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#### Deliverable summary

Probabilistic risk assessment (PRA) and life cycle assessment (LCA) are approaches enabling us to (a) quantify potential effects of products and (b) support decision making in environmental management. The first part of this document illustrates preliminary works performed in the context of PRA which we envision to then transfer to the two field sites analysed in the project (i.e., the Cremona and Bologna Aquifer systems, located in the Po Plain, Northern Italy). A review of the most widely tools used for PRA is provided. Methodologies we describe include: Failure mode and effect analysis, Multi-barrier approach, Event and Fault tree analysis, Bayesian belief network, and Influence diagram. Emphasis is given to the applications of these approaches to subsurface flow and transport phenomena considered in WE-NEED. We then provide a special focus on the Fault tree method. We also propose a procedure to tackle (i) groundwater contamination occurrence and (ii) natural spring depletion issues, tailored to the two showcases considered. In the second part of the document we present and discuss the four main steps at the heart of LCA.





# D5.1

# Report on Groundwater Risk Management Model

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## 1. Introduction

Subsurface heterogeneity, the ubiquitous lack of complete site characterization as well as conceptual and numerical limitations inherent to all modeling approaches are (among others) main reasons rendering deterministic predictions of subsurface flow and transport inadequate. Quantification of these and other sources of uncertainty is key for the design of modern and scientifically-based decision making procedures, in the areas of sustainable use and remediation of groundwater resources. Many pressing environmental problems, such as the selection of an efficient and sustainable water management and development strategy, cannot be realistically tackled without a robust uncertainty quantification and risk analysis. When these modeling components are ignored, failures of action plans engineered to the control of fate and migration of contaminants have already been documented. For example, one should consider the frequency with which contaminant plumes are documented to bypass permeable reactive barriers set in place with a pattern designed by relying on deterministic analyses (ITCR, 2005).

While in subsurface hydrology it is widely recognized that risk analysis must be an integral part of decision making processes, a unique and unambiguous definition of the procedure to be employed in such a context is still subject to lively debate. Scientific/technical disciplines where risks are routinely evaluated to satisfy statutory requirements, e.g., nuclear power generation (NRC, 1983), aerospace industry (Pate-Cornell and Dillon, 2001), and earthquake engineering (NRC, 1997), provide some guidance in this sense.

A comprehensive risk analysis can be defined as a procedure that enables one to answer the following three questions: "What can happen? How likely is it to happen? Given that it occurs, what are the consequences? (Bedford and Cooke, 2003)". The National Research Council's report (NRC, 1997) on seismic hazard analysis explicitly identifies the following attributes of risk assessment (RA): (1) RA must be probabilistic and quantitative; (2) RA must be based on subjective probabilities; and (3) The main focus of any probabilistic RA (PRA) must be on uncertainty quantification.

The reasoning behind these recommendations is also applicable to subsurface hydrology. The emphasis is on the quantitative (as opposed to descriptive or qualitative) nature of PRA. The statement "the contamination is likely to occur" does not provide a complete picture of the issue, as it must include the quantification of the probability of such an occurrence (Garrick, 1989). Additionally, the use of "subjective probabilities", P[A], defined as "a degree of belief, of one individual, in the occurrence of A" (Bedford and Cooke, 2003, p. 24), paves the way to include expert knowledge and additional soft data in the modeling process (NRC, 1997).

A rigorous PRA framework lays out a formal procedure for risk analysis formed by the following steps (Vesely et al., 1981; Bedford and Cooke, 2003):

(1) Definition of the concept of system failure;



- (2) Identification of key components/events (e.g., contaminant release, failure of a permeable reactive barrier to intercept a migrating plume) contributing to a system failure (e.g., aquifer contamination, escape of the sequestered CO<sub>2</sub> into the atmosphere, depletion of a spring);
- (3) Provision of a graphical diagram (e.g., fault or event tree, binary decision diagram, see Section 2) elucidating the dependency structure across the various aspects of the considered problem;
- (4) Development of a mathematical modeling strategy for the system, which allows one to relate the probability of system failure to that of its critical constitutive components,  $P_i$  (subscript *i* indicating a given component according to which the event "system failure" has been destructured);
- (5) Computation of the probabilities defined at point (4).

Application of PRA in complex physical processes, including flow and transport in subsurface environments, poses a set of challenges that are not typically encountered in PRA developed for classical engineered problems (Batchelor et al., 1998; Wang and McTernan, 2002; Tartakovsky, 2007; Winter and Tartakovsky 2008; Bolster and Tartakovsky, 2008). While in manufactured systems (e.g., space shuttles or nuclear power plants) the probability of failure of an individual component (i.e., the probability of the occurrence of an undesired event),  $P_i$ , can often be estimated *a priori*, in analyzing subsurface systems  $P_i$  must be either computed by solving flow and transport problems (with uncertain parameters) or inferred from expert knowledge. The former option typically relies on (numerical) Monte Carlo simulations or alternative mathematical frameworks, including moment equations (Morales-Casique et al., 2006), probability density function (pdf) approaches (Sanchez-Vila et al., 2009; Tartakovsky and Broyda, 2007), stochastic collocation methods (Zhang et al., 2013), and stochastic finite elements (Charrier, 2012). The second option is based on prior experience, knowledge of geology at the site, recharge terms, strength of anthropogenic actions, and of the main processes taking place in the specific application. PRA can facilitate both approaches by replacing a complex problem typically characterized by several uncertain inputs by a set of subsystems, characterized by only a few uncertain parameters. When the probability of failure of a given subsystem cannot be evaluated, it might be possible to compute its upper bound, thus leading to a conservative estimate of risk.

Life Cycle Assessment (LCA) is a RA tool widely used and accepted for quantifying potential effect of a product and supporting decision making during environmentally conscious management. This procedure has been developed in the 1960s and its framework is nowadays coded by the international standard series ISO 14040 and ISO 14044. In essence, LCA consists of four main steps:

(1) Goal and scope definition, where the purpose of the study and its scope are defined;





- (2) Inventory analysis, involving data collection and calculation procedures to quantify relevant inputs and outputs of a product system;
- (3) Impact assessment, providing a link between data (i.e., the results of step 2) and specific environmental impacts;
- (4) Interpretation of the results of steps (2) and (3) to meet the objectives of the study.

The LCA approach has been applied to evaluate the impact caused by diverse groundwater remediation technologies (e.g. Bayer and Finkel, 2006; Cadotte et al., 2007; Lemming et al., 2010). Analyses of methods to assess impacts of water use have been proposed, among others, by Boulay et al. (2015a, b), Pfister et al. (2016) and Núñez et al. (2016).

Although PRA and LCA are characterized by differing key aspects and methodological approaches, they provide a way of structuring and analyzing information relevant to one or more environmental aspects of the decision making procedure. A PRA can be effectively performed at different stages of LCA and the two approaches may benefit from a feedback, one informing (and complementing) the other in the decision process (Cowell et al., 2002; Flemström et al., 2004).

This Deliverable is structured as follows. Section 2 provides a description of alternative probabilistic methodologies for risk assessment. Ongoing activities focusing on the application of PRA for groundwater contamination (at the Bologna pilot site) and natural springs depletion (at the Cremona pilot site) scenarios are summarized in Section 3 and 4, respectively. Section 5 is devoted to illustrate the role of LCA and its main components.

## 2. Probabilistic Risk Assessment

A plethora of methods have been established to perform PRA. Here we report the most widely used approaches as well as their application to subsurface flow and transport phenomena.

#### 2.1 Failure mode and effect analysis

Failure mode and effect analysis (FMEA) is a qualitative tool (Andrews and Moss, 1993; Kunamamoto and Henley, 1996;) identifying all possible failures in a system. The system is divided into elements and failure modes and their resulting effects are identified for each element (in sequence). Each failure mode is associated with potential effects/causes of failure, and detectability modes. All these identified features are in turn associated with quantitative indices indicating their severity (*S*) of impact, probability of occurrence (*O*) and detectability (*D*). *S*, *O* and *D* indices are scored on a scale 1-10 as specified below:





- 1. *S* indicates severity of impact of a failure event, a high score being associated with high impact;
- 2. *O* is associated with the frequency of occurrence of the failure event, a high score being associated with high frequency.
- 3. *D* illustrates the ability of process control to detect the occurrence of failure events; a low score identifies a failure event which can be easily detected while high scores are assigned to inconspicuous failure events.

The key outcome of this methodology is a risk priority number (*RPN*), defined as  $RPN = O \times S \times D$ . High values of *RPN* are associated with the most critical failure modes. A list of actions for reducing the occurrence of the cause of the identified key failure events or aimed at improving their detection is usually provided.

As an example, Figure 1 shows a typical worksheet associated with FMEA for an exemplary element (here termed Element 1 and characterized by three possible failure modes) of a generic system.

System Element	Potential failure mode	Potential effect(s) of failure	S	Potential cause(s) of failure	0	Detecta- bility	D	$RPN = = O \times S \times D$
	In what ways can the system fail?	What is the impact of failure?	How severe is the effect of failure?	What causes the element failure?	How frequently is the cause likely to occur?	What are the existing controls which may prevent failure?	How probable is the detection of the failure mode?	Risk priority number
Element 1		Effect 1		Cause 1	$O_I$	Detection mode 1	$D_{I}$	RPN <sub>1</sub>
	Failure mode 1	Effect 2	$S_{I}$	Cause 2	$O_2$	Detection mode 2	$D_2$	$RPN_2$
		Effect 3		Cause 3	$O_3$	Detection mode 3	$D_3$	RPN <sub>3</sub>
	Failure mode 2	Effect 1 $S_2$	G	Cause 1	$O_l$	Detection mode 1	$D_l$	$RPN_{l}$
			$S_2$	Cause 2	$O_2$	Detection mode 2	$D_2$	$RPN_2$
	Failure mode 3	Effect 1	Effect 1	Cause 1	$O_l$	Detection mode 1	$D_{I}$	RPN <sub>1</sub>
		Effect 2 $S_3$	$S_3$	Cause 2	$O_2$	Detection mode 2	$D_2$	RPN <sub>2</sub>

Figure 1. Example of worksheet associated with FMEA (modified from Stamatis, 2003).

FMEA can be easily applied to diverse fields of interest. It is noted that even as *RPN* provides a ranking of the failure modes, based on expert knowledge, the probability of system failures is not quantified.





## 2.2 Multiple barrier approach

The Multiple barrier approach (MBA) (Hrudey, 2001; 2006) is a qualitative methodology which aims at reducing the risk of contamination of drinking water, increasing the feasibility and the effectiveness of remedial controls and precautionary measures (CCME, 2004). MBA is based on the application of multiple procedures (or barriers) to ensure that pathogenic contaminants or undesirable chemicals do not reach the consumer's tap. Main components of the method include the source water, the drinking water treatment plant and the distribution system. Links between these components and the workflow typically associated with MBA are depicted in Figure 2. First, all potential control barriers in the system are established and their limitations are identified. These barriers can be physical tools (e.g., filtration system in a drinking water treatment plan) or procedures improving the management of a drinking water program (including, e.g., legislation, policies, guidelines, or other). Then, these elements are combined in an integrated manner (see Figure 2) to minimize the likelihood that contaminants pass through the entire system with a concentration that can cause illness to consumers (i.e., exceeding a critical concentration threshold). The risk reduction associated with a multiple barrier approach is depicted in Figure 3. The key strength of MBA relies on the observation that failure of one or more barriers may be compensated by the remaining barriers. However, MBA (as already observed for FMEA) yields a qualitative risk assessment of the system and it has been proposed and applied mainly for drinking water quality issues (Hrudey et al., 2006).



Figure 2. Components of the multiple barrier approach (modified from: CCME, 2004).





Figure 3. Drinking water risk management and the multiple barrier approach (Modified from Hrudey et al., 2001; 2006).

## 2.3 Event tree and Fault tree analysis

Event tree (ETA) and fault tree (FTA) analyses are two of the most widely applied quantitative tools in system analysis (Bedford and Cooke, 2003). Both approaches are based on a graphical representation of the system grounded on Boolean logic. ETA is a forward, bottom-up, logical modeling technique for both success and failure of a system. It begins with an initiating event (an incident) and then propagates this event through the system, considering all possible ways in which it can affect the behavior of the network. An example of ETA, including an initiating event and two safety systems, is depicted in Figure 4.



Figure 4. Event tree graphical representation of the system (modified from Bedford and Cooke, 2003). F and S indicate respectively system failure and success.





FTA is a backward, top-down, methodology using the system failure as a starting point and then establishing a chain of basic events that can cause the system failure. Using Boolean operators (or operations) 'AND', 'OR' and 'NOT', one can write down which events or combination of events leads to the top event and thus to the failure of the system. Figure 5 illustrates a schematic example of a generic fault tree. In this simple case, system failure can be caused by the occurrence of at least two basic events, here identified as events 1 and 3 or events 2 and 3.



Figure 5. Fault tree graphical representation (modified from Bedford and Cooke, 2003).

FTA and ETA are methodologies for PRA which allow to quantitatively estimate the probability of a system failure. FTA aims at replacing an intractable problem of risk assessment characterized by several uncertain parameters with key subsystems, each of which can be described upon relying on only a few uncertain parameters. Due to its intrinsic versatility, FTA has been applied to assess risk within a probabilistic framework and considering several hydrogeological contexts (Tartakowsy, 2007; Bolster et al., 2009; Jurado et al., 2011; Fernàndez-Garcia et al., 2012; Pedretti et al., 2011; Siirila-Woodburn et al., 2015, Henri et al., 2015).

### 2.4 Bayesian belief network and influence diagram

Bayesian belief network (BBN) and influence diagram (ID) are statistical tools used to represent graphically multi-dimensional probability distributions. These methodologies allow to make inference about uncertain states of a system under scarce availability of information. BBN and ID consist of directed acyclic graphs whose nodes represent variables of interest.





Arrows between nodes indicate probabilistic influence of one variable to another, describing the dependency structure of the considered problem. For each variable, which has a finite set of mutually exclusive states, a conditional probability is defined. The main difference between BBN and ID consists on the type of nodes which are allowed (Jensen, 2002). In ID there are four types of nodes: (*i*) decision nodes, i.e., alternatives for the decision-maker (conventionally depicted with a square); (*ii*) chance nodes, i.e., probabilistic quantities (conventionally depicted with a circle); (*iii*) deterministic nodes, i.e., deterministic quantities (conventionally depicted with a square with rounded corners); and (*iv*) value nodes, i.e., associated with the value (or often utility) given the state of other variables in the system (note that these are special kinds of deterministic nodes; they can be depicted with a diamond). In BBN there are only chance nodes.

As an example, Figure 6 depicts a simple BBN in which variable A influences variable B.



Figure 6. Example of BBN (modified from Bedford and Cook,e2003).

For this simple case the probabilistic description of the system includes the marginal probability of A, P[A] and the conditional probability of B given A, P[B|A]. The full joint distribution, P[A, B] can be expressed as

$$P[\mathbf{A},\mathbf{B}] = P[\mathbf{A}]P[\mathbf{B}|\mathbf{A}]$$
(1)

Equation (1) can be generalized to consider *n* variables,  $X_1, ..., X_n$  as

$$P[x_1,...,x_n] = P[x_1]P[x_2|x_1]P[x_3|x_1,x_2]...P[x_n|x_1,...,x_{n-1}]$$
(2)

Note that if the system has Markov properties i.e. for each i,  $X_i$  depends only on  $X_{n-1}$ , Eq. (2), can be simplified as

$$P[x_1, \dots, x_n] = P[x_1]P[x_2|x_1]P[x_3|x_2]\dots P[x_n|x_{n-1}]$$
(3)

Figure 7 shows a simple ID composed by 3 nodes. In this system a decision node A influences a deterministic node C and a chance node B. In this case, the probabilities to be determined are P[A] and P[B|A]. Then it has to be specified the function f(A), which determines the value of the deterministic node C, given the value of A.







Figure 7. Scheme of a simple ID composed by 1 decision node, A, 1 chance nodes, B, 1 deterministic node, C.

In summary, while BBN focuses on (Bayesian) inference (i.e., on the evaluation of the posterior probability of a selected variable on the basis of available observations of the remaining variables), ID must contain a decision node and it is mainly focused on determining the optimal decision. Both BBN and ID have been applied to various engineering aspects, in particular to emergency planning in the context of PRA. Winter and Tartakowsky (2008) and Farmani et al. (2009) applied BBN to assess risk assessment of groundwater contamination problems and optimum management of groundwater resources. The LEAP project (<u>https://uwaterloo.ca/legacies-of-agricultural-pollutant/</u>), funded by Water JPI, Joint call 2016, is developing a BBN framework to evaluate uncertainties in both biophysical and hydro-economic modelling of nutrient legacies, and assess their implications for nutrient risk management.

#### 2.5 Discussion

While the goal of the above mentioned approaches is unique, their philosophy is slightly different. FMEA, MBA and ETA are inductive methodologies, built on the concept of forward logic where an initiating event must occur for a system to fail and then be followed by a series of consequent events. Otherwise, a deductive approach, like FTA, is built on backward logic. In this case one identifies a particular failure of the system, defines the failure as the top event and seeks the combination of all possible events which may contribute to such a top event. Finally, BBN and ID provide an alternative representation of the relationship between basic events and system failure and can be built following both deductive and inductive approaches.

Among all of these alternative methodologies, we plan to rely on the fault tree approach because it allows identifying all basic events contributing to an undesired system failure, thus leading to a reduction of the dimensionality of the parameter space, and a reduction of a markedly complex problem into a set of manageable tasks (see also Sections 4 and 5).



## 3. Fault tree analysis: groundwater contamination problem

Here, we focus on the FTA approach that can be set up for a groundwater contamination setting. This methodology will be applied to one of the field sites analyzed in the project, i.e., the Bologna aquifer.

In order to construct the fault tree, we must first define the meaning of system failure and the events that lead to the failure. In general, a contamination problem involves a mixture of contaminants  $\{C_1, \ldots, C_n\}$  coming from several sources and moving towards several receptors  $\{\Omega_1, \ldots, \Omega_m\}$ . System failure is defined as the event that the concentration of any of the contaminants exceeds some critical value in any given receptor within a legally mandated time interval  $t \le T$ . Defining  $CC_{ij}$  the event of exceeding the critical contaminant concentration  $C_{ij}^*$ for pollutant *i* and receptor *j* at time shorter than (or equal to) *T*, i.e.,

$$CC_{ij} = \left\{ C_i \left( x \in \Omega_j, t \le T \right) > C_{ij}^* \right\}$$
(4)

we can formally write system failure as the occurrence of any of these events, i.e.,

$$SF = \{CC_{11}\} \cup \{CC_{12}\} \cup \dots \cup \{CC_{nm}\}$$

$$\tag{5}$$

For event  $CC_{ij}$  to take place, the following basic events (or sub-events) must occur (see also Figure 7)

• Contaminant sources,  $CS_i$  – a given contaminant must be detected at a given source. We denote this combination contaminant/source with a subscript *i*. In many cases we cannot be certain that a contaminant source exists and we need to apply a probabilistic approach. For example, in a highly agricultural zone there is a non-negligible probability that a contaminant source related to pesticides may exist.

• Potential receptors,  $PR_j$  – a receptor *j* must be susceptible to adverse impact by any of the contaminants. Receptors can include individuals, wildlife, water reservoirs or environmentally sensitive zones.

• **Pathways**,  $PW_{ijp}$  – a path *p* connecting the contaminant source *i* with the receptor *j* must potentially exist. This includes natural flow fields and preferential flow paths.

• Fate and transport,  $FAT_{ijp}$  – mechanisms driving fate and transport including natural attenuation or remediation must not have reduced (below a critical value) the contaminant concentration along the *p* pathway.

The generic fault tree depicted in Figure 7 provides an example of a graphic representation of all events that must occur for the system to fail. The group of events associated with one (potential) contaminant source constitutes one possible risk scenario. This fault tree reveals that two important mechanisms must occur for the system to fail: (1) a





pathway must connect the contamination source with a given receptor, and (2) the transport processes taking place along these pathways cannot preclude the adverse effects of contamination. All processes taking place along a pathway are combined within a single  $FAT_{ijp}$  event.



Figure 7. Generic fault tree of a contamination problem (modified from Fernàndez-Garcia et al., 2011).

A generic fault tree consists of different potential events, whose inter-connections can be represented with Boolean operators. Once a fault tree is constructed, the probability of each individual event and then of the overall system failure can be evaluated. The evaluation of the probability of individual events is not often an easy task and can be performed relying on diverse methods ranging from relatively simple numerical or analytical models (Bolster et al., 2009), to pdf equations (Tartakovsky et al., 2009; Sanchez-Vila et al. 2009; Tartakovsky and Broyda, 2010;), surveys (McClelland et al., 1990), expert opinion (Mosleh and Apostolakis, 1985), and available datasets (EIREDA Tech. Report 1991). In all cases, when estimating the probability of an event it may be advisable to be on the side of caution and choosing the worst-case scenarios. Such conservative approaches are typically employed *a priori*, aiming at





identifying those events leading to the highest probability of occurrence of an adverse event. Additional analyses can then be devoted to study the *selected events* (associated with the highest occurrence of risk) to refine their probability of occurrence.

### 3.1 Minimal cut sets

FTA expresses the system failure as series of basic events using Boolean logic. Introducing the Boolean operators for two basic events A and B as

$$A 'AND' B \equiv A \cdot B \equiv A \cap B \tag{6}$$

$$A 'OR' B \equiv A + B \equiv A \cup B$$

the fault tree in Figure 7 represents the system failure as

$$SF = \sum_{ij} CC_{ij} = \sum_{ij} CS_i \cdot PR_j \cdot PW_{ijp} \cdot FAT_{ijp}$$
(7)

The failure modes or minimal cut sets of the system are the smallest combinations of basic events that cause the failure of the system, i.e.,  $M_a = \{CS_i \cdot PR_i \cdot PW_{iip} \cdot FAT_{iip}\}$ .

System failure can be expressed as the sum of all possible minimal cut sets, i.e.,  $SF = M_1 + M_2 + ...$ , and the probability of system failure is given by

$$P[SF] \approx \sum_{a} P[M_{a}] - \sum_{a < b} P[M_{a} \cdot M_{b}] + \sum_{a < b < c} P[M_{a} \cdot M_{b} \cdot M_{c}] - \cdots$$
(8)

### 3.2 Human health risk assessment

Stakeholders and regulators usually denote the critical contaminant concentration,  $C_{ij}^*$ , maximum contaminant levels, *MCL*. The latter is defined by the United States Environmental Protection Agency as the legal threshold limit of a contaminant concentration allowed in public water systems.

Alternatively, the failure of the system associated with a given scenario is sometimes expressed in terms of cancer risk due to chronic exposure. The probability of system failure is thus defined as the probability that the cancer risk is larger than a mandated critical value (typically ranging between  $10^{-4}$  and  $10^{-6}$ ). This critical risk value is denoted here as  $R_{ii}^*$ .

Following the human health risk assessment guidance (U.S. Environmental Protection Agency, 1989), carcinogenic health risk can be evaluated by a Poisson model for individual cancer occurrence, as

$$R_{ij}\left(x \in \Omega_{j}\right) = 1 - \exp\left(-ADD_{i}\left(\Omega_{j}\right) \times CPF_{i}\right)$$
(9)

where  $R_{ij}(x \in \Omega_j)$  is the incremental lifetime cancer risk (ILCR) to a contaminant *i* at a given position  $\Omega_j$  where the sensitive receptor is located,  $CPF_i$  (kg day/mg) is the metabolized cancer 14





potency factor related to the carcinogenic contaminant *i*, and  $ADD_i$  (mg/(kg day)) is the average daily dose of contaminant *i*. When human exposure occurs by direct ingestion  $ADD_i$  is evaluated as

$$ADD_{i}\left(\Omega_{j}\right) = \overline{c}_{i}\left(\Omega_{j}\right) \left[\frac{IR}{BW}\right] \frac{ED \times EF}{AT}$$

$$\tag{10}$$

where *IR* is the ingestion rate of water (l/day), *BW* is the body weight (kg), *AT* is the expected lifetime (day), *ED* is the exposure duration (year), *EF* is the daily exposure frequency (day/year) and  $\overline{c}_i(\Omega_j)$  (mg/l) is the maximum running averaged concentration given by (Maxwell and Kastenberg, 1999)

$$\overline{c}_{i}(\Omega_{j}) = \max_{t>0} \left\{ \frac{1}{ED} \int_{t}^{t+ED} c_{i}(\tau;\Omega_{j}) d\tau \right\}$$
(11)

Here,  $c_i(\tau; \Omega_j)$  is the flux-averaged concentration. The latter is widely used in human health risk analysis (Andricevic and Cvetkovic, 1996; de Barros and Rubin, 2008) and is defined as the ratio of the mass discharge to the volumetric water flux at a location of interest  $\Omega_j$ . Note that lowercase and uppercase concentrations will, respectively, denote flux-averaged and resident concentrations throughout this work. Typical values of *IR*, *BW*, *AT*, *ED*, *EF* adopted in human health risk analysis are listed in Table 1. As an example, in Table 2 we list values of *CPF<sub>i</sub>* and *MCL<sub>i</sub>* associated with four chlorinated compounds which can cause potential risk to human health: tetrachloroethylene (PCE), trichloroethylene (TCE), cis-Dichloroethylene (DCE) and vinyl chloride (VC). PCE is a common DNAPL product found in groundwater. Under anaerobic conditions PCE can undergo sequential reactions producing the DCE, VCE and VC. Considering multiple risk scenarios, each one contributing to the total risk, the probability of system failure can be written in terms of minimal cut sets as

$$P[SF] \approx \sum_{ij} P[R_{ij} > R_{ij}^*]$$
(12)

Parameter	Value
Ingestion rate, IR (l/day)	1.4
Body weight, BW (kg)	70.0
Exposure duration, ED (year)	30.0
Exposure frequency, EF (day/year)	350.0
Average time of the expected lifetime, $AT$ (day)	25500

Table 1. Risk parameters (Modified from Henry et al., 2015).





Parameter	Value				
	PCE	TCE	DCE	VC	
Cancer potency factor, <i>CPF<sub>i</sub></i> (kg day/mg)	0.0021	0.011	0.6	1.5	
Maximum contaminant level, $MCL_i$ ( $\mu$ g/l)	5.0	5.0	7.0	2.0	

Table 2. Risk parameters associated with tetrachloroethylene (PCE), trichloroethylene (TCE), cis-Dichloroethylene (DCE) and vinyl chloride (VC) (Modified from Henry et al., 2015).

## 3.3 Computation of probabilities

In order to compute probabilities associated with each set of basic components *ijp* (source, receptor, pathway), one needs to solve a stochastic flow and transport model (or a set of likewise stochastic alternative models). These models are typically expressed in terms of stochastic partial differential equations (PDEs)

$$F_{ijp}\left[C_1(\mathbf{x},t),...,C_n(\mathbf{x},t);\boldsymbol{\theta}\right] = 0$$
<sup>(13)</sup>

where  $\theta$  is a vector of system parameters,  $\{C_1, \ldots, C_n\}$  are contaminants migrating from source *i* to receptor *j* through pathway *p*, and  $F_{ijp}$  indicates the functional form of the PDEs associated with a given source, receptor and pathway scenario. When contaminants do not interact with each other, Eq. (13) simplifies as

$$F_{ijp}\left[C_{i}\left(\mathbf{x},t\right);\boldsymbol{\theta}\right] = 0 \tag{14}$$

The randomness of the PDEs stems from structural (arising from errors in a conceptual model) and/or parametric (arising from imperfect knowledge of  $\theta$ ) uncertainties. Structural uncertainty can be implemented in PRA by evaluating the relative performance of several competing models and then ascertaining the degree of reliability among models (e.g., Christakos, 1990; Hoeting et al. 1999; Neuman 2003).

Several methodologies have been proposed to solve stochastic PDEs governing flow and transport phenomena under uncertainty. These range from small-perturbation approaches (Dagan, 1989; Gelhar 1983), to moment (Guadagnini et al., 2003; Riva et al., 2006; Morales-Casique et al., 2006) and PDF (Sanchez-Vila et al., 2009; Tartakovsky and Broyda, 2007) equations, as well as (typically numerical) Monte Carlo simulations (Stauffer et al., 2005; Salamon et al., 2007; Riva et al., 2008). While analyzing a system as a whole is often computationally prohibitive due to the presence of a large number of uncertain parameters (i.e., high dimensionality of the parameter space), evaluating probabilities of basic events within a fault tree logic can be feasible. In general, solutions of a stochastic PDE of subsurface transport for each scenario are given in terms of the PDFs of concentrations or related quantities (e.g., incremental life time cancer risk). From these quantities, the probability of failure can be estimated via Eq. (8).



## 4. Fault tree analysis: spring depletion problem

In this Section we propose a FTA which can be applied to analyze the risk associated with the depletion of a natural springs. We envision to apply this approach at the Cremona site where we developed a steady-state three-dimensional groundwater flow model (see Deliverable 1.4a). A simplified scheme of the system is depicted in Figure 8. The aquifer,  $\Omega$ , is characterized by natural springs located in the region  $\Omega_P$ . Cumulative values of recharge, R, and withdrawals,  $O_P$ , have been evaluated (see Deliverable 1.4a). Hydraulic conductivity,  $K(\mathbf{x})$ , is modeled according to two different approaches: Composite Medium (where each block of the numerical model is considered to be formed by a single geomaterial) and Overlapping Continuum (grounded on the observation that the system can be modeled as a collection of multiple media coexisting in space). Both methodologies rely on the definition of five values of hydraulic conductivity ( $k_i$ , with i = 1, ..., 5), associated with the five geomaterials which have been detected in the area (see Deliverable 1.4a for details). Uncertain system parameters are collected in a vector  $\boldsymbol{\theta} = [k_i, Q_p, R, NBC, DBC]$ , DBC and NBC being, respectively, Dirichlet and Neumann boundary conditions. A forward flow simulation can be performed for a given  $\boldsymbol{\theta}$ , obtaining the distribution of hydraulic head in the investigated domain. Estimates of a sub set of model parameters ( $k_i$ , NBC, DBC, with  $i = 1, \dots, 5$ ) has been obtained against hydraulic heads data collected at 39 observation wells (see Deliverable 1.4a, Section 2.4), setting values of  $O_P$  and R on the basis of available measurements. During the upcoming research period, we envision to assess the joint impact of differing environmental conditions (thus implying different recharge terms, R, and diverse strategies for exploitation of the aquifer, as expressed through  $Q_P$ ) on the aquifer system This analysis aims at optimizing the exploitation of the groundwater resources preserving the natural springs.



Figure 8. Simplified scheme of the problem under investigation.





We envision to tackle this problem according to the following methodology. The system failure, *SF*, is defined as the event corresponding to the hydraulic head, *h*, in  $\Omega_{\rm P}$  dropping below a threshold value,  $h^*$ 

$$SF = \left(h < h^*, \mathbf{x} \in \Omega_p\right) \tag{15}$$

The fault tree analysis shown in Figure 9 will allow evaluating system failure by expressing *SF* as the sum of three minimal cut sets:

- (1)  $M_1 = R < R^*$ , where  $R^*$  is the minimum values of R such that  $h = h^*$  at least in one point of  $\Omega_P$  when  $Q_P = Q_P^{MIN}$ ,  $Q_P^{MIN}$  being the minimum withdrawal selected on the basis of available historical data;
- (2)  $M_2 = Q_P > Q_P^*$ , where  $Q_P^*$  is the maximum values of  $Q_P$  such that  $h = h^*$  at least in one point of  $\Omega_P$  when  $R = R^{MAX}$ ,  $R^{MAX}$  being the maximum recharge selected on the basis of available historical data;
- (3)  $M_3 = (R < R') \cdot (Q_P > Q'_P)$ , where the pair of values  $(R', Q'_P)$  leads to  $h = h^*$  at least in one point of  $\Omega_P$ .



Figure 9. Fault tree of a spring failure problem.

Then, we can express the system failure (15) as  $SF = M_1 + M_2 + M_3.$  (16)

The probability of SF, 
$$P[SF]$$
 can then be quantified making use of (8) and (16) as  

$$P[SF] = P[M_1] + P[M_2] + P[M_3] - P[M_1 \cdot M_2] - P[M_2 \cdot M_3]$$

$$-P[M_1 \cdot M_3] + P[M_1 \cdot M_2 \cdot M_3]$$
(17)





A global sensitivity analysis will be performed to assess the impact on the probability of system failure of uncertain parameters (i.e., the hydraulic parameters and the boundary conditions) as well as of the conceptual model adopted for describing the system.

## 5. Life Cycle Assessment

Life Cycle Assessment (LCA) represents a widely accepted method for assessing the overall environmental aspects and potential impacts related to a product, process or service. Within this kind of analysis, the emissions and resources consumed during the life of the product, process or service are compiled and documented in a Life Cycle Inventory (LCI). An Impact Analysis is performed considering human health, natural environment and natural resources use. Emissions and resources consumed by a given product are assigned to different impact categories that include climate change, ozone depletion, eutrophication, acidification, human toxicity, respiratory inorganics, ionizing radiation, ecotoxicity, photochemical ozone formation, land use and resource depletion. Emissions and resources considered are then converted into indicators using impact assessment models. Life cycle oriented methods were developed in the 1960s and were known as Resource and Environmental Profile Analysis (REPA) or Ecobalances (U.S. EPA, 2006). The structural and procedural components of LCA are nowadays determined by the international standard series ISO 14040, 2006 and ISO 14044, 2006, while ISO 14046, 2014 specifies principles, requirements and guidelines related to water footprint assessment of products, processes and organizations based on LCA. Furthermore, EC-JRC (2010 a, b) provides guidelines for LCA.

LCA consists of four main phases: Goal and scope definition, Inventory analysis (LCI), Impact assessment (LCIA) and Interpretation, as detailed in the following.

#### 5.1 Goal and scope definition

This step requires to (i) define and describe the product, process or activity, (ii) establish the context in which the assessment has to be made, identifying the system (space-time) boundaries and (iii) select the functional unit that appropriately describes the scope and function of the product or process studied, thus determining the environmental effects that need to be considered for the assessment. A functional unit is defined as "quantified performance of a product system for use as a reference unit in a life cycle assessment" according to the international standard ISO 14040, 2006.





## 5.2 Inventory analysis

This is targeted at identifying and quantifying the physical flows in terms of input of resources, materials, and products and the output of emission, waste and valuable products. The analysis is extended to all relevant energy, water and material usage and environmental release identified. A traditional inventory qualifies three categories of environmental releases or emissions: atmospheric emission (e.g., particulate, nitrogen oxides, volatile organic compounds, sulfur oxides, carbon monoxide), waterborne wastes (e.g., BOD, COD, suspended solids, dissolved solids, sulfides, iron, chromium, metal ions, ammonia), solid waste. Inventory practices also usually include substances required by regulatory agencies to be monitored.

## 5.3 Impact assessment

LCIA translates the collected emissions and consumptions into environmental and/or health effects. LCIA is based on the following five steps (ISO 14040):

- Selection and definition of impact categories: one identifies relevant environmental impact categories (e.g., global warming, acidification, terrestrial toxicity). A representative indicator and an environmental model used to quantify the identified impacts on the indicator are chosen for each impact category;
- (2) Classification: the elementary flows from the LCI are assigned to impact categories;
- (3) Characterization: using a science-based conversion factors (characterization factors), the impact of each emission or resource consumption is converted and combined into representative indicators of impact to human and ecological health;
- (4) Normalization (optional): the impact scores determined at step (3) are normalized to facilitate comparison across impact categories;
- (5) Grouping or Weighting (optional): one sorts indicators by characteristics (e.g., type of emission or location) and ranks them according to their relative importance.

The purpose of LCIA is to interpret the life cycle emissions and resource consumption inventory in terms of indicators for the three Areas of Protection of human health, natural environment and natural resources (EC-JRC, 2010a, b). Impacts on the Areas of Protection are modelled by applying knowledge about the relevant pathways or environmental mechanism (cause-effect chain). The indicator of an impact category can be chosen anywhere (midpoint level) along the impact pathway which links inventory data to impacts on the Area of Protection (endpoint level). Characterization at the midpoint level models the impact using an indicator located along the mechanism. Characterization at the endpoint level requires modelling all the environmental mechanism (EC-JRC, 2010b).

Figure 10 shows an example of relationship between the midpoint impact categories and the three Areas of Protection.





Figure 10. Impact categories for characterization modelling at midpoint and endpoint levels (modified from EC-JRC, 2010b).

#### 5.4 Interpretation

Here, one evaluates the results of LCI and LCIA to achieve the goals defined in the first phase (Section 5.1). Sensitivity and uncertainty analysis are applied as part of the interpretation.

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