GUARDIANS

D2.2.5 Reference algorithms for estimating risk maps in fire scenarios

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Abstract.
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This document surveys the current methodologies to estimate the risk level of industrial fires and methods to fuse spatio-temporal sparse risk information into a global continuous risk map.
Keyword list: fire risks, risk assessment, spatio-temporal estimation.

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Executive Summary

This report intends to identify the types of risk found in fire scenarios, how can those risks be measured, and how to estimate a risk map from scattered measurements.

Contents

Chapter 1

Risks in fire scenarios

There are a large number of risks associated to a fire scenario; however, these can be separated and classified into different groups such as explosion, hazardous gases, smoke, temperature and flame.

1.1 Hazardous gases

Many chemicals routinely located in warehouses or industrial buildings can produce toxic, flammable or explosive fumes or vapour by leaking from some containers or reacting with another chemical during a fire. A leaking gas, or vapour evaporating from a spilled liquid, can potentially create a hazardous cloud that travels far downwind from its release point. Usually, the chemicals can be liquid or gas, depending on the temperature of the environment. Knowing this, it is possible to understand how the gases can get into the atmosphere, and how quickly they do so. Another important aspect is related to the toxic and/or flammable/explosive characteristics of the chemical. Basically, a chemical is considered toxic if it can poison people who breathe it; it is considered flammable if it can ignite and burn easily.

1.2 Explosion

As mentioned above, a gas can be hazardous if its concentration in the air reaches a dangerously high level. A toxic gas can be hazardous if its concentration becomes intense enough to poison the people who breathe it. Exposure duration is important for toxic substances: people who breathe a toxic gas for a longer period of time are more likely to be harmed or to sustain worse injury. Similarly, a flammable gas can be hazardous if its concentration reaches the flammable range. This flammable range is the range of concentration of a gas in the air that will burn or explode if ignited. That range is place between the lower explosive limit (LEL) and the

upper explosive limit (UEL). In relation to the risk, the LEL (also known as lower flammability limit) is more important than the UEL mainly because it is the lowest concentration of a flammable vapour in the air at which an explosion or combustion can occur.

1.3 Temperature

In physics and thermodynamics, temperature can be defined as a physical property of a system that underlies the common notions of hot and cold. Usually, something that feels hotter generally has the higher temperature. Specifically, temperature is a property of matter. Many physical properties of materials including the phase (solid, liquid, gaseous or plasma), density, solubility, vapour pressure and electrical conductivity depend on the temperature. Temperature also plays an important role in determining the rate and extent to which chemical reactions occur. Temperature is a key element in the determination of the flammable or explosive limits. Another important aspect is the commonly called material's auto ignition or ignition temperature. This is the temperature at which a material self-ignites without any obvious sources of ignition, such as a spark or flame.

1.4 Flame

A flame can be described as the visible (light-emitting) part of a fire. It is caused by a highly exothermic reaction (e.g. combustion). Flame, as a state of matter, is classified as plasma - partially ionized gas. The colour and temperature of a flame are dependent on the type of fuel involved in the combustion, for instance, when a lighter is held to a candle. The applied heat causes the fuel molecules in the wick to vaporize. In this state, they can then readily react with oxygen (a key element in combustion) in the air, which gives off enough heat in the subsequent exothermic reaction to vaporize yet more fuel, thus sustaining a consistent flame. Therefore, the presence of flames in any scenario represents a real risky situation that might be potentially dangerous.

1.5 Smoke

Smoke is the collection of airborne solid and liquid particulates and gases emitted when a material undergoes combustion, together with the quantity of air that is entrained or otherwise mixed into the mass. It is a very common product of fires (including stoves, candles and fireplaces). Smoke inhalation is perhaps the primary cause of death in victims of indoor fires. Smoke kills by a combination of thermal

damage, poisoning and pulmonary irritation caused by carbon monoxide, hydrogen cyanide and other combustion products. The composition of smoke depends on the nature of the burning fuel and the conditions of combustion. Different chemicals will produce different smokes' compositions, ranging from the material that can be commonly found in houses to industrial buildings or warehouses. As mentioned before, oxygen plays an important role in fire. A fire with high availability of oxygen burns at a high temperature but with a small amount of smoke produced.

Chapter 2

Risk assessment

From the fire risks described in the previous chapter, the explosion risk is the most critical and harder to estimate, so this chapter is mostly focused on the problem of estimating the Lower Explosive Limit (LEL) of gas mixtures.

2.1 Estimating LEL

Many manufacturing processes involve flammable chemicals, making the safety and risk assessment one of the major concerns when working in such environments. The flash point of a flammable liquid is the lowest temperature at which it can form an ignitable mixture with air. It is related to the lower flammability limit which is the minimum concentration of fuel in the fuel-air mixture (as can be seen in Figure 2.1).
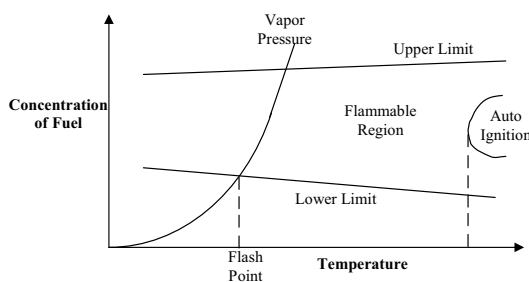

Figure 2.1: Inflammable limits.

In cases which involve processes where mixtures under different conditions of temperature, pressure and oxygen concentrations are used, it is necessary to determine the flash point. The flash point can be used to assess the level of risk over the

time because it is the temperature at which sufficient vapour is generated to bring the concentration of flammable vapour above the lower flammability limit.

Most of the predictive theoretical methods used to determine the flash points of mixtures are based on the Le Chatelier equation together with a vapour-liquid equilibrium model calculation of the vapour composition when liquids are involved.

2.1.1 Predictive methods for flash point of substances

A nonlinear exponential correlation was proposed by Satyarayana and Rao [1] for the estimation of the flash point of organic compounds and petroleum fractions as a function of their boiling temperature capable of predicting the flash point with less than 1% average absolute error. The resulting correlation is:

$$T_f = a + \frac{b\left(\frac{c}{T_b}\right)^2 e^{-\frac{c}{T_b}}}{\left(1 - e^{-\frac{c}{T_b}}\right)^2} \tag{2.1}$$

where T_f denotes the flash point temperature in K; T_b is the normal boiling point in K, and a, b and c are constants. These constants are evaluated by nonlinear regression using the Gauss-Newton iteration method.

Hshieh [2] developed a correlation of closed cup flash points with normal boiling points for silicone and organic compounds. The silicone compounds correlation:

$$T_f = -51.2385 + 0.4994T_b + 0.0004T_b{}^2 \tag{2.2}$$

A correlation for organic compounds was developed using data for 494 compounds. The result is:

$$T_f = -54.5377 + 0.5883T_b + 0.00022T_b{}^2 \tag{2.3}$$

where T_f and T_b are in °C. The correlation coefficient is 0.966 and the standard error of estimate is 11.66° C.

Prugh developed an alternative for the calculation of flash point of pure components [3]. The method consists in the prediction of vapour pressure curves and LFL of organic compounds solely on the basis of their normal boiling points and chemical structures. He calculated the stoichiometric concentration of the vapour in the air needed to calculate the flash point from the value of the normal boiling point.

Flash points of pure compounds can also be obtained from Quantitative Structure Property Relationships (QSPR), which are correlations that relate the flash point value with molecular descriptors [4].

2.1.2   Predictive methods for flash point of mixtures

Mathematically, the flash point is the temperature at which the saturated vapour pressure is equivalent to the LFL composition:

$$LFL_i = \frac{P_{i,fp}^{sat}(T_f)}{P} \tag{2.4}$$

where $P_{i,fp}^{sat}(T)$ is the saturated vapour pressure at the flash point temperature and P is the ambient pressure. Thermodynamically, the relation between an ideal vapour and a non-ideal liquid is represented by the equilibrium condition presented in the following equation, which represents the Le Chatelier rule for the flammable vapour-air mixture of two components:

$$\frac{y_1}{LFL_1} + \frac{y_2}{LFL_2} = 1 \tag{2.5}$$

where y_1 and y_2 refer to the vapour mole fraction of components 1 and 2, and LFL_1 and LFL_2 refer to the lower flammability limit of component 1 and 2. The flash point of a binary mixture can be estimated by the model developed by Liaw:

$$\frac{x_1 \gamma_1 P_1^{sat}}{P_{1,fp}^{sat}} + \frac{x_2 \gamma_2 P_2^{sat}}{P_{2,fp}^{sat}} = 1 \tag{2.6}$$

where x_i, γ_i, P_i, and $P_{i,fp}^{sat}$ are the liquid mole fraction, liquid phase activity coefficient, vapor pressure at temperature T and vapor pressure at Tf of the mixture component, respectively.

Affens and McLaren [5] developed a graphical method to calculate flash points of multi-component hydrocarbon mixtures from the flash points and concentrations of the individual components. This method is based on the assumption that the vapour pressure-temperature relationships are known and that the systems obeys the laws of Raoult, Dalton, and Le Chatelier. This method works well for hydrocarbon mixtures.

Wu and Finkelman [6] calculated the flash point of different binary mixtures using the equations of Le Chatelier and Walsham. Some of the mixtures considered were ethanol-toluene, hexane-ethanol and ethanol-n-propanol.

White [7] reduced Affens and McLaren's model to a simpler equation by ignoring the temperature effect upon LFL. This equation is used to estimate the flash point of jet-fuel mixtures.

Gmehling and Rasmussen [8] have shown that the UNIFAC group contribution method is applicable for the flash points prediction of binary and multi-component liquid mixtures. The method consists in determining the flash point temperature based on the partial pressure of the components. It uses Zebatekis's equation to calculate the temperature and Antoine's equation for the pressure.

Wickey and Chittenden [9] implemented a method for calculating the flash points of petroleum mixtures. Their method is based on the use of flash point indices for the components in the mixture in proportion to their volume fractions.

### 2.1.3 Predictive methods for flammability limits in substances

Flammability limits provide the range of fuel concentration (normally in percentage volume), within which a gaseous mixture can ignite and burn. Below the lower flammability limit, there is not enough fuel to cause ignition. Similarly, with fuel concentrations greater than the Upper Flammability Limit (UFL), there is insufficient oxygen for the reaction to propagate away from the source of ignition. As an example of the equations for the estimation of flammability limits in air, those of Jones are frequently cited [10]:

$$LFL = 0.55C_{est} \tag{2.7}$$

$$UFL = 3.5C_{est} \tag{2.8}$$

where C_{est} is the stoichiometric concentration of the flammable product for complete combustion in air.

The estimate for a general compound CHO is obtained by considering complete combustion to carbon dioxide and water:

$$C_nH_xO_y + \left(n + \frac{x}{4} - \frac{y}{2}\right)O_2 \rightarrow nCO_2 + \left(\frac{x}{2}\right)H_2O \tag{2.9}$$
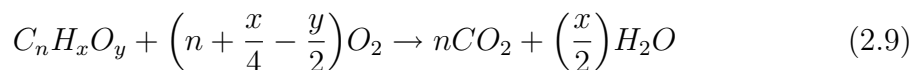
The concentration in air is calculated by correcting the oxygen calculated from the above equation for the accompanying nitrogen.

Another empirical relation frequently used for the prediction of the LFL in air is that of Spakowski [11]:

$$LFL \times (-\Delta H_{comb}) = 4.354 \times 10^3 \tag{2.10}$$

where $(-\Delta H_{comb})$ is the standard heat of combustion, and expressed as kJ/mol.

2.1.4 Predictive methods for flammability limits in mixtures

Given the flammability limits of each of the components in a mixture, the lower flammability limit of a mixture may be calculated by Le Chatelier's rule [12]:

$$MLFL = \frac{100}{\Sigma \frac{C_i}{LFL_i}} \tag{2.11}$$

where $MLFL$ is the mixture lower flammability limit (vol.%); C_i is the concentration of component i in the gas mixture on an air-free basis (vol.%); and LFL_i is the lower flammability limit for compound i in the mixture (vol.%).

Melhem [13] developed a method for the estimation of flammability limits for chemical mixtures based on chemical equilibrium. The impact of the mixture initial temperature and pressure is implicitly accounted for. His methodology uses the concept of a threshold theoretical flame temperature, which is the temperature at which the combustion reaction is able to generate sufficient heat to produce a self-sustaining (propagation) reaction.

Another method is the neural network method implemented by Zhen, Fan and Zuo used to estimate the explosion limits of flammable gas mixture containing H_2, CH_4 and CO.

Chapter 3

Risk mapping

A risk map is a floor plan of the workplace which pinpoints various hazards that can cause any risk. It is similar to a blueprint which gives a visual representation of the location of workplace hazards. The risk mapping findings can be used to identify and prioritize hazards. Risk mapping provides written records of workplace hazards and gives labour/management representatives a better view of problems. Figure 3.1 shows a risk map representing the smoke concentration in an enclosed area.

In a general view, a risk map helps to identify the existence of risks in an area, helping to find solutions or take steps to reduce the risk:

- It will help to identify major hazards

- It will provide authorities and local organizations with information for decision making and planning.

- It can record the effects of any previous disasters.

- It can identify possible solutions to be followed in the case of a disaster.

A broad class of environmental sensing applications requires observing environments that display significant heterogeneity in both space and time. As an example, in terms of the amount of a special type of gas or smoke in an area, observation is useful for answering the questions pertaining to the multi-dimensional area gas modelling. These require high granularity measurements of density of the gas in different points of the under-study area. A spatial field will be partially observed at selected sites and the goal is to infer the field at unobserved sites. This is the problem of spatial estimation, sometimes called spatial prediction.
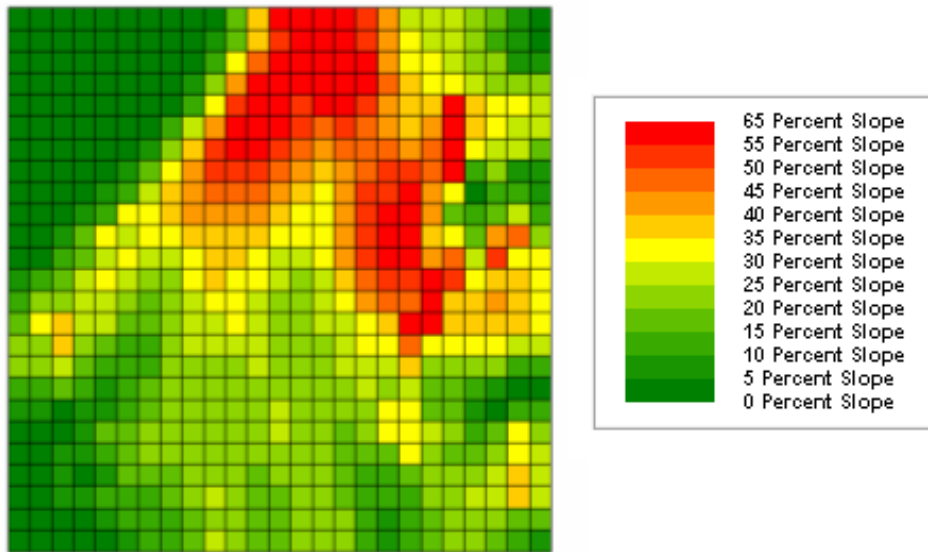
Figure 3.1: A risk map

3.0.5 Spatial estimation

Conventional interpolation methods (Piecewise constant, Linear, Polynomial, Spline), incorrectly assume that data varies linearly between sampled points. Gradients encountered at region boundaries often invalidate the assumption of linearity. Thus, renditions of data that are computed using conventional linear methods are accomplished using a model that is not valid over the entire data domain. Furthermore, these methods do not provide a measure of the estimation error that they introduce to the interpolated data set.

Kriging is a method for converting the data into an estimate of the field together with a measure of error or uncertainty. A Kriging estimate of the field at an unobserved location is an optimized linear combination of the data at the observed locations. The coefficients of the Kriging estimate and the associated error measure, both depend on the spatial configuration of the data, the unobserved location relative to the data locations, and spatial correlation or the degree to which one location can be predicted from a second location as a function of spatial separation. The method has close links to Wiener optimal linear filtering in the theory of random functions, Gandin objective analysis in meteorology, spatial splines and generalized least squares estimation in a spatial context. Kriging methods have been studied and applied extensively since 1970 and have been adapted, extended, and generalized. For example, Kriging has been generalized to classes of nonlinear functions of the observations, modified to increase robustness extended to take advantage of covariate information, adapted for fields whose statistical properties are spatially evolving, and placed into a formal Bayesian framework.

Kriging is a procedure for spatial prediction at an unobserved location, using data at observed locations, optimized with reference to a specific error criterion. The criterion is the squared prediction error at the unobserved location - averaged over a conceptual class of spatial prediction problems that have the same configuration of observed and unobserved locations. The specification of this averaging class is the model under which the optimization is carried out and the estimation error is reported.

The usual model under which Kriging calculations are made is that of a spatial stochastic process that generates spatial fields over the geographical region of interest. A stochastic process model is selected with characteristics that reflect characteristics of the available data. With this averaging model, the stated Kriging properties are purely conceptual - they refer to average prediction errors that would be seen if the same Kriging procedure were applied to the same prediction problem on spatial fields generated repeatedly by the selected stochastic process. Locations of the observed sites within the geographical domain are fixed under this averaging model, but not the values of the observations themselves.

When randomness is deliberately introduced into observation sites, such as stratified random sampling for example, it is common to use the fixed-field averaging model with movable site configurations. If the goal is to estimate an area average value, then the assigned estimation errors will be operationally similar for the fixed field and stochastic field averaging models, even though the stochastic field model will treat the results of the randomized observation sites as fixed locations. However, for estimating (predicting) field values at specified sites, as in interpolation and mapping, an averaging model that uses only randomization of the observation sites would not be meaningful for the computation of estimation error, and a more complete method like Kriging will be required.

In other words, one can say, Kriging is an optimal interpolator based on regression against observed z values of surrounding data points, weighted according to spatial covariance values.

It would seem reasonable to estimate ϕ_u by a weighted average $\sum \lambda_\alpha \phi_\alpha$, with weights λ_α given by some decreasing function of the distance, d_α , from u to data point α.

All interpolation algorithms (inverse distance squared, splines, radial basis functions, triangulation, etc.) estimate the value at a given location as a weighted sum of data values at surrounding locations. Almost all assign weights according to functions that give a decreasing weight with increasing separation distance. Kriging assigns weights according to a (moderately) data-driven weighting function, rather than an arbitrary function, but it is still an interpolation algorithm that in the following cases provides very similar results to the other interpolators [?]:

- If the data locations are fairly dense and uniformly distributed throughout
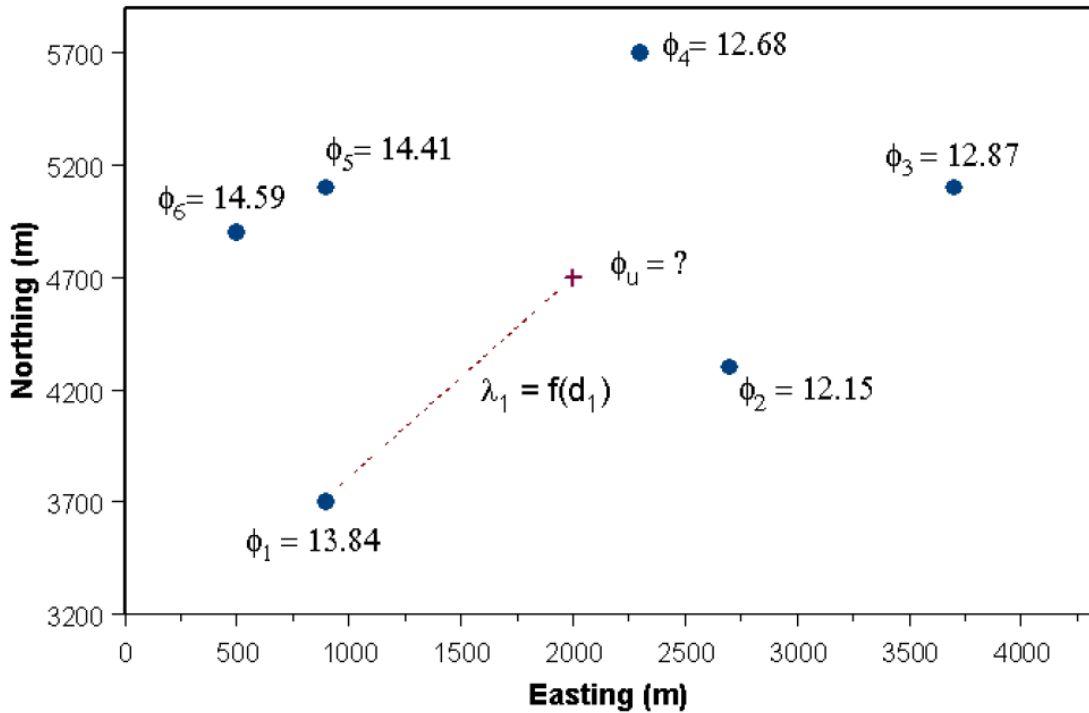
Figure 3.2: Kriging

the study area, you will get fairly good estimates regardless of interpolation algorithm.

- If the data locations fall in a few clusters with large gaps in between, you will get unreliable estimates regardless of interpolation algorithm.

- Almost all interpolation algorithms will underestimate the highs and overestimate the lows; this is inherent to averaging and if an interpolation algorithm didn't average it wouldn't be considered reasonable.

Kriging

All kriging estimators are variants of the basic linear regression estimator $Z^*(u)$ which is defined as:

$$Z^*(u) - m(u) = \sum_{\alpha=1}^{n(u)} \lambda_\alpha Z(u_\alpha) - m(u_\alpha)$$

with u, u_α the location vectors for estimation point and one of the neighboring data points, indexed by α; $n(u)$ the number of data points in a local neighborhood

used for estimation of $Z^*(u)$; $m(u), m(u_\alpha)$ the expected values (means) of $Z(u)$ and $Z(u_\alpha)$; $\lambda_\alpha(u)$ the kriging weight assigned to datum $Z(u_\alpha)$ for estimation location u; same datum will receive different weights for different estimation location; $Z(u)$ is treated as a random field with a trend component, $m(u)$, and a residual component, $R(u) = Z(u) - m(u)$.

Kriging estimates residual at u as a weighted sum of residuals at surrounding data points. Kriging weights, λ_α, are derived from covariance function or semivariogram, which should characterize the residual component. The distinction between trend and residual is somewhat arbitrary; it varies with scale.

The goal is to determine weights, λ_α, that minimize the variance of the estimator $\sigma_E^2 = Var\{Z^*(u) - Z(u)\}$ under the unbiasedness constraint $E\{Z^*(u) - Z(u)\} = 0$.

The random field (RF) $Z(u)$ is decomposed into residual and trend components, $Z(u) = R(u) + m(u)$, with the residual component treated as an RF with a stationary mean of 0 and a stationary covariance (a function of lag, h, but not of position, u):

$E\{R(u)\} = 0$

$Cov\{R(u), R(u+h)\} = E\{R(u)R(u+h)\} = C_R(h)$

The residual covariance function is generally derived from the input semivariogram model, $C_R(h) = C_R(0) - \gamma(h) = Sill - \gamma(h)$. Thus the semivariogram is feed to a kriging program that should represent the residual component of the variable.

Kriging variants

There are three main kriging variants: simple, ordinary, and Kriging with a trend. Their main difference consists in their treatment of the trend component, $m(u)$.

- For simple kriging, we assume that the trend component is a constant and known mean, $m(u) = m$.

- For ordinary kriging, rather than assuming that the mean is constant over the entire domain, we assume that it is constant in the local neighborhood of each estimation point, that is that $m(u_\alpha) = m(u)$ a for each nearby data value, $Z(u_\alpha)$, that we are using to estimate Z(u).

- Kriging with a trend (the method formerly known as universal kriging) is much like ordinary kriging, except that instead of fitting just a local mean in the neighborhood of the estimation point, we fit a linear or higher-order trend in the (x,y) coordinates of the data points. A local linear (a.k.a., first-order) trend model would be given by $m(u) = m(x, y) = a_0 + a_1 x + a_2 y$.

Kriging advantages

- Helps to compensate for the effects of data clustering, assigning individual points within a cluster less weight than isolated data points (or, treating clusters more like single points)

- Gives estimate of estimation error (Kriging variance), along with estimate of the variable, Z, itself (but error map is basically a scaled version of a map of distance to nearest data point, so not that unique)

- Availability of estimation error provides basis for stochastic simulation of possible realizations of $Z(u)$

Chapter 4

Conclusions

Deliverable 2.2.5 has been produced on schedule. However, the methods described in this document have not yet been implemented in the GUARDIANS project. This implementation is foreseen for the last year of the project, and it is expected that enhancements and improvements will arise when the work related to this deliverable is implemented in the GUARDIANS system.

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