerical values in the developed surface soil model, resulted to the same conclusions comparing to the conclusions of the post-accident reports especially regarding the significant concentration of heavy metals in the examined area, which is a 4km radius around the fire location.

In the absence of real-world industrial accident scenarios to test the computational pollutant dispersion models, theoretical scenarios were used in some cases. Specifically, for models concerning soil and underground water, a hypothetical sulfuric acid leak from an industrial pipe was assumed. Based on different scenarios according to the event tree of this accident, the volume of contaminated soil and underground water was calculated for various time steps, ranging from 10 days to 1 year. The contaminated volume of underground water increased over time, indicating the extent of cleanup required.

For surface water models, including lakes and rivers, algorithms developed by the NTUA team were used to simulate pollutant dispersion under two theoretical scenarios. In the first scenario, a continuous sulfuric acid leak into a river over a day was examined. The results showed that constant leakage significantly affects the river, as the pollutant concentration exceeded its toxicity threshold. In the second scenario, an instantaneous sulfuric acid spill into a lake for a tanker truck accident was studied. The simulation revealed that it would take 3 months for the pollutant to contaminate the entire lake up to a depth of around 20 meters.

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Appendix 1 – Handbook Failure Frequences 2009 Flemish Government

Category	Source of danger	Initiating event	Probability of occurrence
Pressure tanks (p. 12)	Storage tanks above ground, road tankers and tankwagons	Small leak (0,1 < d <= 10 mm (deq = 10 mm))	0.000012
		Medium leak (10 < d <= 50 mm (deq = 25 mm))	0.0000011
		Large leak (50 < d <= Dmax (deq = DL, max))	0.0000011
		Complete outflow (Complete outflow in 10 min)	0.00000032
		Rupture	0.00000032
	Underground or mounded	Small leak (0,1 < d <= 10 mm (deq = 10 mm))	0.000012
		Medium leak (10 < d <= 50 mm (deq = 25 mm))	0.0000011
		Complete outflow (Complete outflow in 10 min)	0.0000001
		Rupture	0.0000001
	Process installations and other	Small leak (0,1 < d <= 10 mm (deq = 10 mm))	0.00012
		Medium leak (10 < d <= 50 mm (deq = 25 mm))	0.000011
		Large leak (50 < d <= Dmax (deq = DL, max))	0.000011
		Complete outflow (Complete outflow in 10 min)	0.0000032
Mobile pressure containers (p. 13)	Gas cylinder	Rupture	0.0000011
	Pressure vessel	Leak (deq=Dmax)	0.000011
		Rupture	0.0000011
Atmospheric tanks (p. 14 - 16) Atmospheric tanks (p. 14 - 16)	Storage tank type 1 (incl. road tankers and tankwagons), 2, 3, 4 and underground or mounded	Small leak (0,1 < d <= 10 mm; deq = 10 mm)	0.0024
		Medium leak (10 < d <= 50 mm; deq = 25 mm)	0.00022
		Large leak (50 < d <= Dmax; deq = DL,max)	0.00022
	Process installations and other	Small leak (0,1 < d <= 10 mm; deq = 10 mm)	0.024
		Medium leak (10 < d <= 50 mm; deq = 25 mm)	0.0022
		Large leak (50 < d <= Dmax; deq = DL,max)	0.0022
		Complete outflow in 10 min	0.00005

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Category	Source of danger	Initiating event	Probability of occurrence
		Rupture	0.00005
	Storage tank type 1	Complete outflow in 10 min	0.000005
		Rupture	0.000005
	Storage tank type 2	Complete outflow in 10 min	0.0000005
		Rupture	0.0000005
	Storage tank type 3	Complete outflow in 10 min	0.000000012
		Rupture	0.000000012
	Storage tank type 4	Complete outflow in 10 min	0.00000001
		Rupture	0.00000001
	Underground or mounded storage tanks	Complete outflow in 10 min	0.00000001
		Rupture	0.00000001
	Tank with external floating roof	Tank fire (P1 liquid)	0.00025
		Tank fire (P2 liquid)	0.000076
		Tank fire (P3 and P4 liquids)	0.000023
	Tank with fixed roof without nitrogen blanket	Tank fire (P1 liquid)	0.00069
		Tank fire (P2 liquid)	0.00021
Atmospheric tanks (p. 14 - 16)		Tank fire (P3 and P4 liquids)	0.000062
	Tank with fixed roof with nitrogen blanket	Tank fire (P1 liquid)	0.00025
		Tank fire (P2 liquid)	0.000076
		Tank fire (P3 and P4 liquids)	0.000023
Heat exchangers (p. 17 - 18)	Pipe heat exchangers	Small leak. 0 < d <= 25 mm (deq = 10 mm)	0.006
		Medium leak. 25 < d <= 50 mm (deq = 35 mm)	0.0039
		Large leak. 50 < d <= 150 mm (deq = 100 mm)	0.000016
		Rupture	0.000013
	Plate heat exchangers (Working	Small leak. 0 < d <= 25 mm (deq = 10 mm)	0.0046
		Medium leak. 25 < d <= 50 mm (deq = 35 mm)	0.002
		Rupture	0.0000055

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Category	**Source of danger**	**Initiating event**	**Probability of occurrence**
	pressure (P) < 5 bar)		
	Plate heat exchangers (Working pressure (P) >= 5 - 8 bar)	Small leak. 0 < d <= 25 mm (deq = 10 mm)	0.007
		Medium leak. 25 < d <= 50 mm (deq = 35 mm)	0.003
		Rupture	0.0000083
	Plate heat exchangers (Working pressure (P) >= 8 bar)	Small leak. 0 < d <= 25 mm (deq = 10 mm)	0.018
		Medium leak. 25 < d <= 50 mm (deq = 35 mm)	0.0072
		Rupture	0.00002
Pumps and compressors (p. 19)	Centrifugal pumps with gaskets	Leak. deq = 0,1 Dmax	0.0044
	Centrifugal pumps without gaskets	Leak. deq = 0,1 Dmax	0.0001
	Reciprocating pumps	Leak. deq = 0,1 Dmax	0.0044
		Rupture	0.0001
	Compressors	Leak. deq = 0,1 Dmax	0.0044
		Rupture	0.0001
Pipe systems (p. 20)	Above ground pipeline	Small leak. deq = 0,1 D	0.00000028
		Medium leak. deq = 0,15 D	0.00000012
		Large leak. deq = 0,36 D	0.00000005
		Rupture	0.000000022
	Underground pipeline	Crack. deq = 10 mm	0.000000079
		Hole. deq = 0,5 D	0.000000069
		Rupture	0.000000028
Loading and unloading activities (p.21)	(Un)loading arm	Leak. deq=0,1 D(max. 50 mm)	0.0000003
		Rupture	0.00000003
	Hose	Leak. deq=0,1 D(max. 50 mm)	0.00004
		Rupture	0.000004
	Hose for LPG	Leak. deq=0,1 D(max. 50 mm)	0.0000054
		Rupture	0.00000054
Warehouses (p.22)	Fire in warehouse	Fire	0.0025

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Category	Source of danger	Initiating event	Probability of occurrence
	without an automatic fire fighting system		
	Fire in warehouse with an automatic fire fighting system	Fire	0.00069
Packaging units (p.23)	Packaging unit storage	One packaging unit fails	0.000025
Packaging units (p.23)	Packaging unit handling	One packaging unit fails	0.000025
		All packaging units on a pallet fail	0.0000025

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