UNIVERSIDADE FEDERAL DE PERNAMBUCO

PROGRAMA DE PÓS-GRADUAÇÃO EM ENGENHARIA DE PRODUÇÃO

A NOVEL QUANTITATIVE ECOLOGICAL AND MICROBIAL RISK ASSESSMENT METHODOLOGY: theory and applications.

HEITOR DE OLIVEIRA DUARTE

Recife,
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“We concentrate on things we already know, facts that have already happened before and we can explain. Time and time again we fail to take into consideration what we don't know. We are, therefore, unable to truly estimate risks and opportunities, too vulnerable to the impulse to simplify, narrate, and explain, and not open enough to imagine the improbable.”

N. N. Taleb

ABSTRACT

The environment is a complex system where human, ecological environment (e.g., plants, animals, microbes), materials (eg, pollutants, medical), and meteorological/oceanographic conditions interact. The human impact has potential to cause significant damage to the ecological environment (e.g., potential oil spills on the coast cause risk to coastal ecosystems, tuna industrial fishing cause risk to sharks that are bycaught). Similarly, the human impact may turn against the human itself by favoring the growth of populations of unwanted species (e.g., poor sanitation favors the growth of microbial populations that cause risk of an excessive proportion of sick humans). Therefore, it has been demanded an efficient method of quantifying the risks in systems where plant, animals or microbes populations are involved in order to give support to risk management in environmental issues, fisheries management and public health. First, this paper proposes a methodology capable of quantifying ecological risks (i.e., likelihood of adverse effects on the ecosystem, in the long term, due to exposure to stressors such as chemical, fishing, etc.) or microbial risks (i.e., likelihood of adverse effects in humans, in the long term, due to exposure to microbial pathogens). It uses population modeling to simulate future changes in populations of ecologically important species (e.g., fish, corals, sharks), or undesirable (e.g., parasites), under conditional scenarios simulating the influence humans impacting and/or managing the risks. The risk is calculated in terms of probability of extinction or decline, explosion or growth of these populations over time. Second, the methodology is applied to four case studies in Brazil. Each of them have their specific conclusions, as follows. (1) Ecological Risk Assessment caused by potential maritime accidents in the transportation of oil to the port of Suape. Conclusion: low but significant ecological risk. (2) Ecological Risk Assessment caused by potential maritime accidents in the passage of oil tankers nearby Fernando de Noronha. Conclusion: negligible ecological risk, although a more detailed analysis is required due to limited data. (3) Microbial Risk Assessment to Porto de Galinhas community inherent to sanitation and medical treatment program. Conclusion: high microbial risk, the current sanitation level is not enough to contain the spread of schistosomiasis disease, and periodic treatment of patients is not efficient to reduce risks significantly. (4) Ecological Risk Assessment of tuna industrial fishing in Brazilian waters. Conclusion: industrial tuna fishing does not cause significant risks to the population of Mako sharks in the South Atlantic Ocean. In each case study, several conditional scenarios were simulated for the next 100 years, including adverse scenarios and scenarios with risk control measures. Thus, it was possible to quantify the added risk caused by each adverse condition as well as the reduced risk caused by each control measure. In this way, the manager has objective information to prioritize scenarios and evaluate the cost-effectiveness of control measures. The general conclusion of this work is that the proposed methodology has proven to be practicable, useful and efficient.

Keywords: Quantitative risk assessment. Ecological risk assessment. Microbial risk assessment. Ecological modeling. Maritime accidents.

RESUMO

O meio-ambiente é um sistema complexo onde interagem humanos, meio ecológico (e.g., plantas, animais, micróbios), materiais (e.g., poluentes, medicinais) e condições meteorológicas/oceanográficas. O impacto humano tem potencial para causar danos significativos ao meio ecológico (e.g., potenciais vazamentos de petróleo na costa causam risco ao ecossistema costeiro, pesca industrial de atum causa risco aos tubarões que são pescados por acidente). Similarmente, o impacto humano pode se voltar contra o próprio humano ao favorecer o crescimento de populações de espécies indesejáveis (e.g., saneamento básico precário favorece o crescimento de populações de micróbios que causam risco de haver uma excessiva parcela de humanos doentes). Portanto, tem sido demandado um método eficiente de quantificar os riscos inerentes a sistemas onde populações de plantas, animais ou micróbios estejam envolvidas, de forma a dar suporte para o gerenciamento dos riscos em problemas de gestão ambiental, gestão pesqueira e saúde pública. Em primeiro lugar, este trabalho propõe uma metodologia capaz de quantificar riscos ecológicos (i.e., probabilidade de ocorrência de efeitos adversos no ecossistema, no longo prazo, devido à exposição a estressores como químicos, pesca, entre outros) ou microbianos (i.e., probabilidade de ocorrência de efeitos adversos em humanos, no longo prazo, devido à exposição a patógenos microbianos). Utiliza-se a modelagem populacional para simular futuras mudanças nas populações de espécies ecologicamente importantes (e.g., peixes, corais), ou indesejáveis (e.g., parasitas), quando condicionadas a cenários que simulam a influência do humano causando impacto e/ou gerindo os riscos. O risco é calculado em termos de probabilidade de extinção ou declínio, explosão ou crescimento, dessas populações ao longo do tempo. Em segundo lugar, aplica-se a metodologia para avaliar o risco inerente a quatro estudos de caso no Brasil. Cada um deles tem sua conclusão específica, como segue. (1) Análise de Risco Ecológico causado por potenciais acidentes marítimos no transporte de petróleo para o porto de Suape. Conclusão: baixo risco ecológico, porém significativo. (2) Análise de Risco Ecológico causado por potenciais acidentes marítimos na passagem de navios petroleiros ao largo de Fernando de Noronha. Conclusão: risco ecológico negligenciável, mas uma análise mais detalhada é necessária devido à escassez de dados. (3) Análise de Risco Microbiano à comunidade de Porto de Galinhas inerentes ao sistema de saneamento básico e programa de tratamento medicinal. Conclusão: alto risco microbiano, o nível de saneamento básico atual não é suficiente para conter a proliferação da doença esquistossomose, e o tratamento periódico de doentes não é eficiente para reduzir os riscos significativamente. (4) Análise de Risco Ecológico causado pela pesca industrial de atum em águas brasileiras. Conclusão: a pesca industrial de atuns não causa riscos significativos à população de tubarões Mako no oceano Atlântico Sul. Em cada estudo de caso, foram simulados diversos cenários condicionais para os próximos 100 anos, incluindo cenários adversos e cenários com medidas de controle dos riscos. Assim, foi possível quantificar a adição do risco causada por cada cenário adverso e a redução do risco causada por cada medida de controle. Desta forma, o gestor tem informação objetiva para priorizar cenários e avaliar o custo-benefício das medidas de controle. A principal conclusão deste trabalho é que a metodologia proposta provou-se ser praticável, útil e eficiente.

Palavras-chave: Avaliação quantitativa de risco. Análise de riscos ecológicos. Análise de riscos microbianos. Modelagem ecológica. Acidentes marítimos.

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LIST OF ACRONYMS

CETESB – Environmental Company of the state of São Paulo, Brazil

CPR – Committee for the Prevention of Disasters, Netherlands

EC – Effect Concentration

EEA – European Environmental Agency

ERA – Ecological Risk Assessment

EPA – United States Environmental Protection Agency

ICCAT – International Commission for the Conservation of Atlantic Tunas

IUCN – International Union for Conservation of Nature

LC – Lethal Concentration

LOEL – Lowest Observed Effect Level

NOEL – No Observed Effect Level

PDF – Probability Density Function

PHA – Preliminary Hazard Analysis

QRA – Quantitative Risk Assessment

QERA – Quantitative Ecological Risk Assessment

QMRA – Quantitative Microbial Risk Assessment

RNEST – Abreu e Lima oil refinery

SPIC – Suape Port and Industrial Complex

TIS – Toxicological Information Sheet

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1 INTRODUCTION

This work is within the field of Quantitative Ecological Risk Assessment (QERA) and Microbial Risk Assessment (QMRA). The former is the formal process of estimating the probability of adverse effects to the ecosystem, in the short and long-term, due to exposure to one or more stressors (usually chemicals). The latter is the formal process, analogous to QERA, of estimating the probability of adverse effects to humans, in the short and long-term, due to exposure to one or more microbial pathogens (e.g., bacteria, virus, helminths). Since the latter is analogous to the former, it is possible to use one single methodology for both processes. However, they still have differences, which requires the methodology to be flexible for application to both processes, as we propose here. Table 1.1 presents the similarities and differences between QERA and QMRA.

Table 1.1. Similarities and differences between QERA and QMRA.

Similarities	**QERA**	**QMRA**
Objective	To predict relative risks for future scenarios and/or evaluate efficacy of alternative management actions.	To predict relative risks for future scenarios and/or evaluate efficacy of alternative management actions.
Methodology	Proposed in this work	Proposed in this work
Differences	**QERA**	**QMRA**
Adverse effect	Extinction or quasi-extinction of plants or animals.	High proportion of human infection, disease or mortality.
Applications	Licensing of new industrial activities, conservation of threatened species, and environmental protected areas, pesticide regulatory programs, control of evasive species, risk management	Licensing and requirements for water and food companies, urban water projects, urban sanitation projects, disease treatment plans, safe use of recreational waters (lakes,

	programs to prevent against oil & gas spill in the ocean, recovery of contaminated areas, etc.	rivers or beaches), setting disinfection level for sewage outfall, etc.
Stressor dynamics	Undergoes transformation but does not multiply	Growth, reproduction and death
Stressor fate and transport	Physicochemical model	Ecological model with spatial dynamics included (migration)
Frequency of exposure	Rare events (more difficult to estimate)	Frequent events (e.g., wet weather events)
Adaptation	Chemicals do not evolve genetically	Pathogens can adapt to control measures

Both QERA and QMRA have become an important part of the decision-making process for managing environmental and public health problems [1-4]. They have been considered in programs administered by the US Environmental Protection Agency (EPA) and in similar programs administrated by environmental agencies in Canada, Europe, New Zealand and Australia [2-6]. Both can be based on mathematical models capable of providing quantitative risk results. These models are the so-called population models (i.e., models that simulate the population dynamics of a single predetermined species). The main difference is as follows. For QERAs, the population model usually represents a population of a plant or animal (e.g., corals, fishes, turtles) which humans want to protect in order to reduce risks to the ecosystem's health. For QMRA, the model usually represents a population of a pathogenic microorganism which humans want to extinguish or control (e.g., bacteria, viruses, helminths) in order to reduce risks to public health.

Model-based QERA has been used by engineers in pesticide regulatory programs, support in decision-making about waste discharges, remedial actions to clean up or treat contaminated areas, and installation of new industrial facilities [7-15]. Similarly,model-based QMRA help risk assessors characterize the common exposure sources, causative agents, associated symptoms, contributing immunity factors, and other common threads contributing to chronic illness [3, 4, 16].This makes both QERA and QMRA important fields of study within

Production Engineering, since it is particularly useful for industries and governments to provide information necessary to the processes of licensing, risk management environmental management and public health management. Yet, surprisingly, these are subjects not introduced in the university and so rarely applied to Brazilian problems.

In the recent Brazilian context, QERA is applied for toxic spills only and rely on subjective rules-of-thumb or opinions of biologists. It is usually done by the comparison of the estimated concentration of the toxic substance in an ecosystem with toxicity threshold values for an individual of a given species. These threshold values are given by toxicological information, such as the Toxicological Information Sheet (TIS) provided by CETESB [17-19]. This approach is outdated, misleading and not able to provide useful information for determining risks in a Quantitative ERA (QERA), for several reasons [20]: (i) it can only indicate whether effects on individuals are expected, not the magnitude of effects; (ii) the results are difficult to interpret when the comparison for one endpoint (e.g. mortality) conflicts with that for another endpoint (e.g. fecundity); (iii) results are sometimes ambiguous depending on the toxicity threshold chosen; (iv) usually does not provide enough information to make a management decision; (v) interaction among individuals may compensate for adverse effects on individuals; (vi) the life history and ecology of a species can strongly influence the effects of toxic chemicals at the population level. At best, this approach can only be used to screen out risks that are clearly not a problem.

Still in the recent Brazilian context, the basics of QMRA has been reviewed by Santana and Franco [21]. Also, QMRA has been introduced in workshops at the Public Health Faculty of the University of São Paulo (Faculdade de Saúde Pública, *Universidade de São Paulo - USP*) to pharmacists, doctors and biologists. However, these workshops are just a good translation of the EPA’s guidelines for MRA [4] and do not show any novel approach. Besides that, to our best knowledge, nobody has ever applied a quantitative MRA (QMRA) to Brazilian problems.

This work focuses on quantitative risk assessments (i.e. estimate of quantitative values to the risks), which provides objective basis to decisions in environmental and risk management, so it is highly recommended that readers have good knowledge in calculus, algebra, statistics and probability. Our assessments are model-based and our models are probabilistic in nature. Thus, we consider uncertainties and variability in parameters. The risk results are given in terms of probability, undesirable consequence and time, which is useful for experts. Besides that, we transform probabilistic risk measures into risk categories, which is useful to communicate risk for those less familiar with probabilistic systems (e.g., public authorities, politicians, managers, society).

We propose our own methodology for Quantitative Ecological and Microbial Risk Assessment based on ecological models (i.e., mathematical model that can be used to describe or predict ecological processes or endpoints such as population abundance, geographic distribution, area and/or density [20, 22]). The methodology is flexible for application in every system where humans, materials (e.g., pollutants, medicines, pesticides), physical environment (e.g., soil, ocean, river, lake, atmosphere) and biological environment (e.g., plants, animals, microbes) interact with each other.

Our methodology was originated from the need of a systematic procedure to assess the quantitative ecological risks to a coastal ecosystem as a result of potential maritime accidents in oil transportation to a port (chapter 4). Afterwards, the methodology was being polished and improved by means of application to other three case studies (chapters 5, 6 and 7). In summary, four different problems in the Brazilian context gave birth to our methodology as it is in this work, they are:

1. Ecological risks to a coastal ecosystem as a result of potential maritime accidents in oil transportation to a port (chapter 4).
2. Ecological risks to a coastal ecosystem as a result of potential maritime accidents in coastal navigation of oil tankers nearby an environmental protected area (chapter 5).
3. Microbial risks to human populations as a result of bad sanitation (chapter 6).
4. Ecological risks to shark populations as a result of tuna industrial fisheries (chapter 7).

Note that the third case study is the only within the field of QMRA. However, as we propose here a single flexible methodology for both QERA and QMRA, these terms become just a matter of terminology. All case studies use the same methodology, which is based on population modeling. Thus, we prefer to call it as a methodology for QERA, although also applicable to QMRA.

1.1 Rationale and Contribution

Ecological modeling has proved to be an efficient way to simulate the dynamics of ecosystems and populations [2, 20, 22-27]. In the specific case of ecological modeling at population-level, it is a mathematical expression where the dependent variable (the future population abundance) is predicted through the population abundance at the present time and parameters such as survival and fecundity rates).

For risk assessment, a benchmark ecological model can be integrated to other models that simulate risk scenarios and cause variations in parameters of the benchmark ecological model. Thus, a comparison of scenarios can be made against a benchmark scenario (represented by the no disturbance ecological model with background risks) and quantify the added/reduced risk caused by each scenario. By keeping all other parameters the same (*Ceteris paribus [28, 29]*) as in the benchmark ecological model (benchmark scenario) and varying parameters related to the disturbance and/or control measures we aim to assess, we can quantify the added risk caused by each disturbance scenario and/or the reduced risk caused by each control measure scenarios. This is a novel means of providing a prognosis of the system under several scenarios for the future. Thus, this approach does not aim to provide one prognosis that predicts the most probable future. We go beyond that and propose describing the dynamics of the system under several possible scenarios for the future.

We provide a methodology for describing the dynamics of the system under varying conditions for the future, for assessing the risks of such conditions, and for producing meaningful conclusions that can be used to drive efficient management of such conditions. The methodology is thought to be generic, so that it can be applied to any risk assessment in which populations of any species are involved, be they the victim or the hazard itself. We apply and validate our methodology to four case studies. The methodology has proved to be efficient in every one of them. Until now, there were no such methodology developed and tested (except for a preliminary version of this same methodology proposed here [30]), so this work is innovative in its methods. Besides that, each case study is unprecedented itself and has its specific rationale and contribution, which will are detailed in the introduction of chapters 4, 5, 6 and 7.

1.2 Objectives

1.2.1 General objective

To propose a flexible methodology for Quantitative Ecological and Microbial Risk Assessment based on ecological modelling. By flexible we mean that changes can and must be applied for every specific application.

1.2.2 Specific objectives

To prove the efficiency and practicability of the methodology by applying it to three case studies in the state of Pernambuco, Northeastern Brazil:

- Quantitative Ecological Risk Assessment of industrial accidents: the case of oil ship transportation in the coastal tropical area of northeastern Brazil (chapter 4) [31].
- Quantitative Ecological Risk Assessment of accidental oil spills on ship routes nearby a marine national park in Brazil (chapter 5) [32].
- Quantitative Microbial Risk Assessment for Schistosomiasis: The Case of a Patchy Environment in the Coastal Tropical Area of Northeastern Brazil (chapter 6) [33].

And one case study in the South Atlantic Ocean:

- Population dynamics of the shortfin mako shark in the South Atlantic Ocean: a Quantitative Ecological Risk Assessment under several harvest regimes (chapter 7).

1.3 Expected results

The methodology will be capable of effectively quantifying risks of scenarios in systems where humans, materials, physical environment and biological environment interact with each other. More specifically, the methodology will:

- Make predictions that are relevant to environmental and risk management.
- Provide information that allows the comparison among scenarios, as a basis for prioritizing risk management actions under limited resources.
- Deal with uncertainty, measuring it and communicating it to risk managers on a quantitative basis.
- Deal with environmental variability in time and space.
- Be convenient and practicable in terms of costs, time and data needs.
- Be flexible so it can be adapted for every specific application.

1.4 Structure of the work

This work is organized as follows. Chapter 2 presents a review of the theoretical background for understanding this work. Chapter 3 presents the proposed methodology and explains how it can tackle limitations of other approaches and methodologies. Chapters 4, 5, 6 and 7 present four case studies in the Brazilian context where the proposed methodology is applied with some adaptations for each specific case. Each case study describes its adapted methodology, specific contributions, results and conclusions. We recommend that experts in QERA, step from here directly to the case studies in chapters 4 to 7. Chapter 8 is concerned with the concluding remarks, i.e. the most important goals and limitations of this work, practical implications of the results, summary of the conclusions taken from each case study and proposal for future developments. In the last pages of this document, readers can find a glossary of terms.

2 THEORETICAL BASIS

Here we provide a background on ecology, risks, quantitative risk assessment, quantitative ecological risk assessment, and ecological modeling.

2.1 Basic Concepts of Ecology

Ecology is the science that studies the relations of living beings with one another and with the environment in which they live as well as their reciprocal influences, including the human aspects that affect and interact with the natural systems of the planet [31].

For the purposes of this work, it is important to clarify the definitions of environment and ecological environment. In accordance with EPA, environment is "the sum of all external conditions affecting the life, development and survival of an organism" [34]. So environment encompasses humans, materials, physical environment and the ecological environment itself (plants, animals and microbes).

As stated previously, ecology studies the relations of living organisms to each other and to the environment. The biological world is very complex, so it was divided into biological hierarchy levels, as shown in Figure 2.1. The ecology studies only from individual organism level to higher levels and EPA provides definitions to these [34]:

- Organism refers to "any form of animal or plant life".
- Population refers to "a group of interbreeding organisms occupying a particular space". Each population has its own characteristics such as abundance, birth rate (fecundity), deaths rate (mortality), age distribution, dispersion, growth rate.
- Community refers to "an assemblage of populations of different species within a specified location in space and time. Sometimes, a particular subgrouping may be specified, such as the fish community in a lake or the soil arthropod community in a forest".
- Ecosystem refers to "the interacting system of a biological community and its non-living environmental surroundings".
- And landscape refers to "the traits, patterns, and structure of a specific geographic area, including its biological composition, its physical environment, and its anthropogenic or social patterns. An area where interacting ecosystems are grouped and repeated in similar form".

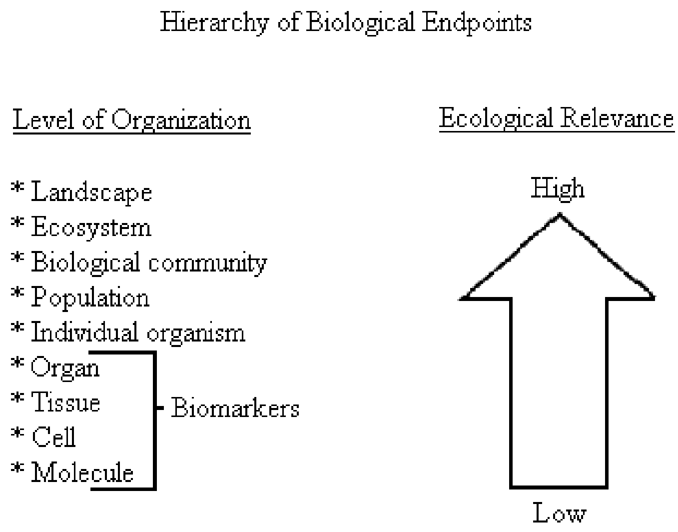

Figure 2.1 - Hierarchy of biological endpoints.
(From the ref. [20])

By the way, habitats used by most species around industrial sites are becoming increasingly fragmented by human activities and, consequently, several distinct populations of same species are living spatially separated, in spite of interacting at some level (e.g. exchange of individuals). In fact, there are relatively few cases where the entire population resides within a same area. Hence, most species are distributed across space as a large population of connected subpopulations, that is, as a metapopulation. According to Pastorok *et al.*, “a metapopulation is a set of populations of the same species in the same general geographic area with a potential for migration among them” [20].

With regard to levels lower than individual organisms, i.e. organ, tissue, cell and molecule, they can be biomarkers. These are measures of body fluids, cells, tissues or measures taken on the whole organism, which indicate (in biochemical, cellular, physiological, compartmental or energetic terms) the presence of contaminants or the magnitude of the response of the target organism [35]. Still, the National Institute of Environmental Health Sciences (NIEHS) states that “biomarkers play an important role in understanding the relationships between exposure to environmental chemicals, the development of chronic human diseases, and the identification of subgroups that are at increased risk for disease” [36].

All these explanations complement each other and help to understand that ERA can be conducted at all levels within the biological hierarchy (including biomarkers). Nevertheless, the methodology proposed in this work focus on population- and metapopulation-level risks, i.e. the potential for adverse effects on (meta)populations. Readers are referred to the reference [20] for models that are potentially useful for risk assessment at higher-levels and to a series of four papers, commissioned by the European Science Foundation [37-40], for the use of biomarkers in ERA.

2.1.1 Ecotoxicology

The term ecotoxicology was proposed in 1969 by the toxicologist René Truhaut during a meeting of the Committee of the International Council of Scientific Unions, in Stockholm. According to Truhaut, ecotoxicology is defined as "the branch of toxicology concerned with the study of toxic effects, caused by natural or synthetic pollutants, to the constituents of ecosystems, animal (including human), vegetable and microbial, in an integral context" [41].

In the 1960s, based on acute toxicity tests results, the Water Quality Act – USA established the first water quality standards in order to protect the aquatic life. In the same period, researches were developed focusing on the selection of sensitive and representative organisms of the aquatic environment and on the cultivation of organisms in laboratory. In the same decade, the book Silent Spring, written by Rachel Carson, was published. It was widely read and began to diffuse to the public concerns about pesticides and environment pollution. In the book, she calls attention to the harming and killing of not only animals and birds but also humans caused by the uncontrolled and unexamined pesticide use.

Throughout 1970s, some American researchers noticed that limits established for many toxic agents separately could not preserve, effectively, the water quality necessary to maintain the aquatic life. With this in mind, the aquatic toxicology had a rapid development due to the knowledge of complex liquid effluents toxicity and the interactions between toxic agents in effluents and its effects on aquatic biota. Besides that, sophisticated systems were developed in order to conduct acute and chronic toxicity tests, using fish eggs and larvae to evaluate the toxic effects of chemical substances on different life stages of organisms. [42]

During the 1980s and 1990s, validation studies of laboratory toxicity tests and collected aquatic water field data results showed the importance of selecting representative species of to evaluate toxic effects on an ecosystem. Afterwards, the implementation of ecotoxicology tests was intensified for the establishment of water quality standards. [42]

Nowadays, the ecotoxicology plays an important role in ERA because it provides basis of knowledge about toxic effects on individual organisms caused by chemical exposure as well as about the representative species in an ecosystem. Knowledge on individual-level effects is essential to predict higher-level effects such as on population abundance (or density), on community species richness, on productivity, or on distributions of organisms. Likewise, because the assessment of all species of an ecosystem would require huge costs and long time, knowledge on which are representative species is necessary to make the assessment tractable.

2.1.2 Population dynamics

Population dynamics is an ecology discipline which studies changes in the population abundance. These studies are important to analyze and understand what happens to the population in natural conditions (without chemical exposure). Incidentally, population models are used to predict and simulate the dynamics of a population. This section will introduce the main components in population dynamics, whereas section 2.5 will present a comprehensive overview of population modeling.

The populations that constitute an ecosystem are open systems, i.e., they exchange energy and matter with the external environment. Hence, any attempt to describe and predict a population dynamics requires knowledge about the interactions between: (*i*) system components, i.e., organisms which compound the population and (*ii*) the system and the external environment [31]. In view of that, to characterize the dynamics of a population it is necessary to define its survival, mortality and fecundity, as well as migration, foraging behavior and density-dependence when appropriate.

Firstly, survival means the number of individuals in a population that are alive after a given period of time and the survival rate indicates the proportion. Pastorok et. al. [20] defines the age-specific survival rate $[S_i\,(t)]$ as “the proportion of individuals present in a given year (t) within a given age class (i) that survives into the next age class $(i+1)$ in the following year $(t+1)$”. Age-specific survival rates can be estimated by the equation below:

$$S_i(t) = N_{i+1}(t+1)/N_i(t) \qquad (2.1)$$

Where

$S_i(t)$ = survival rate of individuals in age classe i at time t

$N_{i+1}(t+1)$ = number of individuals in age class $(i+1)$ at time $(t+1)$

$N_i(t)$ = number of individuals in age class (i) at time (t)

In face of that, mortality is the number of individuals of a population that died in a given period of time. The death rate can be expressed as 1-$S_i(t)$.

With regard to fecundity (F), by definition, it means "the number of live offspring per individual in a given age class that will survive to be counted in the first age class" [43]. Incidentally, calculating fecundity depends on the available data and two brief examples might clarify it. On the one hand, e.g., for oviparous animals, fecundity can be estimated by the equation:

$$F = \mathrm{e} \times p_h \times p_s, \qquad (2.2),$$

where

$e = actual\ eggs\ per\ female$;

$p_h = probability\ of\ hatching$

$p_s = probability\ of\ hatching\ surviving\ to\ age\ 0\ year$

The probability of hatching and the probability of hatching surviving to age 0 year are empirically derived species-specific value between 0 and 1. In this case, it is not enough to derive F on the basis of knowledge about only the actual number of eggs laid, i.e. one has to include the probability of hatching and the probability that the newly hatched fry will survive until the next census to recruit into age class 0.

On the other hand, if sufficient data is available, fecundity can be estimated by the equation:

$$F_{age\ i}(t) = \frac{P_i(t) \times N_0(t+1)}{N_i(t)} \qquad (2.3),$$

where

$P_i(t) = \begin{matrix} proportion\ of\ age\ 0\ year\ juveniles\ that\ were \\ produced\ by\ individuals\ in\ age\ class\ i\ at\ time\ t \end{matrix}$;

$N_0(t+1) = \begin{matrix} \text{number of juveniles at} \\ \text{time } t+1 \end{matrix}$;

$N_i(t) = number\ of\ individuals\ in\ age\ class\ i\ at\ time\ t$

In an effort to estimate survival and fecundity, field data need to be collected. Determining survival rates requires a minimum of two consecutive yearly field censuses; in fact, the results will be more reliable if data from three of more consecutive years are available. In addition to that, Pauwels suggests that the censuses should be consecutive to follow the age classes from one year to the next and to estimate age-specific survival rates, but if data for the target species are insufficient then one could extrapolate the information from the related species to the target species [43].

Let us now examine features concerning the movement of a population, i.e. migration and foraging behavior. The term migration denotes the movement of all or part of a population from one habitat to another [44]. Incidentally, it is the main way of interaction between populations within a metapopulation.

Foraging behavior consists in all methods used by an organism to acquire and utilize sources of energy and nutrients. This encompasses location, storage, consumption and retrieval of resources. Moreover, the foraging theory tries to predict how an animal would choose to forage within its habitat, considering the knowledge of competition, predation risk, and resource availability [45]. The larger the foraging area, more food will be available. In contrast, the organism will spend more energy and take more risk, since the exposure to predators in areas beyond its natural habitat will be greater. It is important to emphasize that the population foraging area should be considered in a QERA when the spatial structure of the environment has important effects on the population dynamics.

Another very important mechanistic process within the population dynamics is its regulation via density dependence on survival, mortality, fecundity and movement of populations. It is the phenomenon of population growth rate depending on the current population density (or abundance). In other words, according to Akçakaya, density dependence "is any non-constant relationship between population growth rate and the current population size" [46].

As is observed in wildlife populations, they are often changing in size, but fluctuating around an equilibrium abundance for long time periods, unless a disturbance occurs (e.g. pollution, harvest, culling, poaching, catastrophe, etc.). Consequently, it is important to incorporate density dependence to describe a population dynamics because it causes the population to reach a stationary state (which may fluctuate due to stochasticity only). The equilibrium abundance is also known as the carrying capacity. In other words, as stated by Akçakaya, "the carrying capacity is the level of abundance above which the population tends to decline" [8].

There are many possible mechanisms that yield density dependence: fecundity may decrease, mortality may increase with competition for limited resources, the crowded conditions may lead to social strife or cannibalisms. Population growth may also be affected negatively as population size reach very low levels. This phenomenon, arising from Allee effects [47, 48], draws a small population away from the carrying capacity and toward extinction.

Usually, to enhance population growth, density dependence factors decrease mortality, increase fecundity, decrease emigration, or increase immigration (i.e. positive density dependence). By contrast, to retard population growth, they increase mortality, decrease fecundity, increase emigration, or decrease immigration (i.e. negative density dependence). A brief example can clarify the concept of density-dependence: on the one hand, when there are too many organisms living in the same space and being part of the same population, food may become less available and competition among the individuals starts. Consequently, negative density dependence manifests itself (e.g., more individuals dying and emigrating) so that the abundance will decrease to a quantity in which food is sufficient for all individuals again.

To conclude, another fundamental component of a population dynamics is the natural variability in all its components. In other words, changes in survival, fecundity, migration and carrying capacity may occur in an unpredictable fashion. For this reason, any attempt to describe a population dynamics should account for stochasticity in those parameters to better represent reality. Section 2.5.2 and section 2.5.3 provide guidance on how to model density dependence and on how to account for stochasticity, respectively.

2.2 Risk, Hazard, Threat, Control Measure, Recovery Measure, Consequences and Accidental Scenario

There are many definitions of risk in the literature, some are complementary, some are supplementary and others are even antagonistic. Each area of knowledge seeks to give its specific meaning; therefore there is no uniformity neither in the interpretations of risk nor in the methodologies to risk assessment.

Camacho [49] transcribes the several definitions of risk which were the theme of discussion and decision of the SRA Committee on Definitions held in San Diego in 1987, entitled “Defining Risk”. It is presented a definition that is considered necessary and sufficient for the interpretation of risk in this work: the American Institute of Chemical Engineers (AIChE) defines risk as a measure of human injury, ecological damage or economic loss in terms of both the accident likelihood and the magnitude of the consequences [50].

As this work focuses on ecological risks, the magnitude of the consequences regards ecological damage and is quantified as a measure of time and population probability of extinction (or decline). This measure is widely accepted and used by the scientific community in ERA as well as is the quantitative measure used by the International Union for Conservation of Nature (IUCN) to classify plants and animals at risk [51].

However, from an economical point of view, this measure does not completely value the magnitude of the consequences in terms of undesirability. Utility theory is used to value an unwanted event and so provide the most objective and relevant measure that a decision maker could have to rationally take decisions while exposed to uncertainty. Describing an unwanted event in terms of time and population probability of extinction (or decline) consists of about 80% of the efforts needed to value such an event in terms of undesirability. To whom it may concern, Campello [52] presents the new methods for assigning value to undesirable events, including a measure of risk aversion.

On the one hand, is the likelihood of occurrence of an undesirable event. On the other hand, is the measured consequence of this event in terms of time and population extinction (or decline). The former is estimated using historical records and reliability analysis techniques (e.g. event tree, Event Sequence Diagrams, Bayesian Belief Networks) and it may involve both equipment failures and human errors. The latter is predicted via exposure and consequence assessment (e.g. fata and transport modeling, exposure-response assessment, population modeling).

It is beyond the scope of this work to provide guidance on reliability analysis; for a general view on reliability theory, models, methods and applications, see the references [51, 53, 54]; and for specific information about techniques such as Event Sequence Diagrams (ESD), Bayesian Belief Networks (BBN) and Human Reliability Analysis, see the references [55-60]. Likewise, human damage are not within the context of this work; for methods to calculate the vulnerability and consequence on human health see the references [61, 62].

It is also important to differentiate between the terms hazard and risk. The former is a potential source of damage whereas the latter is the combination of the likelihood of occurrence of damage and the severity of that damage (in defined circumstances). For example, on the one hand, a great volume of oil under pressure has potential to cause damage, so it is a hazard. On the other hand, overpressure may cause an oil spill with defined circumstances (such as total mass released, time of spill, hydraulic flow) and cause a particular damage that can be measured. The combination of the oil spill's likelihood of occurrence with the magnitude of the damage characterizes the risk.

Concerning threats, control and recovery measures, and consequences, Figure 2.2 is a very interesting way of illustrating it. As already mentioned, hazard is a potential source of damage (usually in the form of energy). Threats are the initiator events, which could cause the hazard to be released, although hazard and threats are sometimes taken to mean the same. Control measures (e.g., safety management systems, alarms, automatic stops) are barriers and preventive actions that can control the threats and avoid the occurrence of the top event, so that they reduce the top event's frequency of occurrence and so reduce the risk. The top event is actually the accident. Recovery measures (e.g. re-routing of spills, burning the oil before it reaches an ecosystem, pollution remediation, habitat protection, translocation or reintroduction of individuals in the population) are mitigation actions, which could reduce the magnitude of the consequences and so reduce the risk. Consequences are the damage, impacts, or effects. Importantly, preventive measures include both control and recovery measures. Finally, an accidental scenario is consolidated by defined circumstances to all this factors.

Figure 2.2 - The bow tie that represents the relationships between hazards, threats, controls, top event, recovery measures and consequences.
(From the ref. [63])

Lastly, there are two types of toxic risks: risk to human health and ecological risk. The former refers to the potential that adverse effects to the human health may occur or are occurring due to exposure to a toxic substance. The latter refers to the potential that adverse ecological effects may occur or are occurring as a result of exposure to a toxic substance.

2.3 Quantitative Risk Assessment

A Quantitative Risk Assessment (QRA) allows the quantification of risks, concerning since the frequent incidents with small impacts to even the rare events with major consequences. Thus, the QRA is necessary for objective decision making related to the security of the establishment, surrounding communities and ecological environment. The major motivation of carrying out a QRA is that in order to optimize risk management measures, they should be taken based on the results of a QRA.

In other words, the QRA is used to demonstrate the risks caused by the establishment and thus help to prioritize which risks require some sort of action and in the decision to choose between different actions to reduce those risks. The actions for risk reduction may be quantitatively evaluated and compared according to their implementation costs through a cost-benefit analysis.

In Brazil, particularly in the state of São Paulo, since the publication of the declaration Nº 1, 01/23/1986 [64], by the Environment National Council (*Conselho Nacional do Meio Ambiente* – CONAMA), which created the requirement of an Environmental Impact Statement (*Estudo de Impactos Ambientais* – EIA/ *Relatório de Impacto Ambiental* - RIMA) for licensing activities significantly affecting the environment, studies of risk assessment started to be incorporated into this process for certain types of industrial activities (e.g., oil refineries [65-67]), so that, besides the problems related to chronic pollution, the prevention of major accidents should be also included in the process of licensing [62]. Thus, one more contribution of QRA is that it also provides the competent authority with relevant information for enabling decisions on the acceptability of risk originating from accidents.

Currently, there are several manuals for implementation of a QRA. The Committee for the Prevention of Disasters (CPR), from the Netherlands, is a worldwide reference in the area. They published four books identified by colors (the purple, yellow, red and green books) [61, 68-70], which are often used in environmental permits, based on the Environmental Protection Law, and in the fields of labor safety, transport safety and fire safety. Those books provide methods for the determination of probabilities, possible damage and physical effects, as well as guidelines for human quantitative risk assessment.

In Brazil, the Environmental Company of the State of São Paulo (*Companhia Ambiental do Estado de Sao Paulo* – CETESB) published a guidelines manual for preparation of studies in risk assessment (version only in Portuguese). This is the main reference on QRA in the country [62, 71].

Although CETESB [62] cites the risk to the environment as a totality (humans, animals, plants, etc.) and highlights several times the importance of considering impacts to the ecological environment, they describe a methodology for QRA capable of quantifying risks to the human health only (surrounding communities), and not to the ecological environment. Likewise, CPR [61] describes in detail a methodology for human QRA and presents separately (in its chapter 7 of only one page), a few basic guidelines and references for Quantitative Ecological Risk Assessment (QERA), which are far from enough to the purposes of this work. Hence, the next section presents our own view about QERA and the main references we used to form it. In advance, to our purposes, a QERA is nothing more than a QRA focused on ecological risks.

2.4 Quantitative Ecological Risk Assessment

Ecological Risk Assessments (ERAs) are conducted in an effort to translate scientific data into meaningful information about risks to the ecological environment. This meaningful information may be provided by assigning values to the risks (i.e. by quantifying the risks), so that an ERA can be addressed as a QERA.

The references [1, 2, 24-26] provide detailed guidelines for the process of ERA. Among them, the main theoretical reference used in this work is the one published by the U.S. Environmental Protection Agency (EPA) [2], for being the most current and on the same plot as the others.

EPA defined ERA as “a process that **evaluates the likelihood (author`s bold)** that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors”. However, for the purposes of this work, it was added the term “quantitative” to emphasize that the assessment attaches a value or a price to the risk, because that is the objective of our proposed methodology. As a result, we adjust EPA’s definition and consider QERA as “a process that **evaluates and quantifies the likelihood** that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors”.

Adverse ecological effects are “changes that are considered undesirable because they alter valued structural or functional characteristics of ecosystems or their components. An evaluation of adversity may consider the type, intensity, and scale of the effect as well as the potential for recovery” [2]. They are evaluated through endpoints, i.e. assessment endpoints and measurement endpoints. According to Pastorok *et al.* [20], "*assessment endpoints* are defined as environmental characteristics or values that are to be protected (e.g. wildlife population abundance, species diversity, or ecosystem productivity) and "*measurement endpoints* are quantitative expressions of an observed or measured biological response, such as the effects of a toxic chemical on survivorship or fecundity, related to the valued environmental characteristic chosen as the assessment endpoint".

Endpoints could be expressed as effects on individual organisms, populations, communities, ecosystems and landscapes. Thus, the definition of QERA allows for risk assessment to be conducted at the various levels within the biological hierarchy (Figure 2.1). However, many QERAs consider only individual endpoints and fail to consider population, ecosystem, or landscape endpoints.

Indeed, the typical QERAs suggests that ecological risk is characterized as a hazard ratio of predicted or measured exposure to predicted no-adverse-effect level expressed as a concentration or dose. This approach is also known as the hazard quotient, which is simply the estimated exposure divided by a toxicity threshold. Thus, one has a value to the risk, which tells whether effects on individuals are expected (in case it is greater than 1) or not (in case it is less than 1). Typically, a measured No-observed-effect-level (NOEL) or Lowest-observed-effect-level (LOEL) – see glossary for details - for the individual-level endpoint of interest are used as toxicity threshold.

Nevertheless, the hazard quotient approach can only evaluate individual-level effects and is not able to provide useful information for determining risks to populations in a QERA. Furthermore, Pastorok *et al.* [20] presents several limitations of the hazard quotient approach, such as:

- it can only indicate whether effects on individuals are expected, not the magnitude of effects;
- the results are difficult to interpret when the hazard quotient for one endpoint (e.g. mortality) conflicts with that for another endpoint (e.g. fecundity);
- results are sometimes ambiguous depending on the toxicity threshold chosen (e.g. LOEL, NOEL);
- usually does not provide enough information to make a management decision;
- population-level processes may compensate for adverse effects on individuals;

- the life history and ecology of a species can strongly influence the effects of toxic chemicals at the population level;
- at best, the hazard quotient can only be used to screen out risks that are clearly not a problem (when the hazard quotient is considerably less than 1).

Hence, a QERA that ignores population-level effects and focuses only on individual-level endpoints may lead to inaccurate risk estimates. This will cause errors in environmental and risk management decisions and lead to inefficiency. Overestimation of risk can lead to waste of resources to mitigate apparent problems that are not really important, whereas the underestimation of risk can lead to inadequate risk management to control and prevent adverse effects to the ecological environment.

As a matter of fact, most toxicity data are expressed as adverse effects on individual organism, i.e. individual-level endpoints. So how to assess higher-level effects, if there are no toxicity data expressed as higher-level endpoints?

Population-level effects or higher-level effects can be obtained with the use of ecological models in the QERA. Such ecological models are essentially used to translate responses in individual-level endpoints into effects on population, ecosystem, or landscapes endpoints. Particularly, when they focus on population-level effects, they are called population models.

In a very simple case, a population model can predict the expected numbers of individuals in a population in the future from estimates of survivorship and fecundity for individual organisms. Thus, chemical effects can be modeled by perturbing the survivorship and fecundity values on the basis of knowledge about changes in these parameters obtained from toxicity test results. [20]

By the way, at the end of August 2009, a group of approximately 30 stakeholders from industry, government regulatory bodies, and academia met for a 2-day workshop in Roskilde, Denmark (RUC09). The purposes of the workshop were to discuss future uses of population modeling in risk assessment by industry as well as its understanding and acceptance by regulators. Forbes *et al.* found that "A major motivation behind this initiative is that, for the sake of more transparency and better risk communication, ecological risks need to be expressed in more relevant (value-relevant) units than hazard ratios, and these units will often be at a population level" [72].

Moreover, the predictive accuracy of population models has already been validated. For instance, Brook et al. [73] validated the prediction of abundance and risks of decline by comparing the historic trajectories of 21 populations (collected from long-term monitoring studies) with the results of population models for these populations. They found that predictions were surprisingly accurate: “the risks of population decline closely matched observed outcomes, there was no significant bias, and population size projections did not differ significantly from reality”.

All things considered, one advocates the QERA approach based on the use of ecological models (particularly population models) to obtain population-level measures, so that risk analysis can assess the probability of a population extinction (or decline) in the future under several environmental conditions, accidental scenarios and management actions. The next section introduces theoretical basis on the use of ecological modeling in risk assessment.

2.5 Ecological Modeling in Risk Assessment

Pastorok *et al.* states that “an ecological model is a mathematical expression that can be used to describe or predict ecological processes or endpoints such as population abundance (or density), community species richness, productivity, or distributions of organisms” [20]. Thus, population and metapopulation (i.e. set of populations of same species living spatially separated but with potential for migration among them) models are a classification of ecological models, in which the mathematical expression is essentially used to translate individual-level effects (e.g., increased mortality, reduced fecundity) into population-level effects (e.g., reduced abundance, increased risk of extinction), so that one can estimate the risk of adverse effects on a population via toxicity data expressed as adverse effects on the individual organism.

The best way to choose the assessment endpoints is to check if they are directly relevant to environmental and risk managers of the enterprise. That is, the risk assessor should keep in contact with these managers to build the ecological model.

With regard to the use of ecological models in the context of QERA, they should also include toxicity extrapolation models, which are used to extrapolate toxicity data in order to describe effects on individuals depending on the species, measurement endpoint and exposure duration. Thus, with the use of ecological models, individual-level effects can be translated into higher-level effects (i.e. effects on population, ecosystem or landscape), and that is the basic rationale for ecological modeling in risk assessment.

As a result, one can estimate the risk of adverse effects on populations, ecosystem or landscape via toxicity data expressed as adverse effects on individual organisms (i.e. individual-level endpoints). Moreover, once formulated the ecological model, it may aid in assessing natural recovery, in developing monitoring programs, in planning restoration of strategies, or in deriving remedial action goals [20].

To sum up, ecological models are used to extrapolate a measurement endpoint to an assessment endpoint. They can predict responses in the population, ecosystem or landscape (using assessment endpoints) via measured individual-level responses (using measurement endpoints). In the specific case of a population model, it is a mathematical expression where the dependent variable (usually the future population abundance) is predicted through measure endpoints (such as survival and fecundity rates) and the population abundance at the present time.

It is important to note that there are several other components in population dynamics rather than survival and fecundity, as described in section 2.1.2, and they can also be incorporated into a population model. Some extensions to a population model are showed below (for more details see the references [8, 20, 46]):

- age or stage structure;
- sex structure;
- parameters vary with time due to stochasticity;
- parameters vary with time due to deterministic trend;
- parameters vary in space: population-specific models for metapopulations (e.g., ref [74]);
- parameters vary with abundance: density dependence;
- additive effects: introduction, harvest, migration between subpopulations in a metapopulation, and catastrophes (e.g., industrial accidents).

Figure 2.3 and Figure 2.4 illustrate the idea of a very simple ecological model at population-level (i.e. population model); the former illustrates the natural dynamics of the population in the future (i.e. without chemical exposure) whereas the latter includes chemical exposure. In this very simple illustration, the future population abundance (assessment endpoint) is predicted through the survival and fecundity rates (measurement endpoints) and the initial population abundance. Once again, there are several other variables which can influence the future population abundance. Sometimes they may not matter much, but sometimes they may matter a lot. It depends mostly on the knowledge of the modeler about the population, on the available data and resources, and on the objectives of the modeling. On the one hand, including other variables makes the model more realistic, on the other, it becomes more complicated and more data is required.

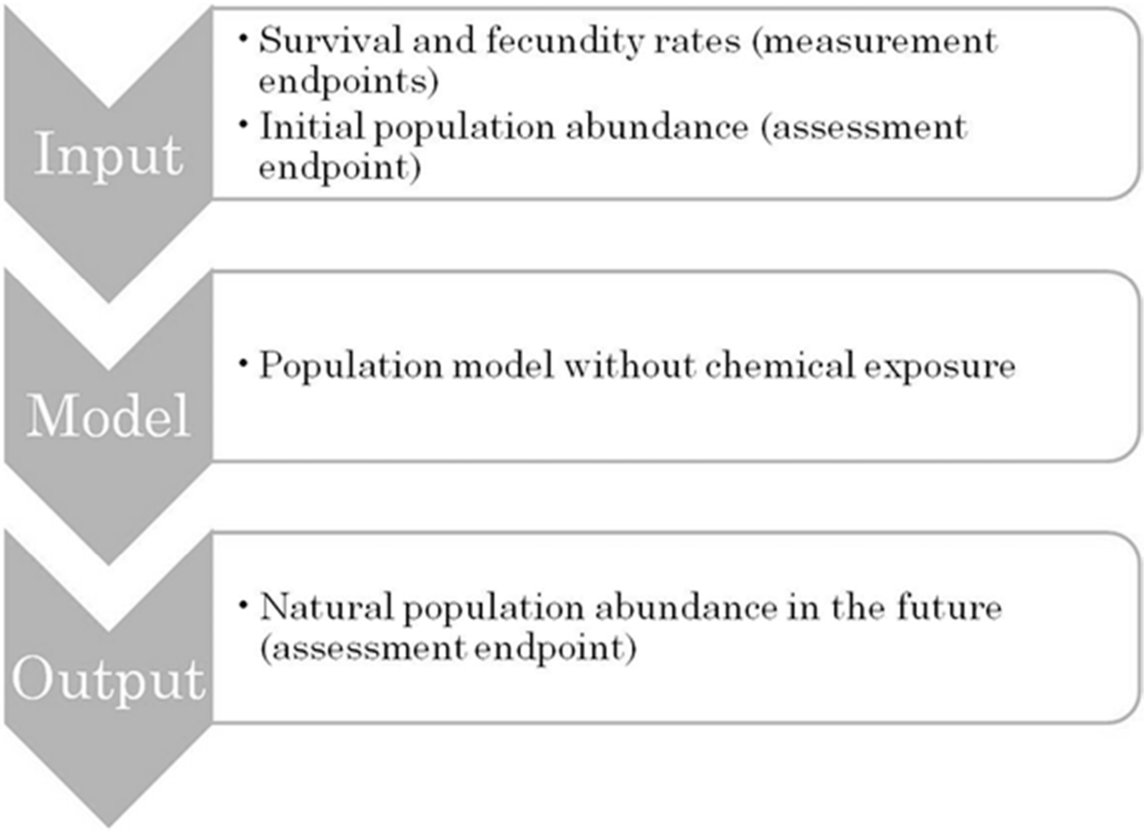

Figure 2.3 - Basic idea of a population model without chemical exposure

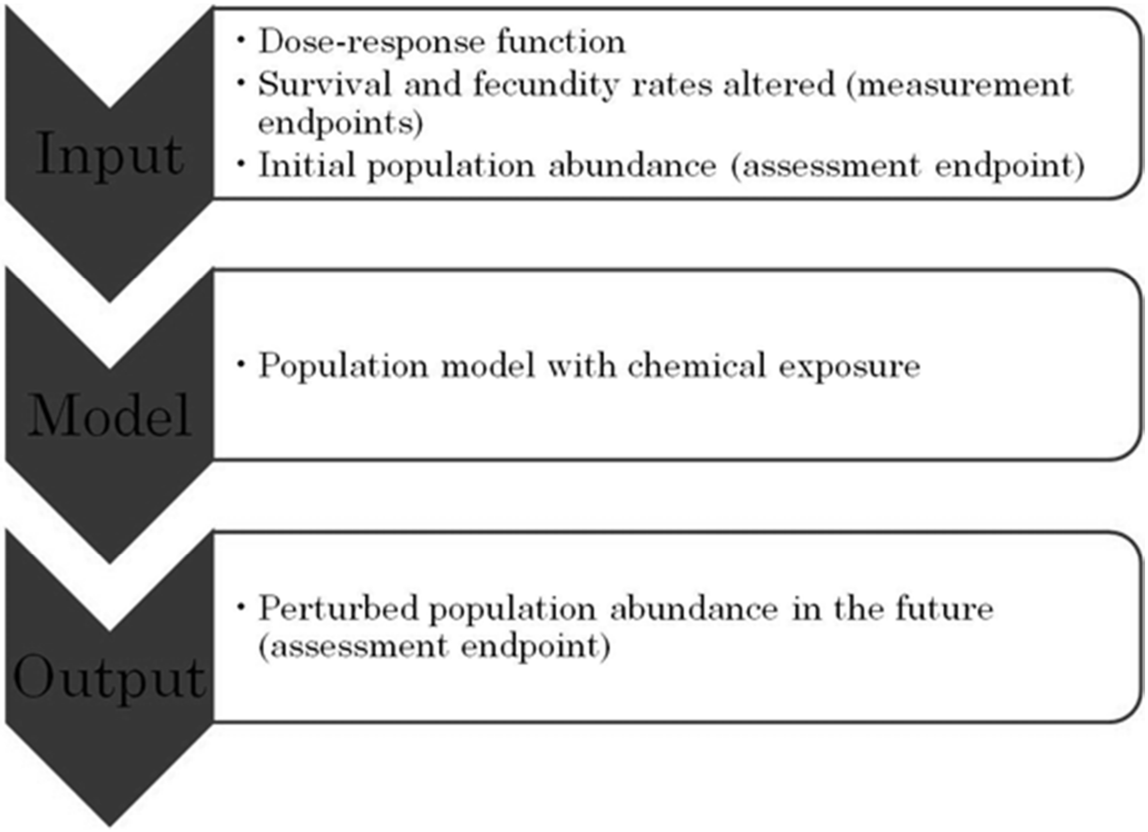

Figure 2.4 - Basic idea of a population model with chemical exposure

Generally, field sampling is used for the estimation of values to the measurement endpoints and the initial conditions of the assessment endpoints, whereas an exposure-response assessment is conducted in order to describe the relationship between the concentration of the chemical and the magnitude of the individual-level responses of native species (represented by changes in measurement endpoints). This relationship is usually specified by a dose-response function, so that it is necessary data on long-term effects of the chemical on the species being analyzed.

Several ecological models and software are already available for use in risk assessment of toxic substances. Pastorok *et al.* [20] conducted a critical evaluation of ecological models that are potentially useful for QERA and ranked the various candidate models based on evaluation criteria that include: realism and complexity of the model (i.e. whether key processes are included and how they are presented); prediction of relevant assessment endpoints and utility relative to regulatory compliance; flexibility; treatment of uncertainty; degree of development, consistency and validation; ease of parameter estimation; regulatory acceptance;

credibility (e.g. prevalence of users, availability or published reviews); and resource efficiency. Furthermore, the best models were selected for a more detailed evaluation and testing.

Nonetheless, selecting the best model depends on the specific problem, so that the modeler must decide it taking into account the management objectives, the ecosystem, chemicals of concern, receptors and endpoints of interest, quality and quantity of available data, and available resources. Thus, model selection is usually site- or issue-specific. Besides that, the level of realism and precision wanted as well as the quality and quantity of data will influence the complexity of the model selected [75].

Habitats used by most species around industrial sites are becoming increasingly fragmented by human activities and, consequently, several distinct populations of same species are living spatially separated, in spite of interacting at some level (e.g. exchange of individuals). In fact, there are relatively few cases where the entire population resides within a same area. Hence, most species are distributed across space as a population of connected populations, i.e. metapopulation. According to Pastorock *et al.*, “a metapopulation is a set of populations of the same species in the same general geographic area with a potential for migration among them” [20]. This way, some ecological models are designed to link Geographic Information System (GIS) with a metapopulation model, combining geographic and demographic data for risk assessment.

By the way, the purpose of the proposed methodology is to conduct a QERA at population-level. Hence, this work does not delve into concepts related to QERA at higher levels and it might be referring to “Population Modeling” instead of “Ecological Modeling”. The reason for choosing (meta)population modeling instead of higher levels modeling is that apart from providing ecologically relevant endpoints, (meta)population models are much more tractable than higher level models. Figure 2.5 illustrates this point of view.

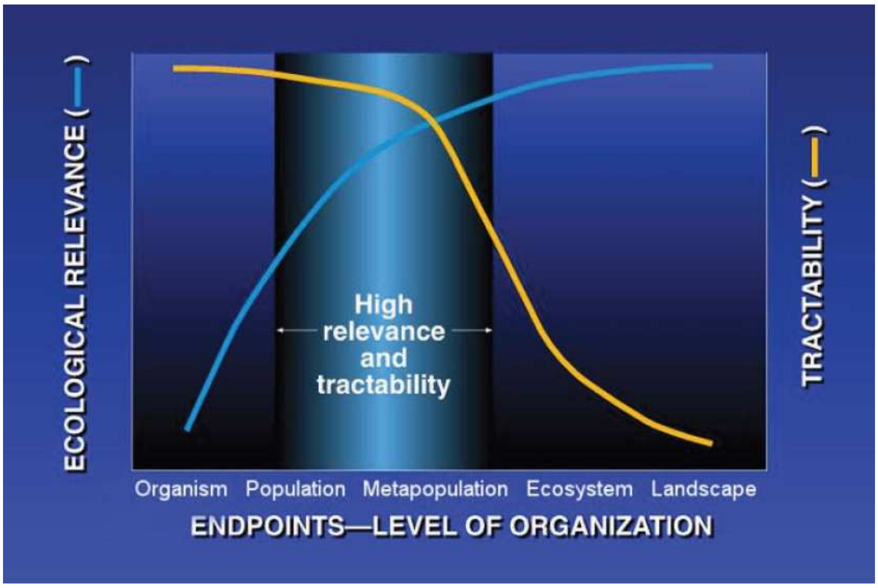

Figure 2.5 - Evaluation of modeling endpoints based on ecological relevance and tractability. (From the ref. [76])

Other several advantages of using population models in risk assessments are related in the reference [76]. Among them, Pastorok *et al.* states that

> "Risk estimation based on population modeling yields value-relevant output (e.g. reduced wildlife population abundance, increased extinction risk) that can be used in cost-benefit analyses to support management decisions concerning siting of facilities and mitigation actions" [76].

It is important to stress here that population modeling will be incorporated into the methodology for QERA proposed in this work, which will then be capable of assessing population-level and metapopulation-level risks only, but not higher-level (ecosystem or landscape) risks. Despite that, it is possible to strategically choose (meta)populations of native species that can effectively represent the ecosystem integrity.

Implementing a population model for a QERA is actually an iterative process that involves data gathering, modeling, model validation, uncertainty and sensitivity analysis. The steps in implementing a population model for a QERA will be described in section 3.5. For a detailed guidance on population modeling see the reference [8] as well as the reference [20] for population modeling applied to risk assessment.

Once a population model is formulated (i.e. a mathematical expression), one has a deterministic model (i.e. no probabilistic components) to predict adverse effects on populations given the exposure to a chemical (in concentration or dose). However, as already mentioned, any realistic attempt to model population dynamics should account for stochasticity, especially because fluctuation is an obvious and often predominant feature of ecological environments. How to model stochasticity will be discussed in section 2.5.3.

2.5.1 Age and stage structure

The age or stage structure of a population refers to age/stage classes within the population. They attempt to consider the fact that individuals of different ages have different characteristics, which are reflected in their vital rates (e.g. survival and fecundities rates), whereas individuals of same age have similar characteristics. For instance, juveniles may have lower survival rates than adults or juveniles may not be able to reproduce until they become adults. Conversely, in an unstructured (scalar) population model, the population is represented by a single age/stage, which denotes the totality of the population. Thus, unstructured models are considered to be a special case of structured models, with only one class of organisms [8].

Structured models are useful if the vital rates of individuals in different classes are different enough to justify the discretization of their life span. Individual classes mean their ages or stages. For example, population model of a fish with a life span of nearly 4 years could be structured by their ages, e.g.: zero year old, one year, two years and three year; or by their stages: juveniles (zero year old) and adults (one year old or more). The criteria to structure a model by stages instead of ages are: individual's ages are unknown; vital rates depend on stage or size rather than age; growth is plastic, some individuals are retarded or have accelerated development of vital rates.

Those individuals that are the same age/stage are assumed to have the same survival and fecundity rates. However, those rates may differ between classes. This way, an structured population model has a survival rate, S_x, a fecundity rate, F_x, and an abundance at time t, $N_x(t)$ for each age/stage class x. The abundances for each class form a vector of numbers (one for each class), whereas the vital rates are combined to form a transition matrix that is used in most population models to account for age/stage structure. In fact, it is a transition matrix which has a special structure, called a Leslie matrix for age-structured models [77, 78] and a Lefkovitch matrix for stage-structured models [79]. Above is an example of a Leslie matrix.

$$L = \begin{bmatrix} F_0 & F_1 & F_2 \\ S_0 & 0 & 0 \\ 0 & S_1 & 0 \end{bmatrix} \tag{2.1}$$

Where

$$S_i = survival\ rate\ of\ individuals\ in\ age\ class\ i$$
$$F_i = fecundity\ rate\ of\ individuals\ in\ age\ classe\ i$$

The reason for arranging the survival rates and fecundities in the form of a matrix is to provide a convenient way to make projections of population's structure from one generation to the next [8]. For example, for an age-structured model the distribution of abundances in the next step is given by the matrix multiplication:

$$\begin{bmatrix} N_0(t+1) \\ N_1(t+1) \\ N_2(t+1) \end{bmatrix} = \begin{bmatrix} F_0 & F_1 & F_2 \\ S_0 & 0 & 0 \\ 0 & S_1 & 0 \end{bmatrix} \times \begin{bmatrix} N_0(t) \\ N_1(t) \\ N_2(t) \end{bmatrix} \tag{2.2}$$

Where

$$N_i(T) = number\ of\ individuals\ at\ age\ classe\ i\ at\ time\ T$$

Assessors may then choose which age/stage classes they are interested in assess. In most case, they will be interest in the total population abundance, which will be the sum of the age abundances. In some cases, however, the may be interested in the abundance of a specific class only.

2.5.2 Density-dependence

Section 2.1.2 introduced the natural mechanism of populations to regulate themselves (i.e. density dependence). This section is particularly concerned about the mathematical modeling of density dependence. For more details on density dependence see the reference [8], chapter 3.

To model density dependence, one must

- Decide which stages will count towards the abundance. At times a great amount of individuals in a certain life stage will not cause impact on the population's vital rates. For example, when adult birds compete for territory, only the adult stage would count towards density dependence. The abundance taken into account may depend on all stages, selected stages or even on an average of all stages weighted by their respective fecundities.

- Determine the vital rates to be altered. Depending on the behavior of the population, density dependence may affect fecundity, survival, migration rates, or a combination of these. This selection needs to be coherent with the transition matrix. For example, in a model with a single stage, density dependence cannot affect survival rates because there are none.
- Choose the form of the density dependence function. Modelers can define a density dependence function themselves, but there are functional forms of density dependence used in the literature, they are [8]:
    - Exponential: no density dependence. All parameters related to density dependence are ignored, only the stage matrix is used in calculations.
    - Scramble: as population size increases, the amount of resources per individual decreases. If the available resources are shared more-or-less equally among the individuals, there will not be enough resources for anybody at very high densities. This process of worsening returns leads to scramble competition, and can be modeled by logistic or Ricker equations [80].
    - Contest: if the available resources are shared unequally so that some individuals always receive enough resources for survival and reproduction at the expense of other individuals, there will always be reproducing individuals in the population. This will be the case, for example, in populations of strongly territorial species, in which the number of territories does not change much even though the number of individuals seeking territories may change a lot. This process of diminishing returns leads to contest competition, and can be modeled by the Beverton-Holt equation [81].
    - Ceiling: exponential growth to a ceiling. At each time step, the population grows exponentially, but if N is greater than the ceiling, then N is set equal to the ceiling.
- Select function parameters. In case of scramble or contest competition, the carrying capacity (K) maximal growth rate (R_{max}) need to be estimated. The carrying capacity is the level of abundance above which the population tends to decline. Therefore one should observe the equilibrium population size for which

the number of individuals at the next time step tends to remain the same. R_{max} is the maximal rate of increase when the population that is regulated by density dependence is not yet influenced by it because of low density. The greatest growth rate observed might be skewed because of stochasticity, causing wrong estimation of the parameter. Therefore a more convenient form of finding the value one wishes for is by making a graph of R(t) as a function of N(t) (number of individuals at time t) and using the y-intercept as R_{max}. Since considering R(t) equal to N(t+1)/ N(t) would cause both the independent and dependent variables to be affected by N(t) measurement errors, a less biased option would be to consider R(t) equal to the geometric average of N around the time step t, i.e. $\sqrt{N(t+1)/N(t-1)}$. In case of Allee effects [47, 48], the A parameter is the population size at which the vital rates are reduced to half of the original value.

It is important to note that including density-dependence in a population model to evaluate the impacts of pollution (i.e. chemical risk assessment) makes the assessment less conservative, because density-dependence effects cause population to recover faster after a pollution episode (except in the case of Allee effects). There is an intuitive way to understand this: after chemical exposure, population suffers from decreasing abundance as long as significant amounts of chemical remain present; on the one hand, if density dependence is ignored, the population growth rate remains the same and population takes longer to recover; on the other hand, if density dependence is considered, then after a decrease in population abundance, the growth rate suffers an increase (positive density dependence), so that population recovers faster.

2.5.3 Stochasticity

The variability and uncertainty in populations and in the environment they live is a fundamental component of population dynamics, so that population models that assume all parameters to be constant (i.e. deterministic models) fail to account for unpredictable fluctuations of real population dynamics. Conversely, stochastic models allow us to consider these fluctuations. They involve replacing constant parameters, such as survival and fecundity rates, and carrying capacity, with random variables responding to a probability distribution function (PDF), usually a normal or lognormal with a certain mean and variance.

There are many different kinds of stochasticity to be incorporated into a stochastic population model, such as:

- environmental temporal fluctuations (i.e. temporal variation in parameters);
- spatial variation (e.g., population-specific parameters for metapopulations);
- measurement and sampling errors that introduce additional uncertainty in parameter estimates of a population;
- demographic stochasticity (because individuals only occur in whole numbers and most parameters may be fractional numbers, there will be additional uncertainty in the number of survivors and births in the next time-step);
- model uncertainty (i.e. uncertainty concerning the structure of the equations used to describe the population)
- catastrophes (i.e. extremely environmental events that adversely affect large proportions of a population, e.g., fire, drought, flood).

Each one of them needs a different approach to modeling the effects of their fluctuations. This work will not delve into each one of them; readers are referred to the reference [8] for details on this issue.

Nevertheless, catastrophes will be an especial type of stochasticity in the proposed methodology, because it allows accidental scenarios to be considered as extremely and rare environmental events included in a population model with a certain probability of occurrence per time step that may either be constant or vary with time. In other words, at each time step a catastrophe (or an accidental scenario) may happen with a certain probability. If it happens, its effects of pollution can be modeled by changes in parameters since the present time step; if not, all parameters remain the same. Section 2.5.5 presents this approach in more details.

Pastorok *et al.* states that there are two kinds of model endpoints: state variables and risk estimates:

> *State variables* are expressed as population, ecosystem, or landscape indicators, such as population abundance, species richness, or landscape fragmentation index, respectively. [...] *Risk estimates* can be derived from the model output for state variables in several ways, but the most common is to run the simulation multiple times in a Monte Carlo analysis to account for variability and uncertainty in input variables as well as initial conditions". [20]

In other words, what Pastorok *et al.* meant is that risk can be estimated through multiple simulations of the ecological model via Monte Carlo. Since a stochastic model has probabilistic components characterized by random variables responding to a PDF, there will be a different result for each single run. Thus, the results will also form a PDF which will characterize the risk estimates (e.g., risk of extinction, risk of population decline). Following such a procedure will allow variability to be evaluated as a degree of confidence, as well as to estimate upper and lower bounds on risk measures to evaluate uncertainty.

A simpler way to deal with uncertainties is to use them to derive worst and best case estimates of extinction risks, based on manual changes on parameters. Such procedure allows estimating a range (upper and lower bounds) to risk measures, such as time to extinction, or risk of decline. The greater are the uncertainties in parameter values, the wider will these bounds be. If they are too wide, uncertainty may be unacceptable and do not meet the needs of risk managers. At best, the bounds should be narrow enough to make decisions taken by risk managers based on the lower bound the same as those based on the upper bound (i.e. the difference between the lower and upper bound should be regardless for risk managers).

All in all, a population model with random variables (and it should be present to better represent reality) is a stochastic model, since the input variables and/or initial conditions respond to a PDF. Hence, the model does not provide a single result, but a distribution of consequences associated to probabilities. The next section presents the ways of expressing the results of a stochastic population model.

2.5.4 Ways of expressing the risk estimates

The most traditional measure to summarize the results of a population model is the expected population trajectory (i.e. the expected number of individuals in a population in the future), which is usually expressed by a mean, a ±1 standard deviation, a minimum and maximum values. However, several ecological-related problems and questions that population models address are phrased in terms of probabilities. For instance, a certain population of a certain species may have a 50% chance of extinction in the next 10 years (i.e. a "critically endangered" population according to IUCN, the International Union for Conservation of Nature [51]).

The probability is usually derived from multiple runs (Monte Carlo) of a population model and may be expressed in many ways as bellow [20]. The selection of a specific expression for the probability depends partly on the objectives of the assessment and partly on available information for the species being modeled [20].

- **Interval decline probability:** the probability of a population declining by as much as a given percentage of its initial value at any time during the period of prediction.
- **Interval extinction probability:** the probability of a population falling as low as a given abundance at any time during the period of prediction.
- **Terminal decline probability:** the probability of a population being as much as a given percentage lower than its initial value at the end of a simulation.
- **Terminal extinction probability:** the probability of a population being as low as a given abundance at the end of a simulation.
- **Interval explosion probability:** the probability of a population equaling or exceeding a given abundance at any time during the period of prediction.
- **Terminal explosion probability:** the probability of a population being as great as or greater than a given abundance at the end of a simulation.
- **Time to extinction:** the time required by a population to decrease to less than a given threshold abundance. This work basically uses two threshold: total extinction (i.e. zero individuals) and “half loss” (i.e. 50% population decline).
- **Time to explosion:** the time required by a population to exceed a given threshold abundance.

Thus, for instance, to estimate the terminal extinction probability, one runs the simulation multiple times and counts the occurrences in which the population ends the simulation lower than a given abundance. The probability (of a population being as low as the given abundance at the end of the period) will be the number of such occurrences divided by the total number of rounds. Clearly, the greater is the number of rounds, the more precise is the probability.

By the way, explosion probabilities and time are especially useful when a population increase may be unwanted. For example, one may want to estimate the probability that a certain seaweed species outbreak will reach an ecological damaging level, because it consumes most oxygen available for fishes in the sea.

Also, explosion probabilities and time are useful to evaluate recovery chances, when the objective is to estimate the recovery of a population under risk management actions. In such cases, it may be useful to estimate the time it will take the population to increase to a certain abundance (i.e. time to recovery, analogous to the time to explosion), or the probability of recovery within a specified time period (analogous to the explosion probability).

To conclude, there are other useful single measures to summarize the predictions of the risk curves [46], i.e.:

- **Expected minimum abundance:** the average (over all replications) of the minimum population abundance of the trajectory. It is an estimate of the smallest population size that is expected to occur within the simulated time period.
- **Median time to extinction:** represents the most likely time required by a population to decrease to less than a given threshold abundance. It is the median value in the PDF of the time to extinction.

2.5.5 Assessing impacts and risks of each accidental scenario

Through evolution, most species go naturally extinct, typically within ten million years or so of their first appearance [82]. Furthermore, human impact may accelerate this time. By human impact one means not only industrial accidents, but several other kinds of human perturbations to the ecosystem that may be continuously affecting a wildlife population, especially if the ecosystem surrounds an industrial activity. Thus, even under the condition that no accidental scenarios might happen, a population has already an implicit risk of extinction.

Therefore, assessing impacts and risks of an accidental scenario alone is not enough. It must be compared against the present environmental condition (i.e. a non-impact scenario) to evaluate the changes in risks. In a non-impact scenario, no future impacts may occur (e.g., accidental scenarios), but only impacts that are already affecting the population.

An accidental scenario can be compared with a non-impact scenario in two ways. Both of them can provide relevant information, so that a QERA should, at best, present results using both approaches. The first one considers only the impacts (i.e. the consequences) of the accidental scenario of concern, whereas the second considers both the frequency of occurrence and the consequences (i.e. the risks).

2.5.5.1 Assessing impact

It considers that the accident is sure to occur at a specified time during the simulation. This approach ignores that the accident is a rare event and considers it as an almost surely event at specified time. This is particularly useful to evaluate the impacts (i.e. consequences) of the accident, because it presents the population dynamics before and after the accident. Hence, one could compare an impact scenario to a non-impact scenario as a means of evaluating the accidental scenario in terms of increase in consequences. Then the results may be used to determine whether the predicted consequences are substantial enough to require pro-active response or action. For instance, this approach provides information to answer questions such as:

- Does the population go extinct before the accident? And what about after the accident?
- What will the population abundance of a species (e.g. sardine) be 1 year after exposure to the concentration of toxic substances (e.g. hydrocarbons) released by the accident?
- How long after the accident would it take for the exposed population to decline by a certain value (say 20 or 30%)?
- What is the probability of extinction in the population after the accident?
- What is the probability of the population dipping below a given threshold (say 20 or 30% from the original population) at some point in the next year after the accident?
- If we invest a certain quantity of money (say U$100,000) in mitigation actions that reduce the magnitude of impacts, what will be the extinction probability decrease?

2.5.5.2 Assessing risks

It considers that the accident might happen with a certain probability (equal to the accident’s frequency of occurrence) at any time during the simulation. This is similar to the catastrophe stochasticity type (section 2.5.3). Thus, the results represents not only the consequences of the accident, but the risks (i.e. a measure that encompasses both consequences and frequency of occurrence). This approach allows the comparison of a non-impact scenario with a potential accidental scenario, in terms of changes in risk measures (e.g., risk of extinction, risk of half loss). Also, it allows the comparison of the accidental scenarios among themselves, which is useful for prioritizing management actions. For instance, this approach provides information to answer questions such as bellow, considering that there is a certain chance of a catastrophic toxic spill:

- How will the population abundance fluctuate during a period of 50 years?
- What is the change in the risk of extinction in the population?
- What is the risk of the population dipping below a given threshold (say 20 or 30% from the original population) at some point in a 50-year simulation?
- How serious are the changes in risk measures in a simulation with a potential accidental scenario when compared to a simulation with a non-impact scenario? Changes may be serious if species jumps categories of risk (risk categorization will be discussed in section 2.5.7).
- If we invest a certain quantity of money (say U$100,000) in mitigation actions, what will be the extinction risk decrease?
- And if we invest the same amount of money in control measures that reduce the accident's frequency of occurrence, what will be the extinction risk decrease?
- If we have only U$100,000 available for risk management, how to allocate this money in an effort to reduce risks the most? Which accidents prioritize?

2.5.6 Cumulating risks of all accidental scenarios

Quantifying risks of each accidental scenario provides a basis for categorizing them, comparing them against a non-impact scenario, and prioritizing management actions. However, it may also be useful to cumulate risks of all accidental scenarios as a basis for communicating the total ecological risk. Therefore, this work also proposes an approach for cumulating risks of all accidental scenarios in only one measure, i.e. the FN risk curve (similar to the FN curve for the social risk in human QRA).

Once again, N is the average population decline number (of native species strategically chosen to represent ecological effects) and F the cumulative frequency of accidents with N or greater abundance decline. This way, the greater the number of accidental scenarios in the assessment, the more points will have the FN curve, and so will it be more continuous. More details on how to build a FN curve will be given in section 3.6.

2.5.7 Risk categorization

Establishing risk criteria for acceptability in the FN curve is a slow and complicated process that requires the participation of society and other interested parties in its judgment. It was not an aim of this work to establish risk criteria for acceptability, which is a proposal for future works though.

Nevertheless, the risk status originated from the approach in section 2.5.5.2 can be categorized according to the International Union for Conservation Nature (IUCN) threat categories [51]. One of the IUCN criteria (the only quantitative one) are expressed in terms of time and risk of extinction, so either risk curves or cumulative time to extinction can be used to categorize risk based on these definitions. This way, a threatened population may be classified into one of the 3 risk categories:

- CRITICALLY ENDANGERED: at least 50% probability of extinction within 10 years or 3 generations: whichever is longer (up to a maximum of 100 years);
- ENDANGERED: at least 20% probability of extinction within 20 years or 5 generations, whichever is longer (up to a maximum of 100 years);
- VULNERABLE: at least 10% probability of extinction within 100 years;

The IUCN risk criteria are expressed in terms of total extinction (zero individuals). However, these criteria are intended to classify species at high risk of global extinction in an effort to convey the urgency of conservation issues to the international community. It is used to classify species affected by a whole range of environmental changes and human impact at global-level, not to classify the interaction of a single establishment with a local population or metapopulation.

In this context, establishing risk criteria for the purposes of a QERA was one of the main themes of discussion and decision in a workshop on ecological modeling at Applied Biomathematics, Setauket, New York, on August 24-26 of 2011. The author of this work was present at this workshop, together with some of the most cited authors in the field of ecological modeling. They concluded that it may be more appropriate to express risk criteria in terms of "half loss" (i.e. 50% population abundance decline) instead of total extinction. As a result, they proposed the following risk categories for the purposes of a QERA:

Table 2.1. Categories for assessing risks of each accidental scenario in a QERA.

Category	**Risk of half loss**	**Years**
Critically Endangered	> 50%	10
Endangered	> 20%	20
Vulnerable	> 10%	100
Low risk	> 0.1%	100
Negligible	> 0.001%	100
Background risk	< 0.001%	100

2.5.8 Bibliographic review of case studies

This section is especially concerned with a bibliographic review of published applications of ecological modeling in risk assessment. For instance, Naito *et al.* applies an ecosystem model for ERA of chemicals in a Japanese lake [7]; Pauwels presents a case study to show how risks to a brook trout (*Salvelinus frontinalis*) population exposed continually to a contaminant (in this case the pesticide toxaphene) can be assessed and quantified using ecological modeling, as well as describes the data needed to parameterize a fish population model [43]; Bartell *et al.* presents an aquatic ecosystem model for estimating ecological risks posed by toxic chemicals in rivers, lakes, and reservoirs in Québec, Canada [14]; finally, Chen uses an aquatic ecological risk assessment model to analyze exposure and ecological effects and to estimate community-level risks to fish, aquatic insects and benthic macroinvertebrates in Keelung River in northern Taiwan, associated with chemicals of potential concern such as ammonia, copper and zinc [15].

All those works were very useful as a basis of knowledge on ecological and toxicity extrapolation models. It is worth noting, however, that none of them are within the context of industrial accidents, as we aim to do in this work.

In addition, there are several other works on using ecological models not specifically in risk assessment related to chemical exposure, but manly in species conservation and management (see reference [83]). They are also very useful though, since they contain demonstrations of how an ecological model is implemented. Such reference was essential as guidance on the application example of this work, because it contains a collection of case studies of models applied to a variety of species (including fishes) and implemented in the population modeling and viability analysis software RAMAS GIS 4.0, which is an older but similar version to the same software that will be used in the application example of this work [46].

3 PROPOSED ECOLOGICAL AND MICROBIAL RISK ASSESSMENT METHODOLOGY

The proposed QRA methodology is based on population modeling and can be used to assess both ecological and microbial risks. The methodology is also capable of considering extreme and unfrequent events, but some arrangements must be made to apply the methodology to every specific case. For example, in some cases (such as in chapters 4 and 5), the extreme events are industrial accidents, whereas in other cases industrial accidents are not involved, but other sources of extreme events, such as: the case of QMRA for schistosomiasis disease (chapter 6), where extremely rainy months may drastically increase schistosomiasis transmission; and the case of QERA for mako sharks (chapter 7), where environmental catastrophes may cause reproduction failure. All case studies use population modeling as basis for quantifying risks.

The methodology considers both the event's frequency of occurrence and the magnitude of the adverse ecological effects, so that it is capable of quantifying ecological risks caused by events with low frequency of occurrence and catastrophic consequences. It is not restricted to assess ecological risks via individual-level endpoints that often leads to inaccurate risk estimates. It is also able to predict the responses of populations to toxic exposure (via population-level endpoints), taking into account the relationships between individuals, the life history and ecology of a species. This way, the methodology can assess the risk of a population extinction (or decline) in the future under the conditions that catastrophic accidents might happen.

There are similarities between the methodology and the basic guidelines for preparation of studies in risk assessment provided by CETESB in the reference [62], which is applicable to the assessment of industrial accidents with potential to cause damage to humans outside the establishment (i.e. harm to people in surrounding areas, located beyond the establishment boundaries). The main similarities are in the qualitative risk assessment step that involves the consolidation of accidental scenarios via techniques such as Preliminary Risk Analysis (PRA); and in the risk quantification expressed as a FN curve, which is similar to the FN curve to quantify social risks used by CETESB. By contrast, the main difference is that the methodology seeks to assess ecological risks only, whereas CETESB focus on human risk assessment.

The steps of the proposed methodology are as follows (shown in Figure 3.1).

1. Problem characterization;
2. Identification of hazards and consolidation of accidental scenarios;
3. Exposure assessment
4. Frequency estimates;
5. Population modeling;
6. Risk quantification and evaluation.

The methodology is interactive, so that revaluation may occur during any part of the assessment, although deficiencies that must be revaluated may jeopardize resources available to complete the QERA (e.g. time and money). The methodology uses objective criteria throughout the second, third and fourth steps in order to rule out accidental scenarios that will not significantly contribute to the final ecological risk, avoiding waste of resources.

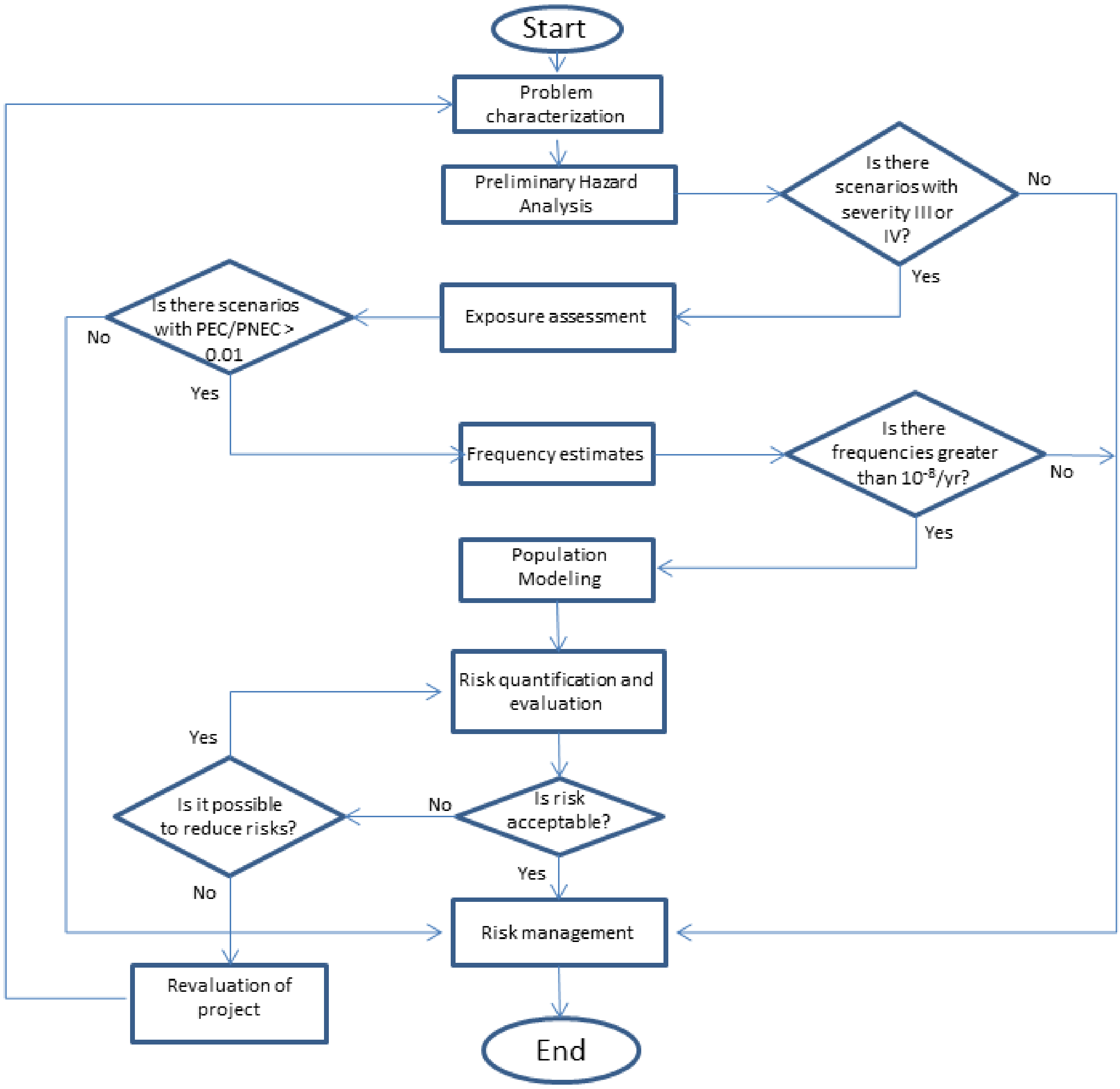

Figure 3.1 – Steps in conducting the methodology to Quantitative Ecological Risk Assessment for industrial accidents.

In the next sections, the aforementioned steps are discussed.

3.1 Problem characterization

The first step is a planning phase on which the entire risk assessment depends. It requires engagement between the risk assessor and other experts such as: risk managers, environmental managers, ecologists, technical managers, operators and other interested parties when appropriate (e.g. industrial leaders, government, environmental groups, any segment of society concerned about ecological risks).

They should be able to (1) define risk assessment issues and objectives, (2) characterize the establishment and installations (e.g. storage tanks, transport units, pipelines, loading equipment) to be included in the QERA and (3) characterize ecological components (habitats, species, life stages) in the region. Information to answer many of these issues may already be available from other studies such as an Environmental Impact Assessment (EIA) or even from a human QRA.

3.1.1 Risk assessment issues and objectives

The risk assessor should ensure that the results of the risk assessment will meet the needs of risk managers, i.e. how will risk assessment help the process of risk management. This way, they should reach a general agreement on characteristics such as:

- Nature of the problem (e.g. licensing process, company's own initiative, providing guidance, legal mandates).
- Objectives for the QERA, including criteria for success.
- Scale of the assessment (e.g. small area evaluated in depth or large area in less detail).
- General spatial (e.g. local, regional, or national) and temporal (i.e. the time frame over which effects will be evaluated) boundaries of the problem.
- Expected outputs of the QERA and the resources available to complete it (e.g. personnel, time, money).
- Policy considerations (corporate policy, societal concerns, environmental laws).
- Data and information already available. When data are few, further field work is needed to collected more data and that requires more resources for the assessment. When more resources are not available and new data cannot be collected, it may be possible to extrapolate from existing data. In this case, the risk assessor and risk managers must reach an agreement about what is known and what will be extrapolated from what is known.
- Acceptable level of uncertainty. If after the end of the QERA, the output does not meet the acceptable level of uncertainty, investment of new resources may be requested in order to develop ways of reducing uncertainty. The obvious way to reduce uncertainty is further field work to collect more data, so that additional

resources will be necessary. This way, the acceptable level of uncertainty should comply with the resources available to complete the assessment.

- Ecological impacts caused by past accidents.

3.1.2 Characteristics of the establishment

Here the risk assessor should collect technical information that characterize the establishment with regard to its physical structure, process conditions, chemicals of potential concern and installations (e.g. storage tanks, transport units, pipelines, loading equipment) in the establishment that deals with those chemicals.

Some installations may not significantly contribute to the risk because they do not deal with a considerable amount of hazardous chemical; therefore it is not worth considering all installations in the QERA. It is the responsibility of the risk assessor to select installations to be included in the QERA, under consultation of competent professionals and experts. The Committee for the Prevention of Disasters provides a selection method to determine which installations should be considered in a human QRA, provided in the second chapter of the reference [61]. This recommends a selection method of installations with potential to cause ecological damage, because this method is not dependent on consequences to humans, but on the amount of substance present in the installations and on the process conditions.

More specifically, the risk assessor should, if possible, gather relevant information about:

- Location of the establishment.
- Layout of the establishment, pointing the hazardous installations to be included in the QERA. If transport units are included as dangerous installations, the transport route should be specified.
- Updated plants or aerial photographs showing ecological environments near dangerous installations.
- Chemicals of potential concern identified by the official nomenclature, including: amount; ways of processing, handling, transport and storage; physicochemical properties. Raw materials, intermediate and finished products, byproducts, residues and wastes should also be considered.
- Description of processes in each hazardous installation and operational routines. If possible, besides a written description, it should include drawings, diagrams and flowcharts.

- Operational data (e.g. flow, pressure, temperature) on the processes with chemicals of potential concern.
- Protection and safety systems.

3.1.3 Characteristics of the ecological components

The purpose here is to gather information about ecological features in the environment possibly affected by accidents in the establishment. Hence, consultants such as environmental managers and ecologists may help the risk assessor out here, who should determine characteristics such as:

- Location of ecosystems possibly affected by accidents in the establishment.
- Area (spatial boundaries) of ecosystems to be evaluated, highlighting zones of permanent preservation.
- Ecological receptors (plants and animals) in the area, highlighting key species, e.g.: indicator species that are thought to be more sensitive and therefore serve as an early warning indicator of ecological effects; species of scientific and economic importance; rare and endangered species; or any species to be protected. For aquatic environments, indicator species are usually fishes, invertebrates or green algae. For sediment and soils, they are terrestrial plants, sediment dwelling organisms or earthworms. For air[1], representative species are typically birds.
- Geographic location and boundaries of populations or metapopulations of key species to be evaluated.
  - Geographic distribution of local populations within the metapopulation (when appropriate).
- Gather relevant information about the biology of key species.
- Define assessment endpoints that can effectively provide information about the population of key species of concern. Population-level endpoints are usually abundance, population growth rate, age/size structure, and spatial distribution

[1]For these types of ecosystems, the toxic concentration in air is usually so low that sophisticated risk assessments are not worth conducting.

[20]. For the purposes of this methodology, at least the population abundance must be considered.

- Define the life stages of the species of concern and the points at which chemicals may affect an individual [20].
- Physical stressors (e.g. hunting, fishing, boat traffic, thermal effluents, extreme weather changes) already affecting the key species.
- Chemical stressors already affecting the key species.

It is important to stress that risk will be quantified via population models that describe the population dynamic of key species chosen here. Consequently, the process of choosing key species should be carefully conducted by the risk assessor and consultants, because it will have a great influence on the results of the QERA. Populations or metapopulations of key species should be strategically chosen in a way that at least: they are representative in the ecosystem possibly affected; there is enough geographic and demographic data on the population to build a population model; and there is enough ecotoxicological data on the key species of concern (or on related species).

When possible, one should build a visual representation of the relationships among representative biotic groups of ecological receptors in order to illustrate the flows of energy, carbon, or contaminants. For example, a food web relationships among representative biotic groups within a ecosystem is useful to illustrate the key species’ position in the food web, which helps to qualitatively understand the ecological adverse effects at higher levels than population-level (i.e. community- and ecosystem-level).

Most information gathered in this phase will be necessary to guide the mathematical representation of the population dynamics, in the sixth step of the methodology.

3.2 Identification of hazards and consolidation of accidental scenarios

This step is similar to the second step of the basic guidelines for human QRA provided by CETESB in the reference [62]. The difference is that here the focus is only on the identification of accidents that may cause damage to the ecological environment.

This is a qualitative step of a risk assessment which aims at identifying all the initiator events of accidents and its possible consequences, i.e. to consolidate accidental scenarios. Structured techniques are applied in order to (1) systematically consolidate all accidental scenarios, to (2) qualitatively rank the risks related to each accidental scenario according to their frequency and severity, and to (3) select those accidental scenarios that should be subjected to a more detailed risk assessment (i.e. quantitative assessment) in the next steps.

The methodology makes use of the technique named Preliminary Hazard Analysis (PHA) to perform this step, although other techniques such as Hazard and Operability Analysis (HazOp), "What If?", Failure Mode and Effect Analysis (FMEA), among others, may be used when the risk assessor finds it is suitable for the installation being studied. More information about PHA and other hazard analysis techniques is provided in the reference [84].

A worksheet is generally used to report the qualitative information that consolidate each accidental scenario, such as: hazard, initiator event (what, where, when), causes, control measures, possible consequences to the ecological environment, as well as frequency and severity classes. A typical PHA worksheet is presented in Table 3.1.

Table 3.1. Typical Preliminary Hazard Analysis worksheet.

Preliminary Hazard Analysis (PHA)								
Identified hazards	Probable causes	Possible effects	*Control Measures*	*Freq.*	*Sev.*	*Risk*	*Recommendations and Observations*	*Accidental Scenario*

Below is the description of information to be filled according to the PHA worksheet above:

- Identified hazards: hazards with potential to cause damage to the ecological environment. At best, it should contain the identification of the substance (CAS number), its temperature, pressure and flow rate.
- Probable causes: description of the causes that may lead to the identified hazard (i.e. initiator events), such as cracking or breaking certain pipeline or equipment.
- Possible effects: possible physical effects from the event (e.g. contamination of the beach nearby, death of fishes, decrease fecundity of fishes, restrict photosynthesis of marine plants, reduce the abundance of affected populations).
- Control measures: barriers and preventive actions which could avoid the occurrence of the initiator event.

- Frequency class: classification of the event on its frequency, according to Table 3.2.
- Severity class: classification of the event on its severity, according to Table 3.3.
- Risk rank: qualitative value to the risk level of each accidental scenario, which is a result of crossing the classes of frequency and severity, as illustrated in the Table 3.4. The risk is classified as Tolerable (T), Moderate (M) or Not Tolerable (NT). For tolerable risks, there is no need for additional measures, i.e., monitoring is necessary and sufficient to ensure that the control and recovery measures are maintained. To risks qualified as moderate, additional control and recovery measures should be evaluated, aiming at risks reduction. The classification as not tolerable risks is an indication that existing control and recovery measures are insufficient. Alternative methods should be considered for reducing the likelihood of occurrence and magnitude of consequences.
- Recommendations and observations: recommendations for control and recovery measures that should be taken to decrease the frequency and/or severity of the accidental scenario.
- Accidental scenario: Identification number to the accidental scenario.

Table 3.2. Frequency classes.
(Adapted from the ref. [85])

Class	Description
A ***Very unlikely***	*Conceptually possible, but extremely unlikely in the lifetime of the installation. Without historical references.*
B ***Remote***	*Not expected to occur during the lifetime of the installation, although there are historical references.*
C ***Ocasional***	*Likely to occur even once during the lifetime of the installation.*
D ***Probable***	*Expected to occur more than once during the lifetime of the installation.*
E ***Frequent***	*Expected to occur several times during the lifetime of the installation.*

Table 3.3. Severity classes.
(Adapted from the ref. [85])

Class	Description
I ***Minor***	*No damage or minor system damage, but does not cause ecological damage.*
II ***Major***	*Irrelevant ecological damage.*

Class	Description
III ***Critical***	*Considerable ecological damage caused by release of chemicals, reaching areas beyond the boundaries of the establishment. Accidental scenario results in ecological damage with short recovery time.*
IV ***Catastrophic***	*Catastrophic ecological damage caused by release of chemicals, reaching areas beyond the boundaries of the establishment. Accidental scenario results in ecological damage with long recovery time.*

Table 3.4. Risk ranking: Tolerable (T), Moderate (M) or Not Tolerable (NT).

		Frequency Categories				
		A	***B***	***C***	***D***	***E***
Severity Categories	***IV***	*M*	*M*	*NT*	*NT*	*NT*
	III	*T*	*M*	*M*	*NT*	*NT*
	II	*T*	*T*	*M*	*M*	*M*
	I	*T*	*T*	*T*	*T*	*M*

After all accidental scenarios have been identified, one should select the most relevant to a more detailed assessment. Therefore, one should clearly establish the criterion considered in the selection of the relevant accidental scenarios. For a conservative approach, one can use a criterion based only on the severity class. Therefore, in this work, it is adopted the criterion of severity III or IV to trigger accidental scenarios for further analysis in the next step [62].

Because PHA is often used as an initial risk study in an early stage of a project, the results of this step may be already available. In fact, in a human QRA, accidents with potential to cause damage to humans are identified and they usually have potential to cause ecological damage as well. In this case, most accidents have been already identified and the risk assessor should just review the ecological effects (i.e. possible consequences) caused by these accidents. Conversely, if a previous PHA was not conducted yet, this is a great opportunity to do it. Likewise, this PHA might be used in a human QRA.

At the end of this step one should have a set of accidental scenarios characterized by qualitative information as in Table 3.1. As already mentioned, all accidental scenarios classified with severity III or IV should be selected for further analysis in the next step. In addition, this step allows to systematically identify the existing accidents and their possible ecological damage, leading to an improved level of preparation to emergencies.

3.3 Exposure assessment

This step should be conducted for all accidental scenarios selected in the previous step to a further and more detailed assessment. Firstly, it consists of applying mathematical models that simulate the occurrence and movement of toxic releases in the water, atmosphere and soil.

More specifically, one must estimate exposure of key species to the chemical released, for each accidental scenario. This includes describing the chemical dispersion and predicting the concentration that reaches key species of concern in each instant of time, i.e. concentrations $C_i(x,y,z,t)$ within a defined area (spatial boundaries), for each accidental scenario, *i*. Chemical fate and transport models have been often used to describe and predict distribution and concentration of chemicals in the environment. Guidance on fate and transport models is beyond the scope of this work; one suggests the references [6, 86] for additional information.

For most accidental scenarios, meteorological conditions may influence the chemical dispersion and, consequently, the estimated exposure concentration. In such cases, it is necessary to generate a set of meteorological scenarios for each accidental scenario, *i*. Thus, if one has *x* accidental scenarios selected from the second step and *y* meteorological scenarios defined here, one has now $x \times y$ new accidental scenarios, each one with a specific function of exposure concentrations $C_i(x,y,z,t)$. In other words, each meteorological scenario defined in this step within each accidental scenario from the previous step will have a specific function of predicted chemical concentration that vary in time and space.

A meteorological scenario is defined by meteorological parameters that depend on the kind of environmental media (e.g. air, soil, water) the chemical moves through. Such meteorological parameters could be, e.g., weather stability class; wind direction and speed; air, soil/bund, water temperature; ambient pressure; humidity; tides of the sea; currents of the ocean; season of the year; etc. To do not yield an exaggerated number of new accidental scenarios for the QERA, it is useful to group the data in a limited number of representative meteorological parameters.

Subsequently, because the next steps of the methodology do require additional costs and special expertise, one should decide whether the chemical concentration estimated is expected to cause ecological adverse effects, for all accidental scenarios. In other words, one should select the accidental scenarios in which population-level effects are likely to occur, so that population-level ecological risks should be quantified. This way, the methodology needs a criterion to trigger accidental scenarios for further QERA. The hazard quotient (i.e. an exposure concentration divided by an effects concentration) is a commonly applied criterion for that [2, 87]. They are quick and simple to use and do not require special expertise from risk assessors.

In this sense, Pastorok *et al.* [20] states that “at best, deterministic hazard quotients […] can only be used to screen out chemicals, receptors, or site areas that are clearly not a problem (when the hazard quotient is considerably less than 1)". In addition to that, EurEco found in recent study that most of the chemicals, pesticides and marine schemes developed for ERA, use the hazard quotient, calculated as the Predicted Environmental Concentration (PEC) divided by the Predicted No Effect Concentration (PNEC), to indicate low risk when it is less than 0.01 [87]. For a conservative approach in the proposed methodology, the PEC will be the local maximum[2] of $C_i(x,y,z,t)$, whereas PNEC is the concentration below which exposure to a substance is not expected to cause adverse effects on an individual organism. The former is provided by the results of chemical fate and transport models and the latter by ecotoxicologial data on the species being assessed, usually as a concentration based endpoint known as No Observed Effect Level (NOEL - see glossary for details). The ECOTOX database can be used as a source for locating single chemical toxicity data for plants and animals [27]. It is important to note that the PNEC is an individual-level endpoint and so is the hazard quotient.

As a result, the proposed methodology uses the criterion PEC/PNEC > 0.01 to pick accidentals scenarios to the next step. Because it is a very conservative approach, it is likely that no accidental scenarios that considerably contribute to the ecological risk will be ruled out. Nonetheless, if it concerns the risk assessor, he might evaluate other chemical aspects such as: persistence and biodegradability; bioaccumulative potential (via bioaccumulation factor); and solubility in water (in case of an aquatic ecosystem). For example, if the chemical is readily degradable, population-level effects are not likely to occur, even if PEC/PNEC is greater than 0.01.

Finally, at the end of this step one should have a set of accidental scenarios that are likely to contribute to cause population-level effects. Several parameters consolidate each accidental scenario, they are mainly: hazard, initiator event, causes, control measures, meteorological parameters, chemical concentration $C_i(x,y,z,t)$, and hazard quotient.

3.4 Frequency estimates

For the selected accidental scenarios in the previous step, the frequency of occurrence should be estimated. The output of the QERA is very dependent on this estimate, so that an under- or sub-estimate of this value can lead to rough errors in calculating the ecological risk.

[2] By local we mean that it is within the spatial boundaries of populations being evaluated as well as within the simulated time period.

In some risk assessments, the frequency of occurrence of an accident can be estimated from historical records contained in databases or references, since they are actually representative to the case. Generic frequencies and times are presented in the reference [61]. In the third chapter of this reference, Loss of Containment Events (LOCs) (caused by e.g., corrosion, construction errors, welding failures, blocking of tanking vents, mechanical impact, natural causes, domino effects, etc.) are described and their generic frequencies of occurrence are estimated, for various systems in an establishment, including stationary installations and transport units such as: pressurized stationary tanks and vessels, atmospheric stationary tanks and vessels, gas cylinders, pipes, pumps, heat exchangers, pressure relief devices, warehouses, storage of explosives, road tankers, tank wagons, and ships.

However, those generic frequencies describe average situations and may need corrections concerning specific circumstances of the installation under assessment. Due to the complexity of some installations, it might be necessary to use expert opinion and Reliability Engineering techniques (e.g., event tree, Event Sequence Diagrams, Bayesian Belief Networks) in order to correct the generic frequencies taking into account the influence of control measures (e.g., safety management systems, alarms, automatic stops), as well as human errors that might contribute to the occurrence of the accidental scenario. In other words, the risk assessment team might need to conduct a reliability analysis involving generic equipment failures, control measures and human error. It is beyond the scope of this work to provide guidance on reliability analysis; for a general view on reliability theory, models, methods and applications, see the references [51, 53, 54, 88]; and for specific information about techniques such as Event Sequence Diagrams (ESD), Bayesian Belief Networks (BBN) and Human Reliability Analysis see the references [55-60].

In addition to that, for each accidental scenario the frequencies concerning meteorological parameters that consolidate each accidental scenario (defined in the previous step) should be also taken into account. Consequently, meteorological statistics (deduced, for example, from a nearby and representative meteorological station) should be used to define fractional frequencies or number of observations to each meteorological scenario.

Finally, only accidental scenarios that contribute significantly to the ecological risk should be included in the QERA under the conditions that (1) the frequency of occurrence is equal to or greater than 10^{-8} per year and (2) PEC/PNEC is greater than 0.01. The criteria therefore are used to trigger accidental scenarios for risk quantification and evaluation via population modeling in the next step. The first criterion is taken from reference [61], where it is stated that "a threshold of 10^{-8} per year as criterion for including LOCs is considered reasonable since generic LOCs leading to the release of the complete inventory have failure frequencies in the range 10^{-5} and 10^{-7} per year". The second criterion is taken from the previous step of the proposed methodology and was already explained.

The output of this step is then a set of accidental scenarios that are likely to contribute to the ecological risk, with their respective frequency estimates of occurrence. Several parameters consolidate each accidental scenario, they are mainly: hazard, initiator event, causes, control measures, meteorological parameters, chemical concentration $C_i(x,y,z,t)$, hazard quotient, and frequency estimate of occurrence (that is equal or greater than 10^{-8} per year).

3.5 Population modeling

This step is an iterative process (see Figure 3.2). Firstly, a population model is formulated (see section 2.5) in an effort to describe the natural population dynamics of key species in the area (without exposure to the chemical of concern). It is necessary to formulate a population model to each key species, if more than one is being analyzed. The population dynamics must be described via assessment endpoints defined in the first step. The predicted chemical concentration, $C_i(x,y,z,t)$ - for each accidental scenario, i, that may affect a population of concern - will be used as input variable to describe the population dynamics with chemical exposure.

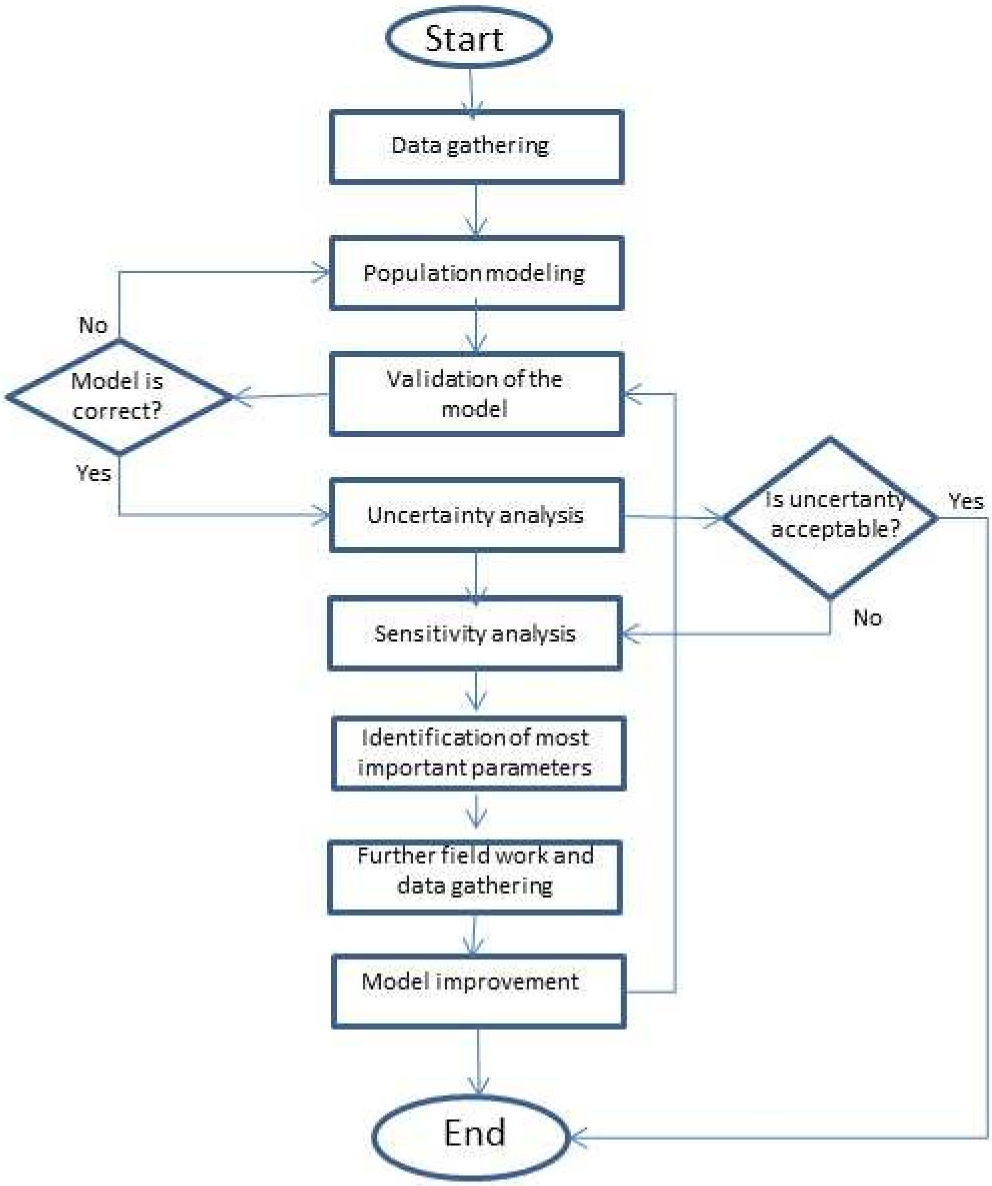

Figure 3.2 - Iterative process of population modeling.

Pastorok *et al.* [20] provides a detailed guidance on ecological modeling in risk assessment. He also makes a critical evaluation of software designed for a QERA, pointing their possible uses and limitations.

Input data will be necessary to parameterize the population model. The quality and predictiveness of the model depends mostly on the quality and quantity of these data. If data for the key species are insufficient, then one could extrapolate the information from related species.

Typically, a population model requires information on the following input variables [20, 43]: age/size structure; specific survival and fecundity rates for each age/size; rates of immigration or emigration; initial abundance for each age/size; estimates of variability for the vital rates and initial abundances; density dependence effects; geographic and habitat distribution of key species; and foraging behavior. The required level of detail for a particular variable depends on the assessment objectives.

Once the population model is formulated, it should be validated in order to make sure that the model is a good approximation of reality and provides reliable predictions. The validation of a model is typically done by measuring the conformance of predictions with empirical data. This measure may be used to characterize the reliability of other predictions.

It is still a limitation of this methodology to provide an effective method for validation. However, there is some ways to validate a model. For example, if there is hardly no chemical/physical stressors currently affecting the population, there is a very simple way to validate the model: to run the population model multiple times for a non-impact scenario and assess its predictions. For non-impact scenarios, it is expected that the population abundance will remain steady (for short and middle-term predictions) or will decrease very slightly (for long-term predictions, because it is expected that every species goes naturally extinct, although it takes thousands of years). This way, if the population model considers no physical and chemical stressors, and the predictions show either high risk of extinction or high risk of explosion, the model may be not correct and should be reviewed.

After validation of the model, an uncertainty analysis of risk estimates should be conducted in order to determine if the level of uncertainty is acceptable. A simple way to deal with uncertainties is to use them to derive worst and best case estimates of extinction risks, based on changes on parameters. Such procedure will let the risk assessor to estimate a range (upper and lower bounds) to risk measures, such as time to extinction, or risk of decline. The greater are the uncertainties in parameter values, the wider will these bounds be. If these bounds are too wide, uncertainty may be unacceptable and do not meet the needs of risk managers. At best, these bounds should be narrow enough to make decisions taken by risk managers based on the lower bound the same as those based on the upper bound (i.e. the difference between the lower and upper bound should be regardless for risk managers).

It is important to stress that there are several other ways to measure and communicate uncertainty. To study them and provide an effective method to evaluate uncertainty is proposal for future developments in this methodology.

If the model is appropriate to describe the population dynamics of concern, uncertainties about risk estimates are mostly because of uncertainties about parameters (e.g., survival rate, fecundity rate, carrying capacity, initial population abundance), what is originated from incomplete knowledge, limited sample size, measurement error and use of surrogate data. More precise estimates for parameters can improve the model by narrowing the ranges of risk measures. This requires further field work and data gathering, what costs resources such as equipment, technology, staff, time, etc.

Obviously, resources are limited, so its allocation should be optimized in a way that uncertainty is reduced the most. With this in mind, a systematic sensitivity analysis can point out to the most important parameters to allocate resources for further data gathering. This can be done by observing the effects of changes in any model parameter on population extinction risk.

In summary, if uncertainty is acceptable, then it is the end of this step. Otherwise, if the present model provides risk estimates with an unacceptable level of uncertainty, then a sensitivity analysis can point out to the most important parameters which need better estimates. Then, further field work and data gathering on these parameters can improve the model. Finally, one has an improved model (with a validated structure and more precise parameters) which must be further analyzed until it is validated and uncertainties are acceptable.

3.6 Risk quantification and evaluation

The output elements from the previous steps are necessary as input for this step, essentially:

- a population model for each key species;
- a predicted concentration $C_i(x,y,z,t)$ within the area of concern for each accidental scenario, *i*; *t* in the same unit as the time-step of the model;
- the frequency estimate of each accidental scenario per time-step of the model;

General temporal boundaries were determined in the first step. The risk assessor should now define specific temporal boundaries for each accidental scenarios, i.e. the expected time frame over which the accidental scenario causes ecological effects, which depends basically on the concentration $C_i(t)$ within the area and on remedial actions to remove chemical from the area. This will also become an input variable (i.e. the time of the simulation).

Subsequently, an exposure-response assessment should be conducted in order to describe the relationship between the concentration, $C(x,y,z,t)$, of the chemical and the magnitude of the individual-level responses of key species (represented by changes in measurement endpoints, e.g., survival rate, fecundity rate, carrying capacity). It will be usually necessary to specify a dose-response function, which can be built from data on long-term effects of the chemical on key species. These are ecotoxicological data at individual-level that basically look at the effects of life-cycle chemical exposure on input variables such as age-specific fecundity, survival and mortality. Because this is a major step in the ecological risk assessment, this topic is not addressed in the reference [20]. Instead, they suggest the references [1, 24, 26] as considerable guidance on how to analyze for toxicity and exposure-response relationships.

By linking exposure-response relationships to the population model, one can now predict how different concentrations of the chemical (note that for each accidental scenario there is a predicted chemical concentration) would cause adverse effects on populations of key species.

The probability of adverse effects may be represented by probability-consequence curves. For example, Figure 3.3 shows the consequences over time on population abundance for three different scenarios of chemical exposure. The several ways of expressing those curves were presented in section 2.5.4 and the two ways of assessing impacts and risks of each accidental scenario were described in section 2.5.5. The risks should also be categorized according to section 2.5.7. Lastly, a sensitivity analysis may add insight to the QERA by exploring the sensitivity to assumptions.

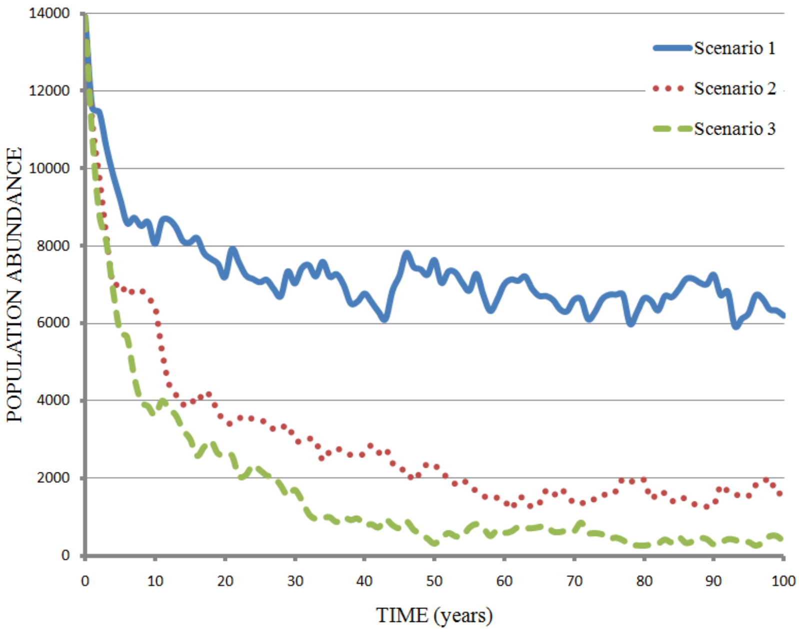

Figure 3.3 – Illustrative example of effects on a fish population for a 100 years simulation, for three different concentrations of oil exposure. Scenarios 1, 2 and 3, respectively: C(x,y,z,t) < 1 ml/L; C(x,y,z,t) = 16 ml/L; C(x,y,z,t) = 30 ml/L.

To quantify the ecological risks of all accidental scenarios in only one measure, the values of the consequence estimates should be combined with cumulative frequency estimate of occurrence. This regard was introduced in section 2.5.6. As a result, one builds a FN curve, where N is the average population decline number and F the cumulative frequency of accidents with N or greater abundance decline. For that, the following steps should be conducted:

a. Select a key species, *s*.

b. Set the average population abundance decline at the end of the simulation, N_{si}, for each accidental scenario, *i*, for each key species, *s*.

c. Build a list of average abundance decline, N_{si}, and its respective frequency estimate of occurrence, $F_{si}(y^{-1})$. It is necessary a list for each key species.

d. The FN curve is now constructed by cumulating all frequencies in each list (i.e. for each key species) for which N_{si} is greater than or equal to N:

$$F_s(N) = \sum_{\forall i: N_{si} \geq N} F_i \qquad (3.1)$$

The Figure 3.4 shows an example of an FN curve that characterizes the ecological risks originating from accidents in an establishment.

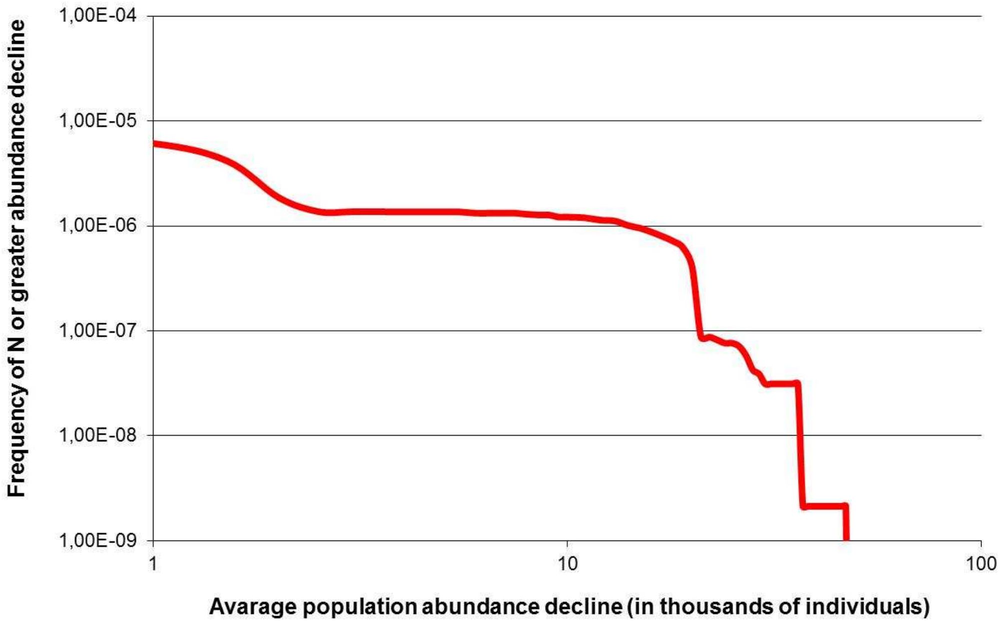

Figure 3.4 - FN curve for representation of the ecological risks related to accidents in an establishment (figure for demonstration purposes only).

Together, the risk curves (for each particular accidental scenario) and the FN curve can be used in making conservation decisions that involve planning future fieldwork, assessing impacts and evaluating management actions. For all these cases, the objective of the decision must be specified. It is assumed that the objective is minimizing the risk. Then a cost-benefit analysis can be made with the results of a series of assessments. The cost is actually the implementation cost of alternatives to reduce risk, and the benefit is the quantified risk reduction itself. Consequently, the selection criterion for the best alternative can be based on minimizing the cost:benefit ratio while satisfying either a cost or a risk constraint.

To sum up, the results of the methodology can support decisions such as for example:

- if we invest a certain quantity of money (say U$100,000) in control measures, what will be the frequency reduction in the FN curve?
- How best to allocate this U$100,000 in order to maximize risk reduction? Which accidental scenarios prioritize?
- If we change the layout of the establishment, setting hazardous installations more distant from ecological environments, what will be the new FN curve?
- What are the best conservation options (e.g., re-routing of spills, pollution remediation, habitat protection, translocation or reintroduction of individuals in the population)?

- To which value an accident's frequency of occurrence must be reduced in order to achieve a risk level of acceptability?

The last question is particularly dependent on risk criteria for acceptability. In fact, after quantification of the risks to populations, they can be evaluated by stakeholders (enterprise leaders, government, environmental agencies, etc.) to determine whether the risks are tolerable or not. However, establishing risk criteria for acceptability is a slow and complicated process that requires the participation of society in its judgment. Once completed the process, there is now a standard, i.e. a value or interval where the risk is considered tolerable. It makes law clearer, so that less money is spent with lawyers and so more money can be spent with environmental and conservation management.

Some scientists believe that the interpretation of the results of a QERA is a political process that requires criteria imposed by the society rather than by the scientific community alone. Others believe that scientists nevertheless have a responsibility to provide guidance [8]. It is not an aim of this work to provide guidance on risk criteria for acceptability. Although it was proposed risk categories for assessing a particular accidental scenario in terms of probability and time to half loss (see section 2.5.7), this work does not devise risk categories in the FN curve that cumulates risks of all accidental scenarios.

Determining risk categories in the FN curve is still a shortcoming of the proposed methodology. With this in mind, the FN curve makes the process of devising risk categories for acceptability less difficult, because it is expressed in the same way as the societal risk in human QRA. For example, one should determine what is the tolerable frequency of a population declining by a given percentage (say 20%), or the tolerable frequency of a population extinction. And that is much more general than, for example, determining risk categories for the volume of contaminated water, as in PROTEUS model [89], because each specific ecosystem has its specific responses caused by exposure to a given volume of contaminated surface water, so that risk categorization relies on a subjective evaluation of ecologists

4 QUANTITATIVE ECOLOGICAL RISK ASSESSMENT OF INDUSTRIAL ACCIDENTS: THE CASE OF OIL SHIP TRANSPORTATION IN THE COASTAL TROPICAL AREA OF NORTHEASTERN BRAZIL

This chapter was published as an original research article in the Human and Ecological Risk Assessment: an International Journal [31].

Accidents such as toxic spills cause massive damage to local ecosystems and hamper the sustainable development of hazardous industries. Models that only consider regularly occurring pollution are unable to truly quantify ecological risks (ecorisks) from these industries. This work presents a methodology capable of quantifying ecorisks related to rare and extreme events such as industrial accidents. We developed a procedure that integrates information from different studies that contribute to characterize ecorisks from industrial accidents: (1) reliability analysis, (2) fate and transport modeling, (3) individual-level toxicological assessment, and (4) population modeling. The methodology is exemplified by an application in the project of oil ship transportation to supply the Suape industrial complex. A fish population was strategically chosen to represent the ecosystem's health of Suape beach. For the critical accidental scenarios, their frequencies of occurrence were estimated and the space-time evolution of oil simulated. The ecorisks were quantified in terms of time and population probability of extinction, categorized and compared against a no-accident scenario. The total ecorisks from all scenarios were presented as a FN curve, where N is the average number of deaths in the population and F the cumulative frequency of accidents with potential to cause N or more deaths.

4.1 Introduction

Recent industrial accidents such as toxic spills have been causing catastrophic damage to local ecosystems (i.e. plants and animals) and consequently great financial losses to the accountable operators. For instance, the British Petroleum spill (Gulf of Mexico, 2011), the wrecks of the oil tankers Prestige (Spain, 2002) and Erika (France, 1999) and the chemical spills at Doñana (Spain, 1998) and Baia Mare (Romania, 2000) [90]. Furthermore, a high number of less harmful (but not negligible) accidents happen every year such as the oil spills in Campos Basin (Brazil, 2011, 2012) [91, 92] and the Rena spill (New Zealand, 2011)

[93].While humans restrict their thinking only to average events (i.e. high-frequency/low-consequence), such large events (i.e. low-frequency/high-consequence) will continue to surprise us and shape our world [94].

A recent perspective for ecological risk assessment (ERA) [95] incorporates the "assessment of the prediction" into the ecological risk (hereafter ecorisk) prediction processes used to grant consent or approval for the construction of major infrastructure projects. If any risk assessment researcher undertake this *post hoc* assessment for the aforementioned industrial activities (e.g., BP's Gulf of Mexico operations), they will likely conclude that there were unaddressed risks remaining, such as ecorisks from catastrophic infrastructure failures. In ERAs for these industries, a bad prediction is very clear when a catastrophic ecological damage happens, penalizing society due to risk assessors who presumably did not considered such events in their ERAs. Conversely, a good prediction is almost indefinable because it takes extremely long to observe that catastrophic ecological damage really does not happen, so society fails to reward those who can assess the "improbable". Gibbs's perspective may help to improve this situation by highlighting ERAs that include catastrophic accidents into their predictions.

In this case study, we develop a methodology for quantitative ERA (QERA) of industrial accidents [96, 97] that uses ecological modeling to explicitly quantify ecological effects caused by industrial accidents. In addition, we present an application of the methodology as a means for exemplifying it. The methodology consists of a procedure that integrates information from four different specific studies that provide relevant information for quantifying ecorisks from industrial accidents, i.e.:

1. Fate and transport modeling that describes and predicts dispersion and concentration of chemicals in the environment (i.e. air, soil, water). For example, we use a model that is able to predict the space-time evolution of chemical concentration in the ocean after a spill.
2. Individual-level toxicological assessment that translates a predicted chemical concentration into effects on individuals (e.g., increased mortality, reduced fecundity).
3. Reliability analysis to predict the occurrence of accidental scenarios and may involve both equipment failures and human error. This is important because industrial accidents are usually complicated to predict given the paucity of relevant data.

4. Ecological modeling at population-level (i.e. population modeling) that translates mortality, growth, and reproductive effects on individuals into population- or metapopulation-level effects (e.g., abundance decline, growth rate decline).

The last topic is particular useful for the sake of more transparency and better risk communication because the expected consequences of an accident to the ecosystem are expressed in more relevant units than individual-level effects [98]. They are expressed in terms of effects on populations (or metapopulations) of an indicator species strategically chosen to represent the ecosystem’s health (e.g., species that are more sensitive, species of scientific and economic importance, rare and endangered species), taking into account the relationships between individuals, the life history and population ecology. This way, the methodology can assess the risk of a population extinction (or decline) under the conditions that catastrophic accidents might happen.

The results of the methodology are risk control measures for each Accidental Scenario (hereafter AS) that take into account both the accident´s frequency of occurrence and the magnitude of the consequence to a population of native species. Such risk control measures are expressed in terms of time and probability of extinction and can be categorized according to the International Union for Conservation of Nature (IUCN) quantitative risk criteria [51].

Quantifying risks of each AS alone provides a basis for categorizing them, comparing them against a no-accident scenario (no-AS), and prioritizing management actions. However, it may also be useful to cumulate risks of all ASs as a basis for communicating the total ecorisk. For that, we propose a FN curve (similar to the FN curve for the social risk in human QRA [61], where N is the average number of deaths in the population and F the cumulative frequency of accidents with potential to cause N or more deaths.

4.1.1 Case study

The methodology is then applied to quantify ecorisks associated with transport and handling of crude oil to the Suape Port and Industrial Complex (SPIC), state of Pernambuco, Northeastern Brazil. The SPIC can be considered as one of the largest center of investments in Brazil. Today, the sum of investments is about U$ 21,3 billion, spent by more than 100 active enterprises and other 35 in their implementation phase, such as the oil refinery, three petrochemical plants and four shipyards. Therefore, it has been seen a great subject of research with the purpose of developing and improving the safe production and operation in SPIC [99].

Indeed oil will be supplied through an offshore harbor in SPIC. This harbour is expected to receive oil tankers up to 170,000 DWT (Deadweight Tons) and is surrounded by very rich aquatic ecosystems such as beaches, estuaries, mangroves, coral reefs and coastal islands. Several native species are important to the Pernambuco state economy and to local human communities. Oil spills may cause catastrophic damage to the ecological health in SPIC and consequently economic and social impairments. Our assessment provides relevant and quantitative information that can support the decision-making process for preventing and managing such catastrophes. Through this case study, we present the methodology step-by-step.

4.1.2 Literature review

Although most approaches for QERA (e.g., [2, 25, 100, 101]) and case studies (e.g., [7, 14, 15, 43, 102, 103]) recommend and use models that are able to quantify ecorisks at population and higher levels, they focus on pollution caused by either regularly occurring events of an industrial activity (e.g., chronic pollution, waste discharge, pesticide use) or events that already occurred (i.e. sites already contaminated). They often ignore the potential occurrence of accidental events that have high consequences, albeit they are much less likely to occur. However, such events do happen at some point, so that any attempt to accurately predict long-term ecorisks should take their potential occurrence into consideration. Indeed there are some QERAs [104, 105] that consider accidental events (in these cases the *Exxon Valdez* oil spill) retrospectively (i.e. after the event occurred), but not preventively as we propose in this chapter.

As a result, it can be argued that the typical limitation consists of the missing link between ecorisks and potential industrial accidents. In order to tackle this drawback, Stam et al. (2000) proposed a model to assess risk for the aquatic ecological environment related to industrial installations[89]. This model considers both a probabilistic approach for accidents (particularly aquatic spills) and adverse ecological effects. The former is calculated based on standard QRA methodology [61] and uses correction factors needed in order to assess the risk from an activity under local circumstances. And the latter is calculated as a volume of potentially contaminated surface water. Although the approach for representing ecological effects predicts a volume of potentially contaminated surface water, the presence of the contaminant does not necessarily mean relevant ecorisk [72], so that it still needs a qualitative evaluation by ecotoxicologists to translate volume of contaminated water into adverse ecological effects. For this reason, one relevant drawback of this model cannot be ignored: it fails to directly and explicitly quantify effects on ecological entities.

The rest of this chapter starts by presenting the proposed methodology. We then follow the steps of this methodology, explaining each of them by means of an example of application. The results were then obtained by the application of the methodology to the example under consideration. The results are given in two ways: ecorisks related to each ASs alone and categorized according to IUCN criteria; and the cumulated ecorisks related to all ASs. A sensitivity analysis is also provided as well as a discussion of the results, its practical implications and potential future improvements. Finally, we conclude by relating the most important goals and shortcomings of the methodology.

4.2 Material and Methods

We propose a QERA methodology directed to industrial accidents with potential to cause ecological adverse effects. It considers both the accident's frequency of occurrence and the magnitude of the adverse ecological effects, so that it is capable of quantifying ecorisks caused by low-frequency/high-consequence events. It is not restricted to assess ecorisks via individual-level endpoints that often leads to inaccurate risk estimates [20]. We incorporated ecological modeling at population-level to predict the responses of populations (or metapopulations) to toxic exposure (via population-level endpoints), taking into account the relationships between individuals, the life history and population ecology. This way, the methodology can assess the risk of a population extinction (or decline) in the future under the conditions that catastrophic accidents might happen. The steps of the proposed methodology are as follows.

1. Problem characterization;
2. Identification of hazards and consolidation of ASs;
3. Prospective exposure assessment;
4. Frequency estimates;
5. Population modeling;
6. Risk quantification and evaluation.

The methodology is interactive so that revaluation may occur during any part of the assessment. The approach uses objective criteria throughout the second, third and fourth steps in order to rule out ASs that will not significantly contribute to the final ecorisk, therefore avoiding waste of resources. The aforementioned steps will be discussed in the following sections by means of a case study.

4.2.1 Problem Characterization

This step aims at providing risk managers objective answers about the ecorisks associated with transport and handling of crude oil to supply the Suape Port and Industrial Complex. To ensure that the results of this assessment would meet the needs of risk managers, the following specific objectives were taken into consideration: identify the significant ecorisks; examine the population dynamics (of a native species in the surrounding environment) when exposed to potential ASs for 100 years from now; quantify ecorisks of accidental events; be as conservative as possible in parameterization, predicting worst-case scenarios; provide numerical basis of knowledge for communicating risks; provide a basis for comparing, ranking and prioritizing ASs; conduct a sensitivity analysis that expresses changes in risks measures as a function of changes in the accidents' frequencies and its consequences; deal with environmental stochasticity in time.

Most of the required data were available in the Environmental Impact Assessment [106] and in public databases [27, 107]. The outputs of our methodology are: risk curves of extinction and time to population extinction for all relevant ASs as well as for a no-AS; comparison of results between ASs and a no-AS; FN curve for cumulating risks of all ASs; point out further work that can effectively improve results.

4.2.1.1 Characteristics of the industrial activity

The SPIC is expected to receive oil tankers up to 170,000 DWT. As this ERA was concerned only with accidents associated with transport and handling of crude oil, only transport units (i.e. oil tankers) and their routes to the offshore harbour were considered. The approach channel of the SPIC was divided into 24 points (Figure 4.1) that represent a possible location for an accidental oil spill. The choice for 24 equally spaced points was subjective, i.e. it was an acceptable trade-off between simulation effort and capability to cover all accidental events in the approach channel. Technical information associated with the activity were also considered, i.e. [99, 106]: transportation ships are double-hull oil tankers; about 1138 ships come in and out the harbour every year; 24 hours is the average duration of unloading per ship; 144 is the average number of transhipments per year. Crude oil was the only chemical of concern in this assessment.

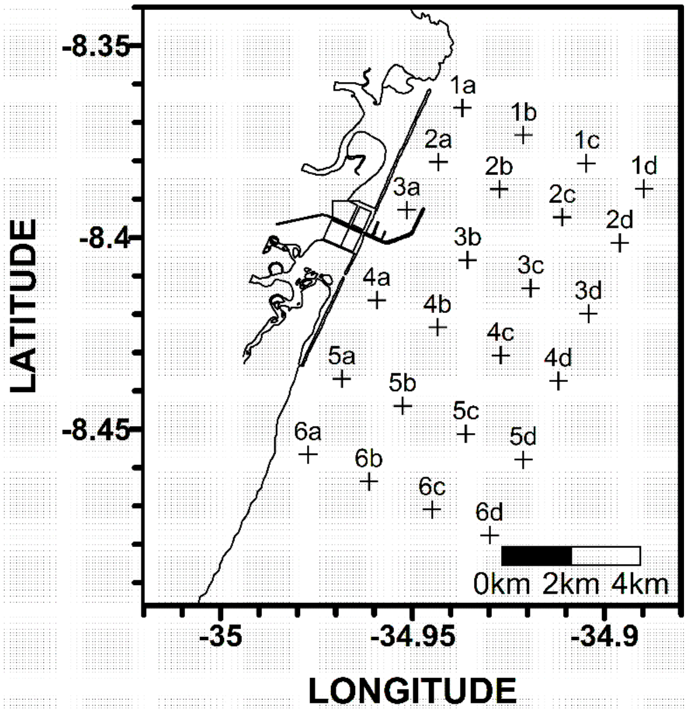

Figure 4.1 - Possible points for an oil spill to be included in the QERA.

4.2.1.2 Characteristics of ecological components

Among the species in the wild fauna and flora of the coastal region of Suape, we chose to analyse fishes because they have numerous advantages as indicator species compared to aquatic invertebrates and diatoms [108, 109], i.e.: they have a relatively large size; short-term effects (i.e. mortality) on fishes caused by oil exposure are often immediately apparent, since thousand (sometimes millions) of dead fish are found floating on the coast; life-history information is extensive for most fish species; their position at the top of the aquatic food web helps to provide an integrative view of the watershed environment; fishes are relatively easy to identify, and therefore tends to decrease observation and measurement errors; and fishes are typically present, even in the most polluted waters. The indicator species selected was a local fish population of a native species known as *Diapterus rhombeus*, order Perciformes, family Gerreidae, common name Carapeba. This is one of the most common Gerreidae species in the estuarine region of Suape, Northeastern Brazil [110]. Local ecologists of the Tropical Fish Ecology Lab of the University of Pernambuco (LEPT) believe that these fishes are thought to be more sensitive and therefore serve as an early warning indicator of ecological impacts. Also, they have significant economic and social importance, since local human communities consume them as well as sell them as a means of livelihood.

The LEPT provided demographic data about juveniles fishes, collected at the Suape shallow waters during 24 consecutive months (from March 2008 until February 2010). Juveniles use shallow waters and mangrove channels for breeding and for the growth phase, and migrate to areas of greater depth as soon as they become adults. Abundance was chosen as an assessment endpoint to provide information about the population of concern. The initial population abundance was estimated at 22,111 based on the aforementioned population demographic data.

4.2.2 Identification of Hazards and Consolidation of Accidental Scenarios

We used Preliminary Hazard Analysis (PHA) to perform this step, although other techniques such as "What If?" may be used when the risk assessor finds it is suitable for the industrial activity being studied. More information about PHA and other hazard analysis techniques is provided by Ericson (2005) [84][84][84][85][85][84].

Each point in Figure 4.1 represents a possible location for an oil spill and so can be used to define an AS. The key inputs for a PHA were frequency and severity of an oil spill. For each location, frequency would be greater if it had the real possibility of Loss of Containment Events (LOCs) during unloading activities and/or due to external impacts (collision with another ship, contact with fixed or floating objects, and grounding), whereas severity took into account the proximity of the location to the Suape beach, i.e. the closer the more severe. The selection of an AS for further assessment was based on severity only, as in human QRA of industrial accidents [61].

After a PHA for the 24 locations, three of them were classified with critical severity (i.e. class III, considerable ecological damage, reaching ecosystems beyond the boundaries of the defined location and short recovery time) or catastrophic severity (i.e. class IV, considerable ecological damage, reaching ecosystems beyond the boundaries of the defined location and long recovery time) and were selected for a more detailed analysis in the next step (i.e. prospective exposure assessment). More specifically, two locations had catastrophic severity class IV (i.e. 1a and 2a) and one had critical severity class III (i.e. 3a).

4.2.3 Prospective Exposure Assessment

Oceanographic and meteorological conditions (i.e. coastal bathymetry, tides, the distribution of water temperature and salinity, currents, winds) influence the dispersion of oil in the ocean and thus the chemical concentration to which the fish population is exposed after an accident. Previous works conducted on the coast of Suape [111, 112] has shown that information on the rainy season (from March to August) could be grouped in one meteorological scenario named “Winter”. Similarly, data on the dry season (from September to February) were grouped in the meteorological scenario named “Summer”. For each season of the year two tidal conditions were considered (Spring or Neap tide) based on information collected by tide gauges installed in the coastal Suape [111, 112]. For a conservative assessment, all scenarios were simulated with the critical initial condition of flood tide, when the transport toward the shore is stronger. Hence, each of the three ASs previously selected was divided into 4 new scenarios dependent on the season of the year (Summer or Winter) and the tidal range (Spring or Neap tide), resulting in the evaluation of 12 ASs.

4.2.3.1 Fate and transport model

A previous study was conducted to describe the ocean circulation at coastal NE-Brazilian waters using a combination of field data and numerical modelling [111]. The results were then used to simulate another model that incorporates the space-time evolution of an oil plume in case of accident in a given location [112].

In short, the Princeton Ocean Model (POM) [113] was used to describe the coastal circulation in the region of concern. It is one of the most tested and used framework by oceanographers to model coastal circulation (e.g., [111, 114-116]). The POM is based on the primitive equations of momentum for a Newtonian fluid. It basically integrates the Reynolds theorem discretized by finite difference method. The prognostic variables are the three components of velocity field, temperature, salinity, and two quantities which characterize the turbulence (i.e. the turbulence kinetic energy and the turbulence macroscale). The original code of the POM does not simulate the dispersion of chemical plumes. For this reason, it was added to the POM routines that calculate the advective-diffusive fate and transport of oil plume [112]. These routines also take into account the main physical-chemical mechanisms influencing on oil balance in tropical seawater: entrainment, emulsification and evaporation [117]. The local variation of oil concentration due to these processes were calculated in the simulation step by step, using a set of routines based on the models of Mackay (1991), Mackay et al. (1992), and Sebastiao and Soares (1995, 1998)[118-121], as described in Nazir et al. (2008). The physicochemical characteristics of the oil were based on the documentation of the ADIOS model, versions 1.1 and 2.0 [122, 123], and CONCAWE (1983)[124].

Once the ocean circulation was previously established by the prognostic variables of the POM, a new simulation was run by continuously injecting oil at the release point (x_r,y_r) on the sea surface, during 7 days, with a constant and normalized flow rate of 1 kg/s. This value (1 kg/s) was based on the inventory study conducted by Araujo et al. (2010). It will lead to the release of about 600 tons of oil.

The simulation grid had its origin at the point of the coastline situated 2800 meters south of the offshore harbour. The x-axis (8 km) was considered perpendicular to the coastline in the northeast direction, the y-axis (10 km) was parallel to the coastline in the northwest direction, and the z-axis was perpendicular upward with the origin at ocean surface. The grid resolution had varying spaces. The more close to the harbour the finer it was. It is worth noting that the simulation grid is not illustrated in Figure 4.1, which is just a map with points that represent possible locations for an oil spill.

The fate and transport model then predicted the time-dependent weight of oil (in kilograms) within each grid cell. By knowing the reference density of this oil (910 kg/m³) and the volume of each grid cell *(dx×dy×dz)*, we calculated the volume of oil within each cell and converted it into millilitres of oil per litre of water. The fish population under assessment is in the Suape beach waters, which covers three of the simulation grid cells and are connected to each other. For each AS, *i*, the concentration as a function of time to which the fish population is exposed, $C_i(x_0, y_0, z_0, t)$, was defined as the arithmetic mean of the predicted concentration in these three cells, i.e.:

$$C_i(x_0, y_0, z_0, t) = [C_i(x_1, y_1, z_1, t)+C_i(x_2, y_2, z_2, t)+C_i(x_3, y_3, z_3, t)]/3 \quad (4.1)$$

4.2.3.2 Hazard quotient

To select only ASs that may significantly contribute to the final ecorisks, we performed a conservative screening assessment of the toxicological effects at individual-level by using the hazard quotient for that, i.e. the ratio of Predicted Environmental Concentration (PEC) to a Predicted No Effect Concentration (PNEC) [87]. More specifically, PEC was the local maximum of $C_i(x_0, y_0, z_0, t)$ whereas PNEC was taken from toxicological data [125]. The value (= 1 ml/L) for the PNEC was the LC_0 to crude oil of a related species that belongs to the same order of the Perciformes, i.e. *Parupeneus barberinus*. This extrapolation was needed because there were no such data on *Diapterus rhombeus*. It was however considered plausible because fishes of the same order present similar toxicological characteristics.

4.2.4 Frequency Estimates

A screening reliability analysis was conducted based on generic frequencies of LOCs for ships, and covering loading and unloading activities, as well as external impact. CPR18E (2005) provides values for such frequencies per year. It is worth noting that such frequencies may overestimate risks because they do not take into account other specific circumstances that could reduce their values (e.g., safety management systems, alarms, automatic stops). Table 4.1 presents the considered LOCs for the selected ASs.

Frequencies to the meteorological conditions were also defined as follows: 0.5 per year for both Summer (6 months) and Winter (6 months); and 0.5 per year for both Spring and Neap tides, because they alternate on a weekly basis. This way, each pair of meteorological condition (season and tide) had a frequency of 0.25 per year.

Table 4.1. Possible LOCs for AS-1a, AS-2a and AS-3a.

Accidental scenario	**Full bore rupture of the unloading arm (L.1)**	**Leak of the unloading arm (L.2)**	**External impact, large spill (E.1)**	**External impact, small spill (E.2)**
1a			X	X
2a			X	X
3a	X	X	X	X

4.2.5 Population Modeling

Data on the population (previously described in the problem characterization) were on one stage class only (i.e. juveniles) provided that they were collected in shallow coastal waters of Suape. These fishes migrate to deeper waters as soon as they become adults. In addition, data provided the total length of each collected fish, so we could estimate their age based on the von Bertalanffy growth function [126], using life history parameter estimates available in FishBase [107], i.e.: L_{inf} = 22 cm; K = 2.21/year; and t_0 = -0.08 years, where L_{inf} is the total length that the fish of a population would reach if they were to grow indefinitely (also known as asymptotic length), K is a parameter that expresses the rate at which the asymptotic length is approached, and t_0 is the hypothetical age the fish would have at zero length, had their early life stages grown in the manner described by the von Bertalanffy growth function. It could be observed that 99.8% of collected individuals were younger than 4 months. As a result, the time-step of the model was 4 months, which is also approximate to this species' generation time (i.e. 4.8 months) provided by life history data on *Diapterus rhombeus* [107].

A population model was then built in the software RAMAS GIS v. 5 [46]. This software is not a model itself, but a computational tool for model building and stochastic simulation with Monte Carlo engine. The model projected the population abundance (N) forward 100 years (or 300 time-steps) from the initial population abundance estimate (22,111 individuals) using the mathematical expression:

$$N(t+1)=R(t)\times N(t) \tag{4.2}$$

, with $R(t)$ the population growth rate at time t. Temporal variability was incorporated into $R(t)$ by establishing a lognormal distribution with a mean equal to 1.001 and a standard deviation (SD) equal to 0.01. These values for the mean and SD were chosen to represent a stationary state for the juvenile fish population. We could deterministically set the mean equal to 1 and so make the population abundance stable over time. Instead, we made the conservative assumption that the abundance is slightly increasing over time with some variations due to environmental stochasticity. This way, this model describes the juvenile population dynamics without chemical exposure, so that it represents a no-AS (benchmark) against which we compared ASs. We made a simulation with 10,000 replications. For each time-step during each replication, a value to $R(t)$ was randomly selected.

4.3 Results and Discussion

4.3.1 Coastal Circulation and Oil Plume Dispersion

Figure 4.2 is one example of the fate and transport model simulation results. It shows the oil plume dispersion in the ocean 19 hours after a spill at location 3a considering meteorological conditions Winter/Spring tide. It is worth mentioning that the oil plume reached the receptor in all simulations of ASs in the Winter season. Conversely, the oil plume moved to the south in all simulations of ASs in the Summer, and did not reach the receptor. It is importantly to mention that we are referring to uncontained oil (i.e. without the implementation of a counter pollution operation, e.g. the deployment of booms).

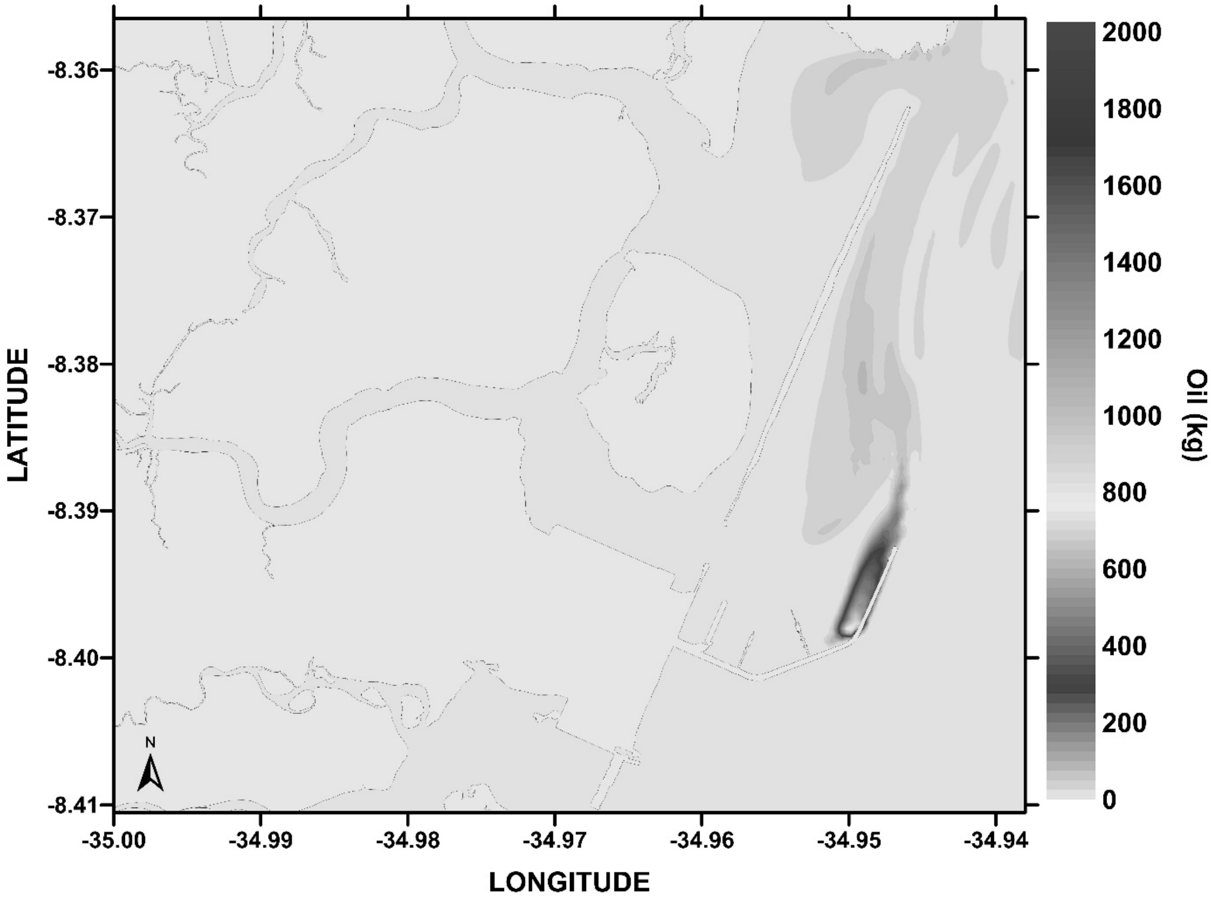

Figure 4.2 - Dispersion of the oil plume 19 h after a spill at location 3a in Winter/Spring tide.

4.3.2 Hazard Quotient

All ASs in the Winter had the hazard quotient PEC/PNEC greater than 10.12. Conversely, all ASs in the Summer had PEC/PNEC equal to zero, because the oil plume moves to the south in this season and does not reach the population of concern. We selected to the next step (frequency estimates) only those ASs which had hazard quotient greater than 0.01.

4.3.3 Frequency Estimates

Table 4.2 presents the resulting frequency estimates together with the predicted concentration from the methods in prospective exposure assessment.

Table 4.2. The concentration as a function of time to which the fish population is exposed, $C_i(x_0, y_0, z_0, t-T)$, where t is the discrete simulation time-step (4 months), T is the time-step at which the accidental scenario i occurs; and $F_i(y^{-1})$ the frequency of occurrence of i.

Accidental scenario	$\boldsymbol{C_i(x_0, y_0, z_0, t-T)}$	$\boldsymbol{F_i(y^{-1})}$
3a-winter-neap tide	$\begin{cases} 17.49, for\ t=T \\ 0, for\ t>T \end{cases}$	0.09504198 × 0.25 = 0.02376049
3a-winter-spring tide	$\begin{cases} 10.12, for\ t=T \\ 0, for\ t>T \end{cases}$	0.09504198 × 0.25 = 0.02376049
2a-winter-neap tide	$\begin{cases} 21.47, for\ t=T \\ 0, for\ t>T \end{cases}$	$1.98\times10^{-6} \times 0.25 = 4.9\times10^{-7}$
2a-winter- spring tide	$\begin{cases} 14.91, for\ t=T \\ 0, for\ t>T \end{cases}$	$1.98\times10^{-6} \times 0.25 = 4.9\times10^{-7}$
1a-winter-neap tide	$\begin{cases} 23.79, for\ t=T \\ 0, for\ t>T \end{cases}$	$1.98\times10^{-6} \times 0.25 = 4.9\times10^{-7}$
1a-winter- spring tide	$\begin{cases} 18.10, for\ t=T \\ 0, for\ t>T \end{cases}$	$1.98\times10^{-6} \times 0.25 = 4.9\times10^{-7}$

4.3.4 Exposure-Response Assessment

Data from a related fish species (i.e. *Parupeneus barberinus*) provided three lethal concentrations (i.e LC_0, LC_{50} and LC_{100}) to crude oil [125] that were used to fit a logarithmic dose-response function as it was expected that the function rate of change quickly increases and then levels out. Also, it was the best-fit curved line among several attempts of other different trend or regression types. The R^2 value was 0.9953, which indicates a good fit of the dose-response data. The fitted curve was then defined as a dose-response function to the species of concern, i.e.:

$$M_i(t) = 0.2926 \cdot ln\big(C_i(x_0, y_0, z_0, t)\big) - 0.0173 \qquad (4.3),$$

where M_i is the fraction of mortality caused by the occurrence of AS *i*.

4.3.5 Assessing Risks Of Each Accidental Scenario

Three new models were implemented to represent AS-1a, AS-2a and AS-3a. To do so, we incorporated to the no-AS model a source of environmental stochasticity (known as *catastrophe*) that is independent of the year-to-year temporal variation of the growth rate *R(t)*. We included two catastrophes for each of the three new models, representing their possible meteorological conditions in the Winter (i.e. Neap tide or Spring tide). ASs in the Summer were not included because in this season the oil plume moves to the south and does not reach the population of concern.

All catastrophes had a given frequency of occurrence and predicted exposure (Table 4.2). Thus, for each time-step of each replication (total of 10,000 replications), each of the two catastrophes was randomly selected to strike (or not) according to its frequency of occurrence. If it does, it causes a certain fraction of mortality (originated from the dose-response function) to the population from that time-step on. This is modeled by the following mathematical expression:

$$N(t+1) = R(t) \cdot N(t) \cdot [1 - M_k(t-T)] \quad (4.4),$$

where k is the randomly selected AS to strike, $M_k(t-T) = 0.2926 \times ln(C_k(x_0, y_0, z_0, t-T)) - 0.0173$, and T the time-step at which k strikes. Table 4.2 shows the parameter values for each AS. Figure 4.3 illustrates this simulation process for one replication.

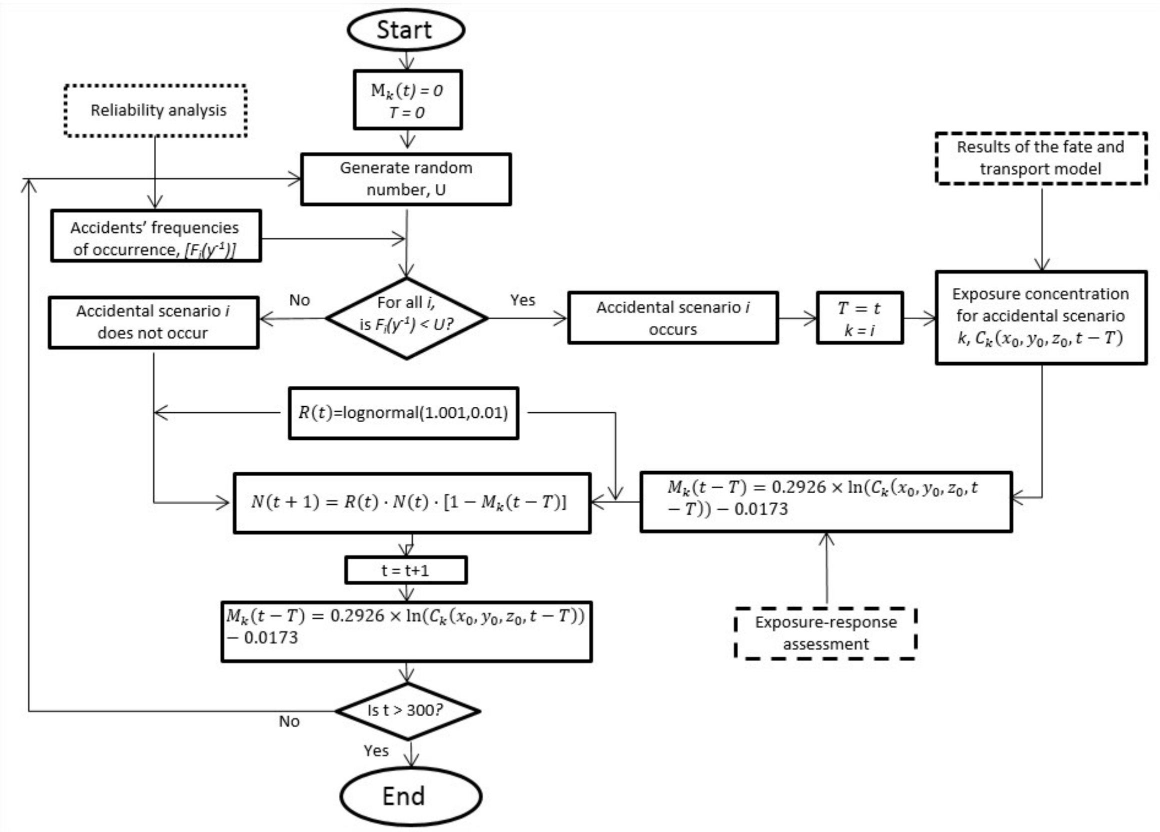

Figure 4.3 - Conceptual diagram that represents one replication out of 10,000 for stochastically simulating impact of potential ASs.

Over a given time period, there is a chance that any population will naturally become extinct. This chance is termed the background risk [8]. If the risks of different ASs are measured in terms of time and probability of extinction, it is possible to compare them against the background risks of a no-AS. The stochastic models predictions were used to construct probability-consequence curves such as the terminal extinction risk curve shown in Figure 4.4. Each point in the curve can be interpreted as "there is a Y% probability that, 100 years from now, the population abundance will be less than X." The dotted line indicates the average value, whereas the solid lines the 95% confidence intervals. The 3 vertical bars with two horizontal tabs represent the maximum vertical difference between a no-AS and an AS. The value of the maximum difference is reported for AS-3a. The reported number is the Kolmogorov-Smirnov test statistic D (which is the maximum vertical difference), the asterisks give the significance level (***: 0.001), based on two-sample Kolmogorov-Smirnov test [96]

The resulting curve for each AS model could be compared to the curve of the no-AS model. Extinction risk curves for no-AS, AS-1a and AS-2a are statistically superimposed, so the potential occurrence of these ASs cause the fish population of concern to face background risks only. Conversely, the potential occurrence of AS-3a causes a significant added risk of extinction.

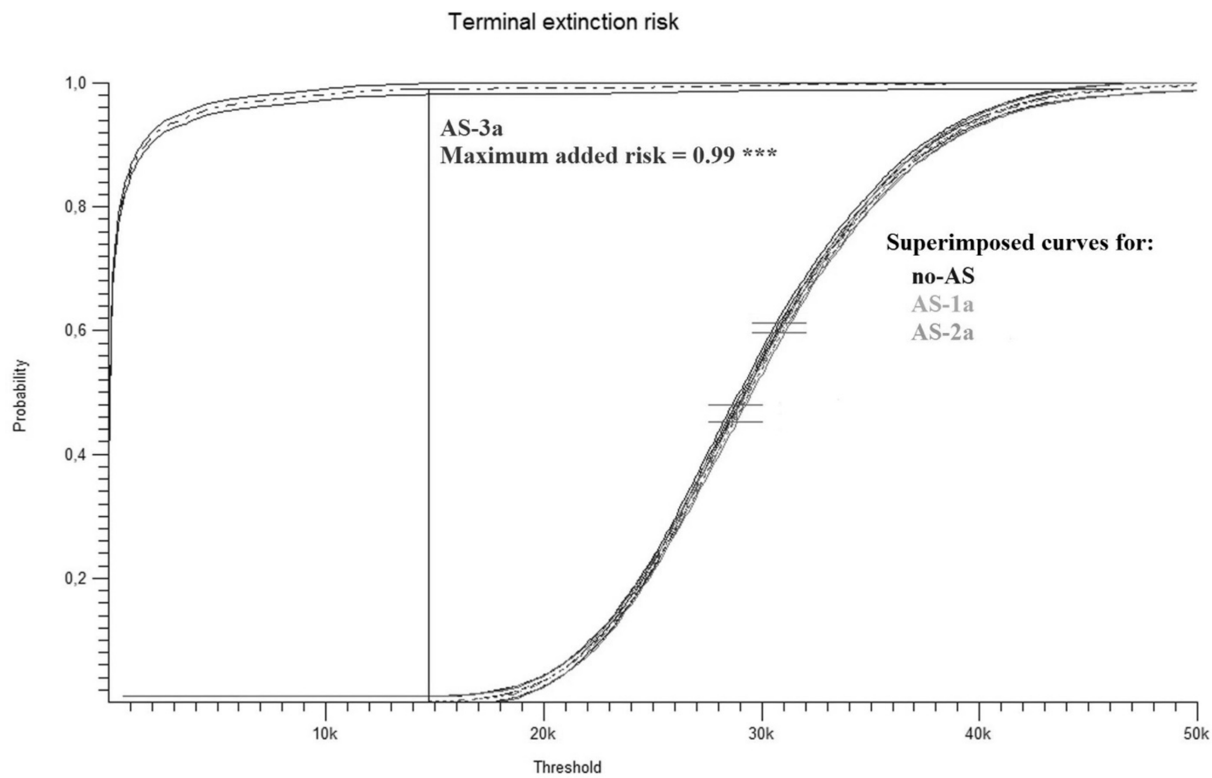

Figure 4.4 – Comparison of a no-AS with each of the ASs, in terms of terminal extinction risk.

4.3.5.1 Risk categorization

According to the IUCN risk criteria [51], the potential occurrence of AS-3a causes the fish population to be categorized as "Vulnerable" (Figure 4.5). Risk categories are provided by IUCN [127]. Each point in the curve can be interpreted as "there is a Y% probability that the population abundance will be extinct in or before time-step X".

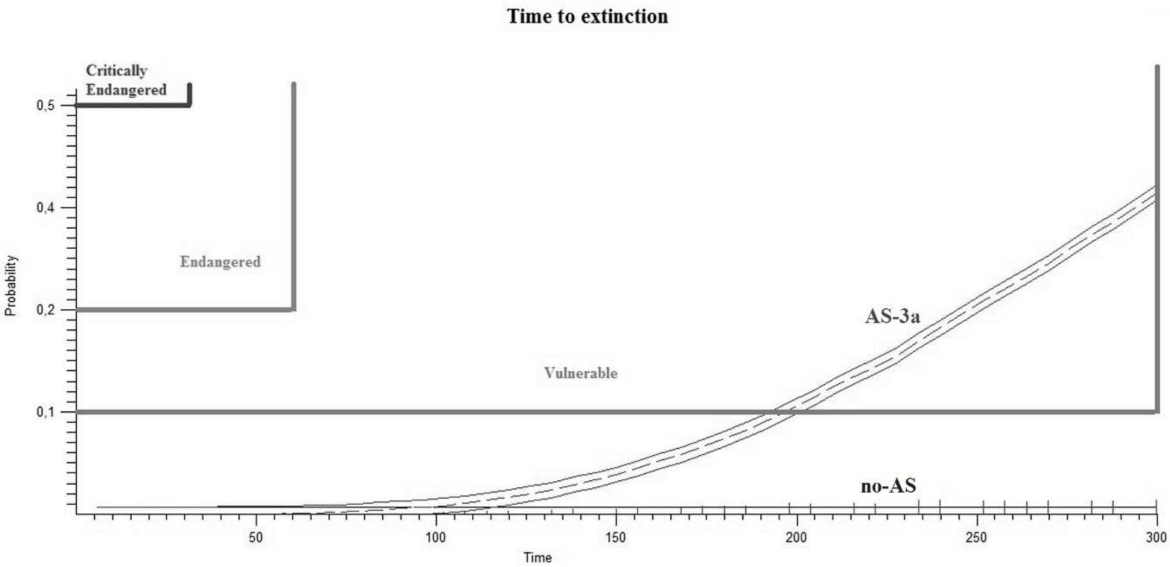

Figure 4.5 - Risk categorization for no-AS and AS-3a.

4.3.6 Sensitivity Analysis

We explored the sensitivity of the AS-3a model to key-parameter changes which allowed understanding how changes on specific parameter cause changes in results. Firstly, we analysed the risk sensitivity to reductions in the frequency of occurrence. Several simulations were made with the primary model for AS-3a, gradually reducing the catastrophes' frequencies of occurrence. It was observed that the frequency of accidental scenario 3a should be reduced by at least 42% in order to achieve a "Not Threatened" IUCN risk category (i.e. less than 10% probability of extinction within 100 years). Secondly, we analysed how reductions in the consequences can reduce risks by gradually reducing the fraction of mortality caused by AS-3a. It was observed that the magnitude of consequences should be reduced by at least 20% to achieve a "Not Threatened" IUCN risk category.

4.3.7 Cumulating Risks Of All Accidental Scenarios

It is considered here all the six critical ASs, i.e. AS-1a, As-2a and AS-3a in the Winter, Neap and Spring tide. Table 4.3 shows a list of these ASs (and the number of deaths caused by each of them) sorted by their frequencies of occurrence. By cumulating the sorted list of frequencies, it was obtained the frequency of *N* or more deaths. This result was used to build the FN curve in Figure 4.6, which presents the frequency to which it is expected to see *N* or more dead fishes. It informs in a single graph, the total ecorisks associated to the industrial activity of concern, using the number of deaths in the fish population as an environmental bioindicator. The y-axis is in logarithmic scale and that is because the frequency of occurrence of 20121 or more deaths was defined at 10^{-8}/year instead of zero. The value of 10^{-8}/year is the frequency criterion (in the fourth step of the methodology, i.e. frequency estimates) to screen out accidental scenarios that are irrelevant in terms of risk. Therefore, ecorisks from any event that occurs with a frequency less than that threshold are considered to be zero.

Table 4.3. List of accidental scenarios and their respective number of deaths (N) sorted by their frequencies (per year).

Accidental Scenario	**Number of deaths (N)**	**Frequency (per year)**	**Frequency of N or more deaths (per year)**
1a-winter-neap tide	20121	0.00000049	1E-8
2a-winter-neap tide	19458	0.00000049	0.00000049
1a-winter-spring tide	18352	0.00000049	0.00000098
3a-winter-neap tide	18131	0.02376049	0.00000147
2a-winter-spring tide	17025	0.00000049	0.02376196
3a-winter-spring tide	14593	0.02376049	0.02376245
	0	---------------	0.04752294

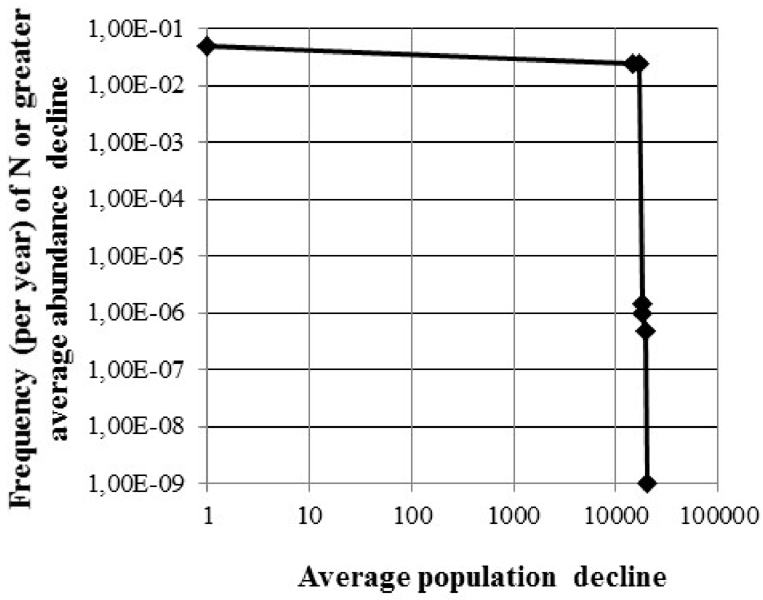

Figure 4.6 - FN curve for cumulating ecorisks of all ASs.

4.3.8 Discussion

The results showed that ecorisks from AS-3a cause the bioindicator population to be categorized as “Vulnerable” (Figure 4.5). Conversely, other accidental scenarios cause background risks only (Figure 4.4). From this point of view, management actions should be taken to reduce the frequency of occurrence and/or the magnitude of the consequences of AS-3a until risks reach a tolerable level (e.g., “Not Threatened” IUCN risk category).

There are some limitations in this QERA, i.e.: (1) frequencies were estimated based on average situations and did not take into account specific circumstances of the AS under assessment (e.g., control measures); (2) fate and transport model was deterministic for each group of meteorological condition (total of four groups); (3) toxicological data to build a dose-response curve was extrapolated from a related species and data on the related species was very scarce; (4) ecorisks related to ASs in the Summer were not considered because the oil plume does not reach the population chosen as bioindicator, although it may reach other populations to the south.

As the methodology is interactive, any new information and revaluation can be incorporated into the assessment at any time, starting a new round in order to improve results. The sensitivity analysis showed, for example, that changes in both frequency and consequence of AS-3a cause significant changes in risk estimates. Hence, some further work to effectively address the aforementioned limitations are: (1) conduct a more detailed reliability analysis for estimating more accurate frequencies; (2) incorporate meteorological stochasticity into the fate and transport model for a more accurate prospective exposure assessment; (3) perform toxicological tests with *Diapterus rhombeus* and crude oil; (4) include another fish population to the south of the release points and build a metapopulation model with potential for migration between the two populations so that ecorisks related to ASs in the Summer could be also quantified.

An uncertainty analysis was not conducted for this QERA. Since all parameters for the case study were defined from a conservative/pessimistic point of view, a simple way to measure uncertainty would be to conduct an optimistic simulation for significant ASs and to estimate a range (lower bound and upper bound) to quantified risk.

4.4 Conclusions

This chapter presented a methodology capable of quantifying ecorisks caused by events with low frequency of occurrence but that may cause catastrophic ecological damage. By means of an application, we showed that the methodology proves to be applicable, flexible, uses data efficiently and gives answers in a useful format. The main goal of the methodology was to integrate information from four different studies that can contribute to quantify ecorisks originating from low-frequency/high-consequence events, namely (1) fate and transport modeling, (2) individual-level toxicological assessment, (3) reliability analysis and (4) population modeling. Also, it is an iterative process, so that new information can be incorporated into risk assessments in order to improve the results.

The main potential benefits for an entity (e.g, government, industry, etc.) that conducts a QERA through this methodology are to: systematically identify the existing ecorisks from industrial accidents; express changes in the ecorisks as a function of changes in management actions that can reduce either the frequency of accidents or the magnitude of their consequences, i.e. sensitivity analysis; provide a basis for comparing and ranking ASs, and prioritizing risk management actions; provide numerical basis of knowledge for communicating to stakeholders the total ecorisks related to all ASs in a single graph, i.e. FN curve; deal with stochasticity; and examine the population dynamics of native species in surrounding ecosystems, what provides relevant information to tackle many other key gaps in environmental management beyond QERA of industrial accidents (e.g., QERA of regularly occurring events, support in decision-making about industrial waste discharges, optimal resource allocation for monitoring affected areas, optimal conservation of native species). As a shortcoming, no risk criteria were proposed in the FN risk curve (Figure 4.6). Although risk criteria were given for categorizing each AS alone, no risk criteria were proposed for the cumulative risks of all ASs in the FN curve.

5 QUANTITATIVE ECOLOGICAL RISK ASSESSMENT OF ACCIDENTAL OIL SPILLS ON SHIP ROUTES NEARBY A MARINE NATIONAL PARK IN BRAZIL

This chapter was published as an original research article in the Human and Ecological Risk Assessment: an International Journal [32].

Fernando de Noronha (FN) is a marine protected area off the coast of Brazil. The study of risks caused by nearby ship routes is new to authorities concerned in preserving FN. We identify nearby ship routes that cause FN to be potentially exposed to oil spills from tankers. A coral species is chosen as bioindicator of the ecosystem's health, which aids quantitative approaches. We simulate oil leakage scenarios with pessimistic occurrence frequencies and corals' mortality in case of accident. A metapopulation coral model is integrated to quantify measures of ecological risk under the potential occurrence of accidental scenarios. The categorization of risk results according to the International Union for the Conservation of Nature quantitative criteria shows that risks are negligible. Due to the considerable uncertainty in the results, we propose a more conservative categorization of risks based not on total metapopulation extinction, but on half loss. As a result, risks were considered not tolerable. The presented methodology and results are useful in supporting authorities in their preservation efforts such as the prioritization of sources of hazard, and selection of the most cost-effective conservation measures for maintaining good environmental health on a realistic budget, using this methodology as an exploratory tool.

5.1 Introduction

Fernando de Noronha (FN) is an archipelago 360 km off the northeast coast of Brazil (03°51'S, 03°30'W). It consists of 21 islands, although the main island alone, also named FN, occupies 17 km^2 of the archipelago's total 26 km^2, and is the only inhabited island [128]. Two thirds of Noronha consists of the Marine National Park of FN (PARNAMAR-FN), a marine protected area (MPA) that reaches to the 50 meter isobathic line [129]. The basic objective of the creation of PARNAMAR-FN is to preserve natural ecosystems with great ecological significance and scenic beauty, enabling scientific research, activities of environmental education, recreation and ecotourism [114].

Most projects devised and developed for preserving PARNAMAR-FN focus on the conservation of a single representative species (e.g., spinner dolphin, turtles, sharks, coral reefs) [97, 130-135]. Much effort has been made in research, planning, management, control and supervision to minimize the adverse ecological effects (i.e., changes that are considered undesirable because they alter the structure or function of ecosystems and its components [2]) caused by human activities within PARNAMAR-FN (e.g., tourism, diving, fishing) [91, 110, 116, 136-145].

Managers need to assess and manage ecological risks (hereafter ecorisks) caused by routine (i.e., high frequency/low consequence) human activities within PARNAMAR-FN. These assessments should also contemplate improbable, large events (i.e., low frequency/high consequence). Taleb [94] argues that surprises shape the world's history more than average events, mainly because humans restrict their thinking primarily to the "average/usual/common/probable" and are always surprised by the "improbable". Recent research efforts have shown the importance and feasibility of including improbable large events in model-based ecological risk assessments [31, 146].

In average, 75 ships navigate daily on routes near FN [147], using landmarks to determine the ship's position at sea more precisely and consistently. Many of these ships are oil tankers. We assess the accidental event of an oil spill from tankers navigating near FN. Thus, this chapter aims to quantify the ecorisks to PARNAMAR-FN caused by potential oil spills nearby. We conduct a Quantitative Ecological Risk Assessment (QERA) of industrial accidents [31] focusing on whether the risks of catastrophic oil spills are tolerable, or whether they need management (i.e., recovery or control measures that may reduce risks). Figure 5.1 shows identified ship routes nearby PARNAMAR. It shows six landmarks used for obtaining Lines Of Position (LOPs): Pico's Hill (A); FN Lighthouse (B); São Pedro's Church (C); Antenna (D); Ovo's Island (E); Pontinha (F). We use three LOPs to estimate the ship position in each point of each route. The LOPs were alignments, distances and/or directions. Ships drawn with increased size for better illustration. Prevailing current between 0.8 and 2 knots to W. Prevailing winds from direction SE (44%) and E (37%), force Beaufort 2.

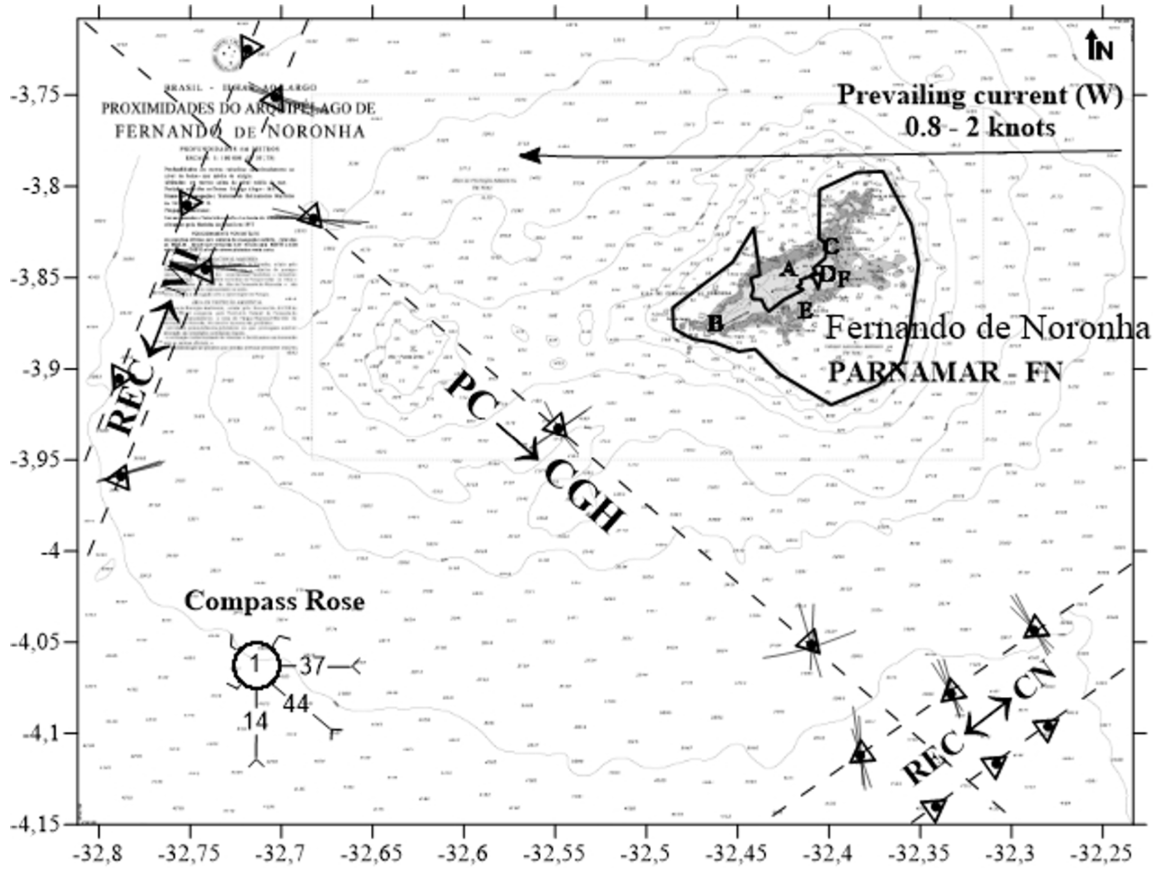

Figure 5.1 – Scale 1:4222. Routes near PARNAMAR-FN: Ponce and Colón – Cape of Good Hope (PC – CGH, going); Recife – Madeira Island (REC – MI, going and return); Recife – Cape Nouadhibou (REC – CN, going and return).

The rest of this chapter is structured as follows. Firstly, we present the methodology used for systematically conducting this QREA. Secondly, we apply the methodology to our study region using *S.stellata* as key-species, present results, categorize risks and discuss their implications. Lastly, we present concluding remarks about the QERA results, its advantages and limitations.

5.2 Methodology

Most approaches to QERA (*e.g.*, [2, 25, 100, 101] and case studies (*e.g.*, [7, 8, 14, 15, 102, 103, 148, 149] focus on pollution caused by either regularly occurring events of an industrial activity (e.g., chronic pollution, waste discharge, pesticide use) or events that have already occurred (i.e., sites that are already contaminated; e.g., [103, 148, 149]. They often ignore the potential occurrence of accidental events that have high consequences, albeit they are much less likely to occur.

In contrast, the methodology for QERA of industrial accidents presented in Duarte et al. [31] is especially applicable to situations in which the ecosystem is vulnerable to unlikely events involving exposure to pollutants, which is the case for PARNAMAR-FN and accidental oil spills. Our case study is based on this methodology, although we make some modifications for situations in which a preliminary (screening) step of the QERA must be conducted due to scarce resources for conducting a detailed analysis, as suggested by Duarte et al. [31].

The methodology requires a key population of a native species to be chosen to represent the ecosystem's health (*e.g.*, species that are more sensitive, species of scientific and economic importance, rare and endangered species, keystone, flagships or umbrella species [150-152]), because constructing and parameterizing a model that represents the entire ecosystem is unrealistic (Forbes et al. 2010, Forbes et al. 2011).

We propose an approach that describes the key population for the next 100 years under varying conditions, i.e.: (i) a benchmark scenario (Scn-0) that simulates the natural population dynamics under no perturbation and causes background risks; (ii) varying accidental scenarios (ASs) with different frequency and consequence parameters. By keeping all other parameters the same (Ceteris paribus [28, 29]) as in Scn-0 and varying parameters related to ASs, we aim at assessing the added/reduced risk caused by each AS, and not the absolute risk caused by a whole range of stressors together (e.g., fishing, global warming, pollution, diving, surfing, predatory tourism).

Here we differentiate between the terms hazard and risk as follows. The former is a potential source of damage whereas the latter is the combination of the likelihood of occurrence of damage and the severity of that damage [50]. For example, the potential oil spill from tankers on a nearby route is a hazard to PARNAMAR-FN. The combination of an oil spill's likelihood of occurrence with the magnitude of the damage to PARNAMAR-FN characterizes the risk [153].

5.2.1 Key-species

The key-species chosen to represent the ecosystem was *Siderastrea stellata*, an endemic, common coral species in Brazil. It occurs in all the Brazilian reefs from Maranhão (00°53N S, 044°16N W) to Rio de Janeiro State (23°S, 042°W) [154]. It is the main reef building organism in the oceanic islands of Atol das Rocas (03ºE 52´S, 033ºE 49´W) and FN [131, 155]. It usually occurs in shallow waters up to 10 meters depth [156, 157].

Corals are sessile; if the region is affected by a pollutant, they will be exposed and suffer the effects of pollution [118]. Corals serve as food and shelter to many types of animals such as worms, crustaceans, sponges, sea urchins, and many species of fish [118]. The loss of coral will affect both humans and terrestrial organisms because it protects the shoreline, supports tourism, and facilitates fisheries [118].

5.2.2 Preliminary Hazard Analysis

Table 5.1, Table 5.2 and Table 5.3 show distances and directions from landmarks in FN to ships that navigates on routes nearby. These routes were identified on Pilot Charts, which show the most recommended routes to navigation (i.e., those taking best advantage of currents, winds and, if possible, nearby landmarks to better determine the ships' position) for each month of the year based on meteorological and oceanographic data observed by the Brazilian Navy from 1951 to 1972 [158]. We considered the month when the routes are closest to PARNAMAR-FN. The three identified routes are: Ponce and Colón – Cape of Good Hope (PC – CGH - November - going); Recife – Madeira Island (REC – MI - August – going and return); Recife – Cape Nouadhibou (REC – CN - March – going and return). To draw the routes, we determined three point of ship's positions on each route. We considered the first point as the one where the ship's crew see any landmark for the first time. To easily measure the distance between points on a route, we also considered that at the first waypoint the ship's odometer is zero. We calculate the ship courses for each waypoint, not only on going routes (CGH, REC - MI, REC - CN), but also on returning ones (REC - MI, REC - CN).

A Line of Position (LOP) is defined as the geometrical locus of all the positions that a ship can occupy, having made a certain observation, in a given moment [159]. A LOP can be originated from an alignment of two landmarks, a direction or distance to a landmark, and other methods out of the scope of this work. It is recommended the use of at least three LOPs of the same type or from different natures (e.g., one distance and two directions; one alignment, one distance and one direction) to reduce the uncertainty [159]. The LOP from an alignment is the most accurate one, so we use alignments when available.

We determine alignments, distances and directions of routes to the following landmarks: Pico's Hill (A); FN Lighthouse (B); São Pedro's Church (C); Antenna (D); Egg's Island (E); Pontinha (F). The courses and directions are the true ones, from 000º to 360º, measured clockwise from the true North [159].

The prevailing current at the region is to West, with a speed from 0.7 to 2.0 knots [158, 160]. This is the South Equatorial Current, i.e., a superficial warm oceanic current that flows continuously [161]. In accordance, more detailed studies [162] show that the current usually flows to direction between NNW and WSW, varying in speed up to 2 knots, occasionally exceeding this value.

Regarding winds, we register them based on Compass Rose on Pilot Charts for each month of the year [158]; we build a new Compass Rose for representing the distribution of winds throughout the entire year. Our Compass Rose indicates the frequency (%) per year of wind direction from the 8 octancts (N, NE, E, SE, S, SW, W, NW) and of dead wind, and the average wind strength. We verify that the prevailing winds are from directions E and SE, with average frequency of, respectively, 44% and 37%, and average force Beaufort 2 (i.e., wind speed between 4 and 6 knots [161]) for both. The third prevailing wind is from direction S, with average frequency of 14% and average force Beaufort 2. Thus, it is expected that winds of 4 to 6 knots from between E and S will be blowing 95% of the year.

The route with the minimum distance to PARNAMAR-FN is PC – CGH, with a distance of 4.96 nautical miles (nm). However, given the prevailing currents and winds, this route was considered an insignificant hazard. Any quantity of oil potentially spilled would probably be transported away from PARNAMAR-FN. The same applies to the route REC – MI.

REC – CN is considered a significant hazard. This route passes from south to east of the Island, for so, the oil potentially spilled on this route is likely to be transported to the coast by the prevailing winds and currents (Figure 5.2). Four basic ASs could occur on route REC – CN, i.e.: (i) a head-on parallel collision of two ships, (ii) an overtaking parallel collision, (iii) a crossing collision with another ship on route PC – CGH, (iv) fire/explosion.

Table 5.1. Route Ponce and Colón - Cape of Good Hope (November).

<table>
<tr><td colspan="2" rowspan="2"></td><td>Landmark</td><td>Pico's Hill (A)</td><td>FN Lighthouse (B)</td><td>São Pedro's Church (C)</td></tr>
<tr><td>Coordinates</td><td>32º 25' 18" W, 3º 50' 42" S</td><td>32º 27' 42.17" W, 3º 52' 31.264" S</td><td>32º 23' 55.753" W, 3º 49' 59.398" S</td></tr>
<tr><td rowspan="10">Route Ponce and Colón - Cape of Good Hope (November)</td><td></td><td>Minimum distance to PARNAMAR (nm)</td><td colspan="3">4.96</td></tr>
<tr><td rowspan="3">Odometer = 0</td><td>Ship course (degrees)</td><td colspan="3">130.6</td></tr>
<tr><td>Distance (nm)</td><td>Alignment between A – Antenna (D)</td><td>X</td><td>X</td></tr>
<tr><td>Directions (degrees)</td><td>X</td><td>104.6</td><td>93.31</td></tr>
<tr><td rowspan="3">Odometer = 10.56 nm</td><td>Ship course (degrees)</td><td colspan="3">129.3</td></tr>
<tr><td>Distance (nm)</td><td>X</td><td>6.214</td><td>Alignment between B – C</td></tr>
<tr><td>Directions (degrees)</td><td>55.12</td><td>X</td><td>X</td></tr>
<tr><td rowspan="3">Odometer = 21.49 nm</td><td>Ship course (degrees)</td><td colspan="3">130.93</td></tr>
<tr><td>Distance (nm)</td><td>X</td><td>11.08</td><td>X</td></tr>
<tr><td>Directions (degrees)</td><td>357.07</td><td>X</td><td>2.69</td></tr>
</table>

Table 5.2. Route Recife – Madeira Island (August).

		Landmark	**Pico's Hill (A)**	**FN Lighthouse (B)**	**São Pedro's Church (C)**
		Coordinates	32º 25' 18" W, 3º 50' 42" S	32º 27' 42.17" W, 3º 52' 31.264" S	32º 23' 55.753" W, 3º 49' 59.398" S
Route Recife – Madeira Island (August)		Minimum distance to PARNAMAR (nm)	16.38		
	Odometer = 0	Ship course (degrees)	21.32 (going) – 201.32 (return)		
		Distance (nm)	X	X	X
		Directions (degrees)	80.74	85.59	79.59
	Odometer = 5.70 nm	Ship course (degrees)	21.59 (going) – 201.59 (return)		
		Distance (nm)	Alignment between A - D	X	X
		Directions (degrees)	X	102.39	93.78
	Odometer = 11.63 nm	Ship course (degrees)	21.75 (going) – 201.75 (return)		
		Distance (nm)	X	X	X
		Directions (degrees)	111.46	116.64	109.41

Table 5.3. Route Recife – Cape Nouadhibou (March).

<table>
<tr><td colspan="2" rowspan="2"></td><td>Landmark</td><td>Pico’s Hill (A)</td><td>FN Lighthouse (B)</td><td>São Pedro’s Church (C)</td></tr>
<tr><td>Coordinates</td><td>32º 25' 18" W, 3º 50' 42" S</td><td>32º 27' 42.17" W, 3º 52' 31.264" S</td><td>32º 23' 55.753" W, 3º 49' 59.398" S</td></tr>
<tr><td rowspan="10">Route Recife – Cape Nouadhibou (March)</td><td></td><td>Minimum distance to PARNAMAR (nm)</td><td colspan="3">12.58 NM</td></tr>
<tr><td rowspan="3">Odometer = 0</td><td>Ship course (degrees)</td><td colspan="3">54.92 (going) – 234.92 (return)</td></tr>
<tr><td>Distance (nm)</td><td>X</td><td>X</td><td>X</td></tr>
<tr><td>Directions (degrees)</td><td>343.02</td><td>334.03</td><td>346.92</td></tr>
<tr><td rowspan="3">Odometer = 2.44 nm</td><td>Ship course (degrees)</td><td colspan="3">55.87 (going) – 235.87 (return)</td></tr>
<tr><td>Distance (nm)</td><td>Alignment between A - Ovo’s Island (E)</td><td>X</td><td>X</td></tr>
<tr><td>Directions (degrees)</td><td>X</td><td>327.79</td><td>343.29</td></tr>
<tr><td rowspan="3">Odometer = 5.04 nm</td><td>Ship course (degrees)</td><td colspan="3">54.16 (going) – 234.16 (return)</td></tr>
<tr><td>Distance (nm)</td><td>X</td><td>X</td><td>Alignment between C – Pontinha (F)</td></tr>
<tr><td>Directions (degrees)</td><td>330.19</td><td>320.14</td><td>X</td></tr>
</table>

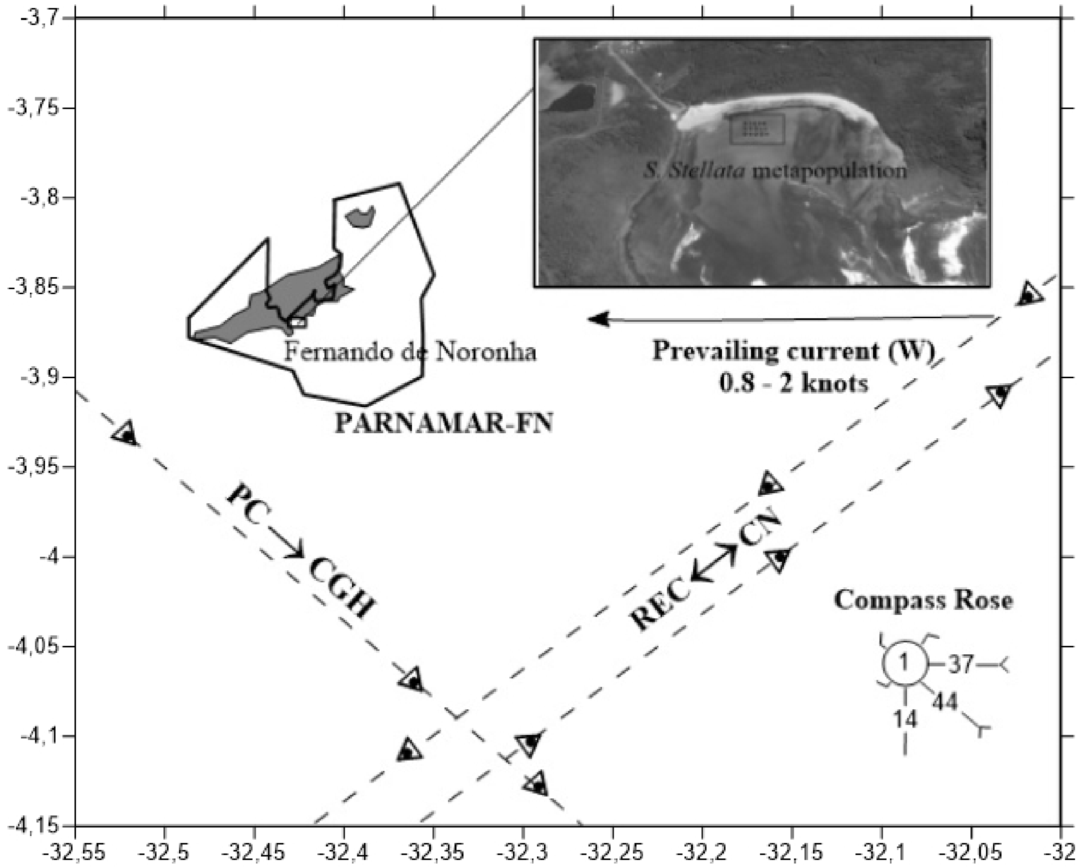

Figure 5.2 - Most hazardous route (REC - CN, going and return) and key coral reef metapopulation at Sueste Bay chosen as bioindicator of PARNAMAR-FN ecosystem's health.

The chances of occurring collision scenarios are likely to be very low, given the large lateral sea room that permits a great distance of ships from each other as well as a hard-over turn in an emergency to avoid collision. However, they are still possible to occur due to human error (e.g., crew communication failure, command failure, helmsman failure, nautical officer gives wrong order, no visual detection) [163, 164]. The overtaking potential collision should be treated with more caution, since the lower is the relative velocity between meeting ships, the more likely is that problems in ship control will occur [165].

Fire/explosions are possible to occur. According to historical records, these scenarios are less frequent than collision [166-171]. Grounding of ships is considered impossible to occur since the shallowest area (i.e., Alto-Fundo Drina on the PC-CGH route) has more than 50 meters depth.

Based on the previous discussion, we choose to model an *S.stellata* metapopulation at Sueste Bay (zoom in Figure 5.2) given that it is a significantly exposed location to potential oil spills on route REC – CN.

5.2.3 Frequency and Exposure Estimates

Li & Meng et al. [164] conducted an extensive review of eighty-seven quantitative risk assessment models for maritime waterways. Although none of them provided quantitative assessments of ecological consequences, models were proposed for estimating frequency of ASs such as head-on parallel collision, overtaking parallel collision, crossing collision, grounding, fire, and explosion. The estimated frequencies fall in the range from E-05 to E-04 per year. Most of these models consider a restricted narrow waterway, which is the utmost concern to the maritime authorities, due to its higher probability of accident when compared to wide-open sea areas (our case). Thus, it is expected that the application of such models to our case would result in frequencies lower than E-05 per year.

On the other hand, the International Maritime Organization (IMO) has reported historical accident frequency statistics for various types of ships world-wide covering the period form 1990s to 2007 [166-171]. The frequency of collision and fire/explosion for double hull oil tankers are, respectively, 8.60E-03 and 1.10E-03 per year. Also, a formal safety assessment with human reliability analysis that used fault trees to model the frequency of ship collision due to human error on another route (with more traffic than on REC-CN) gave results in the order of E-04 [163]. Therefore, we shall simulate very conservative scenarios with a frequency of occurrence not smaller than 1.00E-03 which is nearly the most conservative frequency estimate found in the literature (i.e., 1.10E-03 per year from the statistics by IMO).

Again, for efficient use of the available resources to perform the QERA, firstly exposure should be conservatively estimated. We base the exposure assessment on a very conservative point of view. If the ecorisks are negligible even with a very pessimistic consequence in case of accident, one has a reasonable basis to skip exposure modeling. Otherwise, a more detailed risk assessment is required.

5.2.4 Metapopulation Modeling

The variables, parameters and initial conditions of the metapopulation model are summarized in Table 5.4. To reduce the complexity of a continuous model, changes are considered to happen as discrete, equally spaced, events in time. This is applicable to species with seasonal behaviors. Our model’s time-step is one year, since corals are known to have an annual spawning period and most of their biological parameters are given in units of year [156, 172].

A coral's life cycle is made of two phases: larva and adult [119]. Keeping track of the abundance of larvae is not only troublesome but also ineffective. Our model is built considering the corals as having only one life phase (adult) for several reasons: a *S.stellata* individual generally spends 72 hours to 15 days in larval form [120], which is a small fraction of the one year time-step of our model; 90 to 99% of larvae die of natural causes before reaching the adult phase [121]; larvae are free swimming [156, 173, 174], so they do not add to our assessment endpoint, i.e., the area of colonies.

Adults live, on average, 10 years. The mortality and recruitment rates of the larvae are taken into account only as influencing the fecundity rate of the adults. This causes the mean number of the area of a colony i at the next time-step, $A_i(t+1)$, when in equilibrium (undisturbed reef), to depend solely on the area and growth rate at the present time-step, respectively ($A_i(t)$)) and ($R_i(t)$), as described by the equation:

$$A_i(t+1) = R_i(t) \times A_i(t) \tag{5.1}$$

The metapopulation model consists of 15 colonies distributed in 3 rows parallel to the coast (zoom in Figure 5.2). The initial area of the metapopulation is $\sum A_i(0) = 150\ cm^2$. The location and size of each colony were hypothetically defined by expert opinion. As literature data were given in terms of the radial growth [156], we interpreted the coral as a circle and calculated the mean growth rate for the area as a function of time, i.e., for all i:

$$R_i(t) = \frac{\pi \times r_i(t+1)^2}{\pi \times r_i(t)^2} \tag{5.2}$$

where $r_i(t) = r_i(0) + y \times t$.

Note that $R_i(t)$ decreases with time since corals allocate more energy to growth during early stages of life [173-178].

Table 5.4. Variables, parameters and initial conditions. The time-step is 1 year.

Variable	**Symbol**	**Description**		
Area of colony *i* at time t	$A_i(t)$	Population area at time *t*. $A_i(t) = \pi \times r_i(t)^2$		
Parameter	**Symbol**	**Description and data source**	**Value**	**Standard deviation**
Radius growth	y	The radius growth rate [156].	0.273 cm/year	0.035 cm/year
Radius of colony *i* at time t	$r_i(t)$	Colony radius at time t.	$r_i(t) = r_i(0) + y \times t$	
Growth rate of colony *i* at time *t*	$R_i(t)$	The area growth rate function	$Equation\ 2$	$Equation\ 3$
Carrying capacity	K	The maximum area of a colony (Barros and Pires 2006).	255 cm^2	
Half loss	HL	A threshold used to categorize risks (section 5.2.5).	$HL = 0.5 \times \sum A_i(0)$	$75\ cm^2$
Initial conditions			**Description**	**Value**
$A(0) = \{A_1(0); A_2(0); A_3(0); A_4(0); A_5(0); A_6(0); A_7(0); A_8(0); A_9(0); A_{10}(0); A_{11}(0); A_{12}(0); A_{13}(0); A_{14}(0); A_{15}(0)\}$			Set of the initial areas of each colony.	$A(0) = \{8; 4; 6; 7; 11; 10; 9; 5; 14; 12; 13; 11; 15; 20; 5\}$
$r(0) = \{r_1(0); r_2(0); r_3(0); r_4(0); r_5(0); r_6(0); r_7(0); r_8(0); r_9(0); r_{10}(0); r_{11}(0); r_{12}(0); r_{13}(0); r_{14}(0); r_{15}(0)\}$			Set of the initial radius of each colony.	$r(0) = \{1.60; 1.13; 1.38; 1.49; 1.87; 1.78; 1.69; 1.26; 2.11; 1.95; 2.03; 1.87; 2.18; 2.52; 1.26\}$

Uncertainty about the growth rate parameter is taken into account by calculating its standard deviation and considering that it is normally distributed. Indeed, according to the formula for the propagation of uncertainty [179], we have that:

$$\sigma_{R_i}(t) = \sqrt{\left(\frac{\partial R_i(t)}{\partial(\pi \times r_i(t+1)^2)}\right)^2 \times \left(\frac{\partial(\pi \times r_i(t+1)^2}{\partial r_i(t+1)}\sigma_r\right)^2 + \left(\frac{\partial R_i(t)}{\partial(\pi \times r_i(t)^2)}\right)^2 \times \left(\frac{\partial(\pi \times r_i(t)^2)}{\partial r_i(t)}\sigma_r\right)^2} \quad (5.3).$$

A recent study [156] collected data from 80 *S.stellata* colonies at Canudos reef (16°53.816'S; 039° 04.965'W), South of Bahia, Brazil, and it was considered to be the biggest colony found as an outlier, since it was 7.87 times bigger than the mean colony size and almost twice as big as the second biggest colony. We use the second biggest colony size as the carrying capacity parameter for our model (Table 5.4).

The simulations for each AS were made by the software RAMAS Metapop v. 6.0 [96], that is not a model itself, but a computational tool for stochastic simulation of a population model via Monte Carlo methods [180].

5.2.5 Ecological Risk Categories

As we show later in this paper, we believe that classifying ecorisks according to the International Union for the Conservation of Nature (IUCN) quantitative risk criteria [127] may be too optimistic. The IUCN categories are used to classify species affected by a whole range of environmental changes and human disturbance at regional [181] or global-level, but not to classify the risk caused by a single disturbance (potential oil spill) to a single population, which is our case. Thus, added to the ecorisks quantified in this QERA there will be other risks caused by other sources of disturbances (e.g., global warming, chronic pollution).

Therefore, we propose a classification system for the ecorisks quantified in this QERA such that the results can be better interpreted by risk managers, society, and other interested parties. This is accomplished by implementing some changes to the IUCN categories to adapt them to cases dealing with undesirable consequence of type "half loss" (HL) (i.e., 50% of the initial area killed) instead of "extinction"; and we also use additional risk instead of absolute risk. As it will be shown in the next section, the proposed categories are more conservative than the IUCN categories.

Thus, we propose the following risk categories: CRITICALLY ENDANGERED (CR): more than 50% additional probability of HL within 60 years (i.e., median time to HL is shorter than 100 years); ENDANGERED (EN): more than 20% additional probability of HL within 100 years; VULNERABLE (VU): more than 10% additional probability of HL within 100 years; NEGLIGIBLE (NE): less than 10% additional probability of HL within 5 generations.

5.3 Results and Discussion

5.3.1 Frequency Estimates

We assume frequencies for three ASs (Scn-1, Scn-2 and Scn-3) based on a very conservative point of view, i.e., respectively 0.001, 0.005 and 0.01 per year. These probabilities are thought to be pessimistic (conservative) based on the aforementioned model results and historical statistics in section 5.2.3.

5.3.2 Exposure Assessment

For all three ASs, we assume that an accident would cause the whole coral reef population to be exposed to 1% concentration of oil and kill 90% of the individuals. Exposure is a plausible, conservative assumption, since we consider the worst percentage of mortality observed for the considered species and for the most toxic type of oil. This assumption is based on the fact that dose-response studies between oil and corals are scarce. Shafir et al. (2007) employed a “nubbin assay” on more than 10,000 coral fragments to evaluate the long-term (after 50 days) effect of dispersed oil fractions on two coral species (*Stylophora pistillata* and *Pocillopora damicornis*). Out of the six tested dispersants in Shafir et al. (2007), we assume that the oil type considered in our analysis is similar to Dispolen, which is the most toxic to corals [182]. In their work, an exposure to 1% concentration of Dispolen dispersant, which is already a worst-case assumption, caused an average 47% of mortality on *Stylophora pistillata* and 90% on *P.damicornis*. We assume that *S.stellata* is more related to *P.damicornis*m, since the latter showed a greater rate of mortality than the *Stylophora pistillata*. Hence, we consider that *S.stellata* would have the same rate of mortality (90%) when exposed to 1% oil concentration.

5.3.3 Ecological Risks

Three ASs Scn-1, Scn-2, Scn-3 were introduced into the metapopulation model (section 5.2.4), resulting in a total of four ASs models (Table 5.5) with frequencies of occurrence and consequences as described in sections 5.3.1 and 5.3.2. For each model simulation, the AS was selected to occur (or not) every time-step according to its frequency of occurrence. If it occurs, it is assumed to kill 90% of each population in the metapopulation. All simulated scenarios had 10,000 replications. Figure 5.3 illustrates the simulation process of an ASs model for one replication.

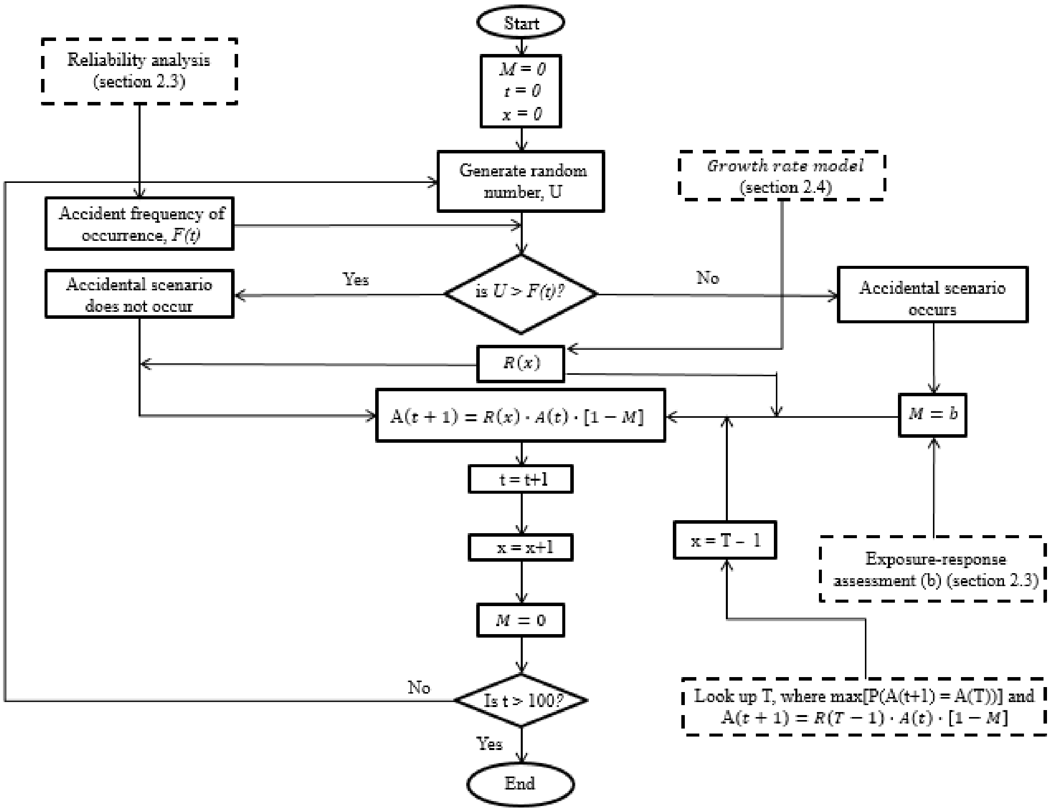

Figure 5.3 - Conceptual diagram that represents one replication out of 10,000 for stochastically simulating impact of potential ASs. Dashed boxes indicate specific studies.

The results for the coral average area over time and probability-consequence curves such as the interval quasi-extinction risk (i.e., the probability that the population abundance will fall below a certain level at least once in the next 100 years) are shown in Figure 5.4 and Figure 5.5, respectively. When compared to the benchmark Scn-0, the maximum added quasi-extinction risk caused by each AS (i.e., the maximum vertical difference between Scn-1, Scn-2, Scn3 curves and Scn-0 curve in Figure 5.5) are, respectively, 79.7%, 82.4% and 85.5%. These values are the Kolmogorov-Smirnov test statistic D (which is the maximum vertical difference) [96]. The location of the maximum difference (the threshold abundance at which the difference is maximum) is different for each scenario, i.e., respectively: 181, 179 and 177 cm².

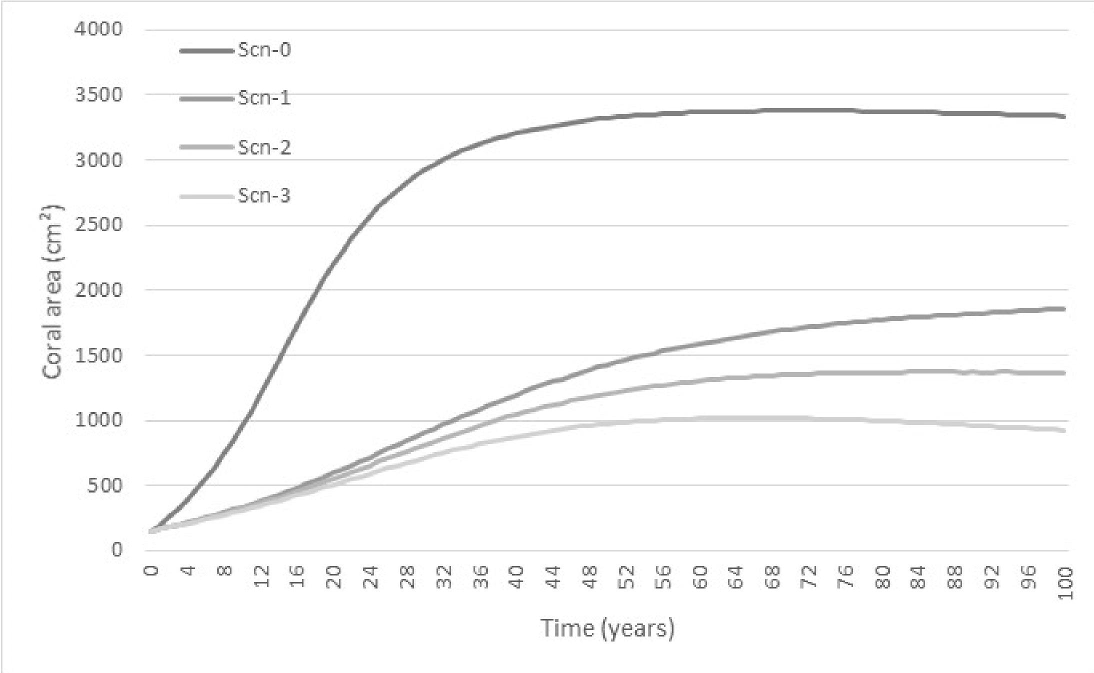

Figure 5.4 - Summary of the S.Stellata average metapopulation area as it changes over time for the benchmark scenario (Snc-0) compared to ASs (Scn-1, Scn-2, Scn-3).

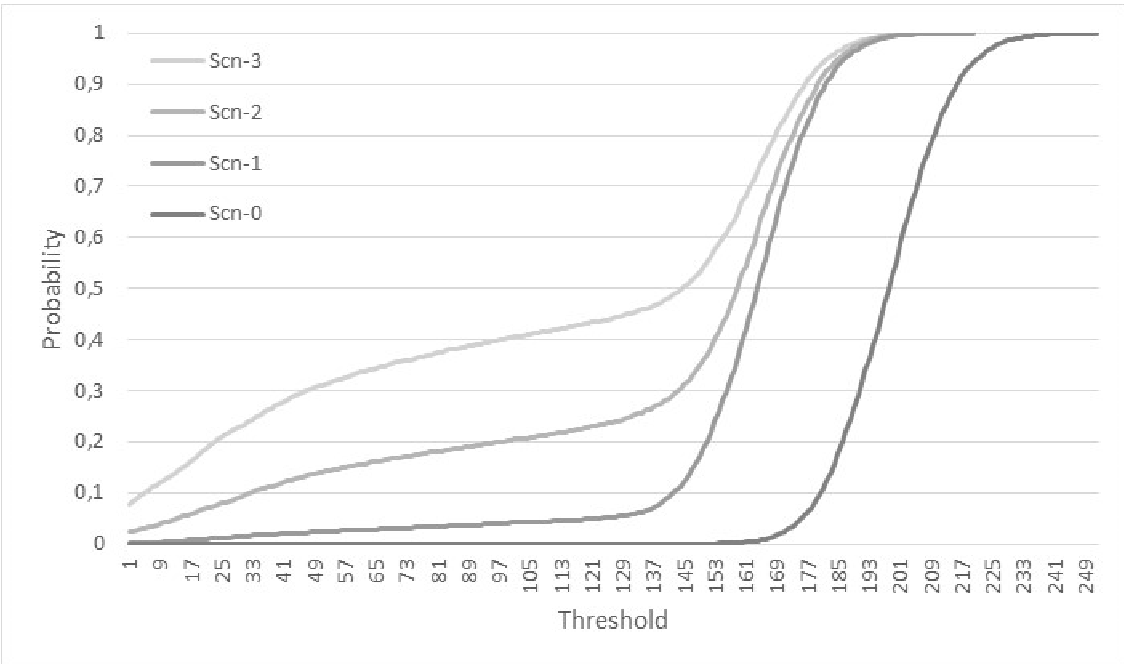

Figure 5.5 - S.Stellata metapopulation interval extinction risk. Each point in the curve can be interpreted as "there is a Y probability that, at least once during the next 100 years, the metapopulation abundance will be less than X".

Other relevant results are summarized in Table 5.5. Our model is probabilistic in nature, so risk results follow a non-parametric probability density function (PDF). We also provide the average value of the PDF in Table 5.5.

Table 5.5. ASs, their parameters and risk results to S.Stellata metapopulation. The parameter $F_j(t)$ is the frequency per year of each A; M_j is the mortality rate to all colonies in case of accident j. Values with a + or – symbol me mean that they are being compared to the benchmark Scn-0.

Accidental scenario parameters				
Scenario	Scn-0	Scn-1	Scn-2	Scn-3
$F_j(t)$	0	0.001	0.005¨	0.01
M_j	Not applicable	90%	90%	90%
Results				
Scenario	Scn-0	Scn-1	Scn-2	Scn-3
Risk of 20% population decline	0	+0.0491	+0.2304	+0.4333
Risk of population HL	0	+0.0317	+0.1751	+0.3642
Extinction risk	0	+0.002	+0.0227	+0.0765
Median time (years) to HL	>100	>100	>100	>100
Expected minimum abundance	198.5	-39.7	-62.5	-91.4
IUCN risk category	Negligible	Negligible	Negligible	Negligible
Proposed risk category (section 5.2.5)	Negligible	Negligible	Vulnerable	Endangered

5.3.4 Discussion

The no-accident scenario (Scn-0) shows significant stability in population behavior, with zero risk of extinction and HL. This indicates that any extinction risk estimated while analyzing the other scenarios is due solely to the added risk of potential oil spills.

Due to the considerable uncertainty in the results, we categorize risk using two different criteria: IUCN and our proposed criteria (section 5.2.5). The former is internationally accepted to classify species at risk [127] exposed to several stressors. However, it may be too optimistic to classify risks from a single stressor (as is the case in this work). The latter is more conservative since the undesirable consequence is HL instead of total extinction.

None of the three ASs caused the *S.stellata* metapopulation more than 10% probability of extinction in the next 100 years, which would have been enough to classify an AS as vulnerable according to the IUCN risk criteria [127]. This indicates that, according to the IUCN criteria, PARNAMAR-FN population of *Siderastrea stellata* is not exposed to significant risk due to potential oil spills on nearby ship routes.

Scn-2 and Scn-3 cause, respectively, additional 17.5% and 36.4% risk of HL. According to the proposed criteria, these scenarios are categorized as VU and EN, respectively. This indicates that the nearby ship route REC-CN causes untolerable risk to PARNAMAR-FN. Note, however, that the chosen probabilities of accidents were conservative, thus likely overestimating occurrences of oil spills on this route. Therefore, a more detailed QERA should be conducted before further taking preventive measures.

5.4 Conclusion

We have developed a QERA model for accidental oil spills on ship routes nearby the Fernando de Noronha marine national park in Brazil based on the methodology for QERA of industrial accidents proposed by [31]. Our methods are very conservative and make an interesting case for more conservative risk managers to utilize.

The parameterization of our model was based on considerable conservative estimates due to the lack of directly relevant data regarding: (i) the occurrence frequency of considered ASs, (ii) meteorological and oceanographic data to model oil fate and transport and (iii) dose-response data between oil and native coral species. Therefore, we believe that a full fledge QERA would likely provide reduced risks results for PARNAMAR-FN, given that more realistic ASs would likely be less conservative.

Most biological parameters involved in the QERA modeling and simulation were based on literature information from other locations and communication with local experts. Neither direct observation nor in situ data collection were conducted with *S.stellata* metapopulation at Sueste Bay, PARNAMAR-FN (Figure 5.2). This limitation has been circumvented at some degree for two reasons: (i) the effect of uncertainty on results has been bounded by making biological parameters vary within their range of plausibility; and (ii) the *Ceteris paribus* [28, 29] approach has minimized output errors originated from input errors in the chosen range of plausibility for biological assumptions. The latter has an important implication when interpreting results. Risk managers should know that we quantify the additional risk caused by a single stressor (i.e., potential oil spill), and not the absolute risk caused by a whole range of stressors (e.g., potential oil spill, noise of ships' propellers, tourism, fishing, diving/surfing, regular occurring exposure to oil and other toxics, global warming, navigation in restricted waters).

According to the IUCN risk categories, the risks are negligible. On the other hand, we have proposed more conservative risk categories to communicate risks, where the undesirable consequence is not 'total population extinction' as in IUCN categories, but 'half loss'. By using our categories, we conclude that the industrial activity under consideration causes the marine ecosystem of PARNAMAR-FN to be endangered; and a more detailed QERA is required, including:

- Collaboration of the Brazilian Navy to provide access to the database of the Maritime Monitoring System of Support to the Oil Activities (SIMMAP) [183].
- More data gathering about oceanographic and meteorological characteristics (i.e., other observed currents, sea surface temperature and salinity).
- In situ study of the *S.stellata* in PARNAMAR-FN (e.g., [156].
- Frequency modeling including human error. The accident frequency models for ships include estimates of the frequency of ship collision, grounding, fire, explosion and other accidents in a specific water area. Through a carefully constructed Bayesian network, historical data collected in different locations and expert judgment, a frequency model can incorporate human error, hardware failure, and other factors [163, 184-186].
- Fate and transport modeling to describe the space-time evolution of oil in case of accident (e.g., [31, 112, 187].

Finally, this work has secondary contributions such as:

- The preliminary hazard analysis may be useful to evaluate other ecorisks not caused by potential oil spills, but also related to the navigation of ships on the routes. For example, the noise of the propellers of passing ships may interfere in the breeding, feeding and rest of dolphins and other animals in PARNAMAR-FN [188]). Also, the suspected criminal action of vessels spilling small amounts of hydrocarbons in the coastal region when they clean their tanks (reported by local experts who have found pieces of oil sludge on beaches in PARNAMAR-FN) may be causing ecological adverse effects. The methodology and results in this chapter are potentially useful in supporting regulatory authorities such as Instituto Chico Mendes de Conservação da Biodiversidade – ICMBio in their preservation efforts of the marine ecosystem such as the prioritization of sources of hazard, and selection of the most cost-effective conservation measures for maintaining good environmental health on a realistic budget, using this model as an exploratory (not decision-making) tool.

6 QUANTITATIVE MICROBIAL RISK ASSESSMENT FOR SCHISTOSOMIASIS: THE CASE OF A PATCHY ENVIRONMENT IN THE COASTAL TROPICAL AREA OF NORTHEASTERN BRAZIL

This chapter was published as an original research article in the Journal of Risk Analysis [33].

This chapter describes the development of a stochastic model for QMRA for the *Schistosoma mansoni (SM)* parasite, which causes an endemic disease of public concern. The model provides answers in a useful format for public health decisions, uses data and expert opinion, and can be applied to any landscape where the snail *Biomphalaria glabrata* is the main intermediate host (South and Central America, the Caribbean, and Africa). It incorporates several realistic and case-specific features: stage-structured parasite populations, periodic praziquantel (PZQ) drug treatment for humans, density dependence, extreme events (prolonged rainfall), site-specific sanitation quality, environmental stochasticity, monthly rainfall variation, uncertainty in parameters, and spatial dynamics. We parameterize the model through a real-world application in the district of Porto de Galinhas (PG), one of the main touristic destinations in Brazil, where previous studies identified four parasite populations within the metapopulation. The results provide a good approximation of the dynamics of the system and are in agreement with our field observations, i.e., the lack of basic infrastructure (sanitation level and health programs) makes PG a suitable habitat for the persistence and growth of a parasite metapopulation. We quantify the risk of SM metapopulation explosion and quasi-extinction and the time to metapopulation explosion and quasi-extinction. We evaluate the sensitivity of the results under varying scenarios of future periodic PZQ treatment (based on the Brazilian Ministry of Health's plan) and sanitation quality. We conclude that the plan might be useful to slow SM metapopulation growth but not to control it. Additional investments in better sanitation are necessary.

6.1 Introduction

Schistosomiasis is a family of diseases caused by flatworms of the genus Schistosoma. It is possibly the most widespread public health problem in the world: there are approximately 200 million infected people worldwide [189] and more than 700 million people living in endemic areas [190]. *Schistosoma mansoni* (SM) is one of the three most common schistosomes and affects large geographical areas in several countries. Its prevalence is estimated to be 8-10 million people in Brazil alone, the northeast region being the most endemic area [191].

SM has the following simplified life cycle composed of four life-stages [192] (Figure 6.1): Adult parasites (male and female) live within humans (definitive host), and they breed and release eggs through human feces; viable eggs hatch and release miracidia into the aquatic environment; miracidia penetrate susceptible snails (i.e., those living in water) where they multiply in the form of sporocysts (snails are SM's intermediate host, usually the species *Biomphalaria glabrata*); sporocysts are released into the environment in the form of cercariae; and (5) cercariae penetrate the skin of exposed humans, migrate to internal veins, and mature into adult parasites.

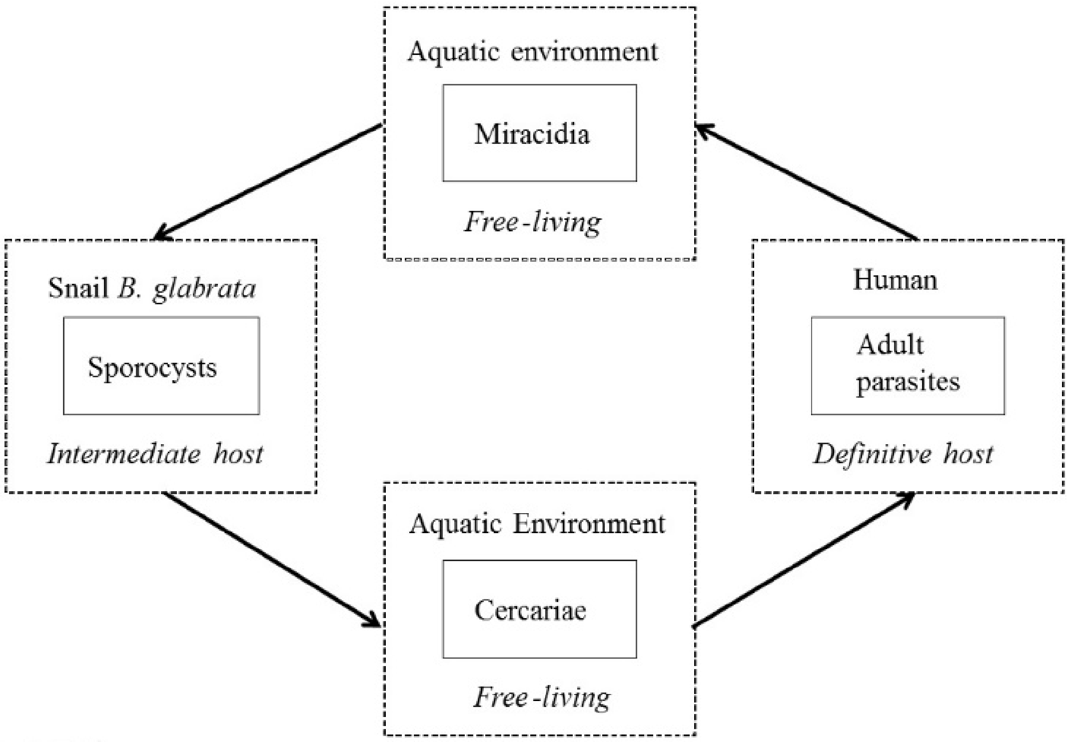

Figure 6.1 - Simplified schematic representation of the life cycle of SM.

Since 1975, when the schistosomiasis control program was implemented in Brazil, the main strategy to control this disease has been focused on treatment. Currently, the recommendation from the Brazilian Ministry of Health (BMH) is to treat cases using the drug Praziquantel (PZQ) to reduce the number of infected people and the parasite load [193]. An additional strategy to control this parasitosis is focused on sanitation because the lack of this environmental infrastructure is identified as a determinant for schistosomiasis as it permits fecal contamination of snail breeding sites [194].

Generally, to model an ecosystem, such as those involved in the transmission of SM, some simplifying assumptions are necessary. For example, traditional approaches for epidemiological modeling are based on deterministic models that often have the number of human hosts as the assessment endpoint and that use differential equations to describe the movement of individuals between states, such as susceptible, latent, infected and recovered [195]. Similarly, the most recent methods for schistosomiasis modeling also focus on evaluating the number of infected humans [149, 196-198]. To resolve these host-focused approaches, additional assumptions have to be made regarding both the resulting intricate indirect-cycle equations that model the dynamics of schistosomiasis (e.g., they assume that parasites are over-dispersed and have a negative binomial distribution among human hosts) and consequently the estimation of additional parameters (e.g., the clumping parameter related to the distribution of parasites). However, these methods do not employ a sensitivity analysis to evaluate changes in the results as a function of changes in the assumptions and parameters, nor is an uncertainty analysis conducted to measure the bounds of the results.

In this context, this chapter aims to develop an epidemiological model that overcomes the aforementioned drawbacks and that is tailored for Quantitative Risk Assessment (QRA) of *Schistosoma mansoni*. To the best of our knowledge, this is the first time that QRA has been used in a Brazilian context for schistosomiasis. In the proposed model, the important features of SM population dynamics are handled from a very different standpoint than from the abovementioned traditional assumptions. First, the proposed ecological model for schistosomiasis focuses on the parasite population abundance itself rather than taking the usual host-focused approach. This parasite-based approach was originally proposed by Milner-Gulland et al. [127] to examine the population dynamics of a tapeworm in Kazakhstan's desert areas and is adopted here for the following reasons: the results are sufficiently relevant for a QRA; it reduces the number of simplifying assumptions; it can more effectively address uncertain changes due to environmental factors (e.g., the incorporation of effects of rainfall variability); the impact of spatial heterogeneity may be evaluated in the dynamics of the transmission of parasites [127, 163, 164, 199, 200]; case-specific data becomes more tractable when focusing on single species; and parameter estimation becomes a simpler task in real case applications.

Secondly, the proposed model is probabilistic in nature and thus may be used to provide useful information to the decision-makers because it allows for the following: *i*) the assessment of uncertainty through the specification of lower and upper bounds on the results of interest; *ii*) modeling the behavior of SM living within a patchy environment, i.e., the dispersion of parasites among patches is considered to occur through infected snails that migrate from one patch to another, thus migration is stage-specific for sporocysts; and *iii*) it allows for quantification of the probability of extinction (i.e., zero individuals), quasi-extinction and explosion (i.e., abundance crosses a defined threshold) under scenarios regarding different control strategies, thus assessing their effectiveness in terms of the probability of undesirable and/or desirable events (i.e., risk). By using this approach, it is possible identify the most suitable patches where SM might be able to persist, and hence help to target public control strategies to reduce human infections in those areas.

Some regions in Brazil still have poor sanitation conditions [12], which contributes to both the persistence and growth of schistosomiasis. Recent findings from a spatial analysis [133] identified the district of Porto de Galinhas (PG) as a site where SM is a hazard of concern due to the considerable numbers of snail breeding sites and schistosomiasis cases that have been registered in the last ten years [133, 142]. PG is located in the southern coast of the state of Pernambuco, northeastern Brazil (Figure 6.2), at a distance of approximately 60 km from the state capital (Recife), and it is one of the most visited places by Brazilians and foreign tourists due to its beautiful beaches and warm sea. Despite the attractiveness of the site, a recent study [201] identified four critical patches for SM populations in PG (Figure 6.2), i.e., Merepe III (ME), Socó (SO), Pantanal (PA), and Salinas (SA). Sanitation quality is extremely low in these patches; most houses discharge their sewage to individual cesspits, whereas some houses simply dump their sewage outdoors without any treatment. The latter situation will be considered to characterize an important feature of the proposed model: the impact of sanitation level.

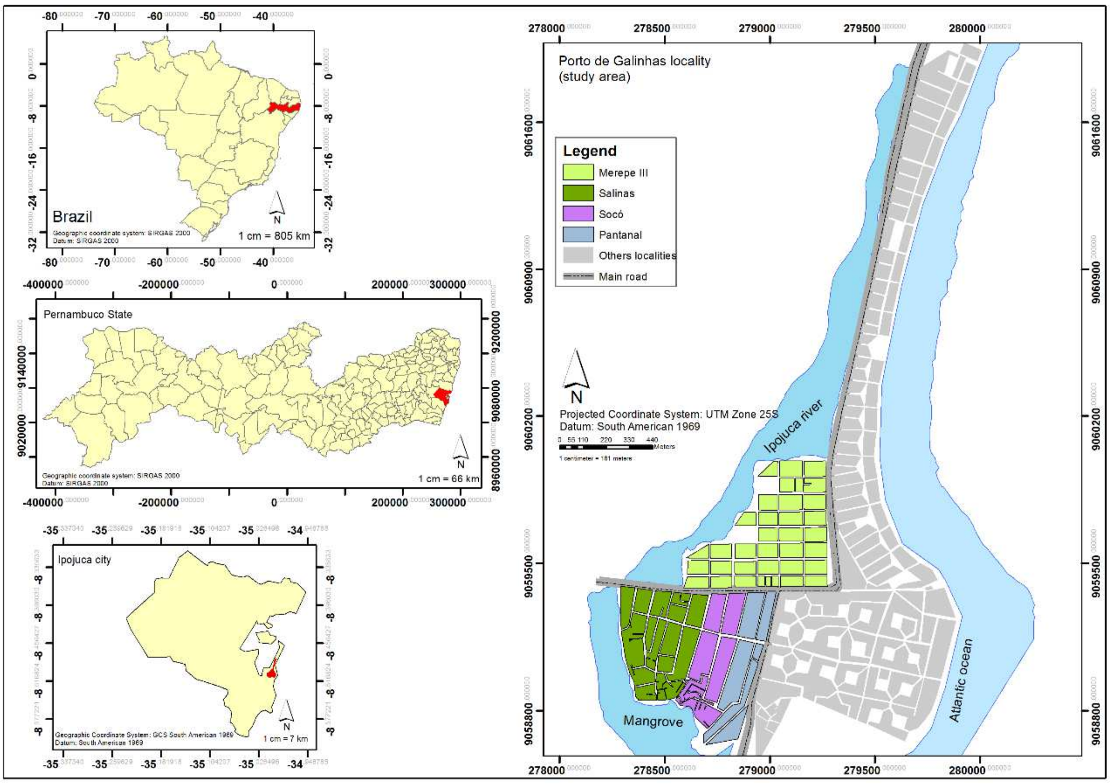

Figure 6.2 - Map of Porto de Galinhas, Pernambuco, Brazil, and its four critical patches for schistosomiasis [from the reference [201]*].*

To estimate the model parameters, field observations and data from the literature have been gathered to fulfill the requirements of the approach. However, due to the lack of published and empirical data to model the dynamics governing the transmission of schistosomiasis, educated guesses by experts have also been used. It will be shown that the outcomes of the approach provide a very good approximation of the dynamics of the case-specific system.

Regarding the public policies imposed to reduce the rates of *Schistosoma mansoni* infection, the BMH recently established quantitative criteria for taking actions against schistosomiasis [129], i.e., to treat only people with positive tests for SM in localities where the prevalence rate is less than 15%; to treat infected people and all of their cohabiters if the rate is between 15% and 25%; and to collectively treat the greatest number of individuals over the age of 5 if the rate is greater than 25%. These criteria will be used to construct different scenarios to evaluate BMH's policy against a do-nothing plan in the district of Porto de Galinhas-PE; the 5% and 25% prevalence limits are used to define the thresholds for metapopulation quasi-extinction and explosion, respectively. Thus, from this applied example, it will be shown that the proposed approach can provide useful answers for public health decision-makers responsible for endemic areas (e.g., municipalities, neighborhoods, districts, rural communities, farms, and villages) where the snail *Biomphalaria glabrata* is the main intermediate host (e.g., South and Central America, the Caribbean, and Africa).

6.2 The Model Structure

Although the proposed model structure is thought to be generic, it can be tailored to incorporate many realistic and case-specific features, such as i) the spatial structure of the specific SM metapopulation (i.e., the set of local populations of the same species in the same general geographic area with a potential for migration among one another [20]); ii) a stage-structured SM population; iii) periodic drug programs to treat humans; iv) density dependence (DD) (i.e., a change in the influence of any factor that affects population growth as the population density changes [8, 202]); v) rare events (e.g., periods of extreme rainfall or drought); and vi) site-specific sanitation quality.

Note that focusing on the parasite population does not mean that the snail's density and human exposure will be ignored. These features will implicitly be modeled to some extent by assuming that both the parasite carrying capacity and vital rates are stochastic and dependent on monthly variations in susceptible snail density, the probability of a cercaria finding a human to infect, the probability of untreated feces entering water ("water" is used here in the sense of a flooded area, usually puddles or ponds on the surface of a patch), and rainfall.

Therefore, we construct a model that is flexible in parameterization and that can predict the patch-specific population abundance of SM under the following conditions: monthly variations in human exposure, probability of untreated feces entering water and abundance of susceptible snails; periodic PZQ drug treatment in a certain percentage of infected humans; changes in patch-specific sanitation level; parasite migration among local populations; and stochasticity in parameters. All monthly variations in the parameters are proportional to a discrete, annually periodic function that describes rainfall, r_t.

The model describes a metapopulation composed of four populations in the patches ME, SO, PA and SA, with potential for migration from one patch to another. Each population is stage-structured by (1) miracidium (viable only), (2) sporocyst (sporocysts have three life-stages, but we only model the first because it is sufficient for our purposes), (3) cercaria, and (4) adult parasites. Migration is stage-specific for sporocysts. Let $N_s^i(t)$ denote the number of *s*-stage parasites in patch i at time t. The model projects the adult parasite abundance, $N_4^i(t)$, for all *i*, forward 240 months (20 years) from June 2011 (t = 0) until July 2031 (t = 240).

Because parasites occupy individual hosts, DD occurs at the intra-host level. We do not model DD in the definitive host, although we do in the intermediate host by making sporocyst abundance dependent on snail density. The DD type is Ceiling (i.e., exponential growth to the carrying capacity of population *i*, K_t^i [8, 202]), so that the maximum number of Sporocysts in population *i* at time-step *t+1* is K_{t+1}^i.

To model K_t^i, we proceed as follows. It is not important to count the exact number of sporocysts, $N_2^i(t)$, but only the number of cercariae that they produce per time-step. Neves [192] states that there is a significantly greater mass of SM tissue within snails infected with two miracidia when compared to snails infected with a single miracidium; however, no significant increase in SM tissue was observed within snails infected with increasing loads of miracidia (more than 2). Thus, we assume that cercarial production by a snail infected with a single miracidium is *x*, whereas that by two or more miracidia is *2x*, i.e., the asymptotic number of sporocysts per snail that makes a significant difference in cercarial productivity is 2. Then, K_t^i is assumed to be the product of the abundance of susceptible *B. glabrata* within patch *i*, S_t^i; the proportion of snails that are not refractory to SM, ρ; and the asymptotic number of Sporocysts per snail, 2; i.e., $K_t^i = 2 \cdot \rho \cdot S_t^i$.

The following algorithm represents one replication for stochastically simulating the metapopulation model. For each iteration, repeat the following steps for all *i*:

1) Project population-specific stage abundances:

$$\begin{bmatrix} N_1^i(t+1) \\ N''^i_2(t+1) \\ N_3^i(t+1) \\ N_4^i(t+1) \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & a_{14}^i(t+1) \\ a_{21} & a_{22} & 0 & 0 \\ 0 & a_{32} & 0 & 0 \\ 0 & 0 & a_{43}^i(t+1) & a_{44} \end{bmatrix} \begin{bmatrix} N_1^i(t) \\ N_2^i(t) \\ N_3^i(t) \\ N_4^i(t) \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 0 \\ \alpha_t \cdot N_4^i(t) \end{bmatrix}$$

2) Update projections of $N''^i_2(t+1)$ to account for DD: $N'^i_2(t+1) = \max\{N''^i_2(t+1), K_{t+1}^i\}$.

3) Update projections of $N'^i_2(t+1)$ to account for the migration of sporocysts by adding the number of immigrants and subtracting the number of emigrants for each population:

$$\begin{bmatrix} N_2^{ME}(t+1) \\ N_2^{SA}(t+1) \\ N_2^{SO}(t+1) \\ N_2^{PA}(t+1) \end{bmatrix} = \begin{bmatrix} N'^{ME}_2(t+1) \\ N'^{SA}_2(t+1) \\ N'^{SO}_2(t+1) \\ N'^{PA}_2(t+1) \end{bmatrix} + [M]_{4x4} \begin{bmatrix} N'^{ME}_2(t+1) \\ N'^{SA}_2(t+1) \\ N'^{SO}_2(t+1) \\ N'^{PA}_2(t+1) \end{bmatrix} - [M]^T_{4x4} \begin{bmatrix} N'^{ME}_2(t+1) \\ N'^{SA}_2(t+1) \\ N'^{SO}_2(t+1) \\ N'^{PA}_2(t+1) \end{bmatrix},$$

where a_{su} is the transition rate from stage u to s, α_t is the periodic mortality of adult parasites caused by PZQ, and $[M]_{4x4}$ is the migration matrix composed of the migration rates of sporocysts from patch j to patch i, m_{ij}. Most transition rates are random variables that are constant over time; therefore, a value is randomly selected for a replication and held constant for the entire 240 iterations of this replication, except for $a_{14}^i(t)$ and $a_{43}^i(t)$, which are non-parametric stochastic processes because they are both random and dependent on, respectively, the probability of untreated feces entering water and the probability of a cercaria finding a human to infect. These probabilities vary according to time-dependent rainfall.

The software RAMAS Metapop v.5.0 [46] is used for the simulations. This software is not a model itself but a computational tool for metapopulation model construction and probabilistic simulation via the Monte Carlo method [30].

6.3 QRA for schistosomiasis in PORTO DE GALINHAS

Ecological modeling has been used for chemical QRA [20, 203]. After a review of the methods for microbial QRA [130], we realized that an ecological model would also be useful to underpin the microbial QRA in this chapter. We subsequently used the model structure described in section 2 to conduct a QRA for SM through the following steps: problem characterization, consolidation of scenarios, exposure assessment, exposure-response assessment, model parameterization and initial conditions, and risk quantification and evaluation.

6.3.1 Problem characterization

The problem consists of quantitatively assessing the risks of SM to provide public health managers with objective answers about schistosomiasis dynamics in PG under several control strategies. To ensure that the results of this assessment would meet the needs of managers, we chose the adult parasite abundance within each population and within the entire metapopulation of PG as an assessment endpoint. We omitted the other life-stage abundances from the final results because the stage length is too short and public health managers are most interested in the number of infected humans, which can be estimated from the number of adult parasites.

This assessment is based on a probabilistic model that provides risk results as a probability distribution for assessment endpoints over time, with an average value, a 95% confidence interval, and lower and upper limits. This QRA is intended to be conservative in the sense of not underestimating risks.

The outputs of this QRA are as follows: time series of population and metapopulation abundance for 20 years; risk curves of extinction, quasi-extinction and explosion; time to metapopulation extinction, quasi-extinction and explosion; and a comparison of these results for all scenarios defined in the next section.

The Laboratory of Schistosomiasis, Aggeu Magalhães Research Centre-Fiocruz (CPqAM) provided the following empirical data: susceptible snail density per month in 36 breeding sites and their geographic coordinates, collected from July 2010 to June 2011 [201]; an epidemiological survey on the number of infected human individuals per patch in PG (i.e., ME = 14, SO = 96, PA = 40, and SA = 259) collected from a sample of 2757 people out of 5607 registered people, collected between August-December 2010 [201]; Figure 6.3, which was constructed based on field observations and defines the maximum flooded area in PG during the rainiest period of the year (June); and the proportion of residences within each patch that have no sewage collection system (SWCS) (i.e., feces are simply discharged outdoors), originating from a sanitary survey in 479 residences (53 in ME, 126 in SO, 64 in PA, and 236 in SA) in 2011 [16]. Data on monthly rainfall (mm) were also collected at the meteorological station of Ipojuca from 1956 to 2010, which were provided by the Meteorological Laboratory of Pernambuco (LAMEPE). Regional rainfall information (and variability) were also confirmed from Global Precipitation Analysis – the GPCP database [186]. The main sources of information used to understand SM ecology in PG were Neves [192] and personal communications with researchers at CPqAM who have extensive knowledge about the transmission dynamics of schistosomiasis. The literature and empirical data do not provide sufficient information to estimate all parameters governing the transmission dynamics of schistosomiasis. We estimated the missing parameters via educated guesses by CPqAM's experts (section 6.3.5).

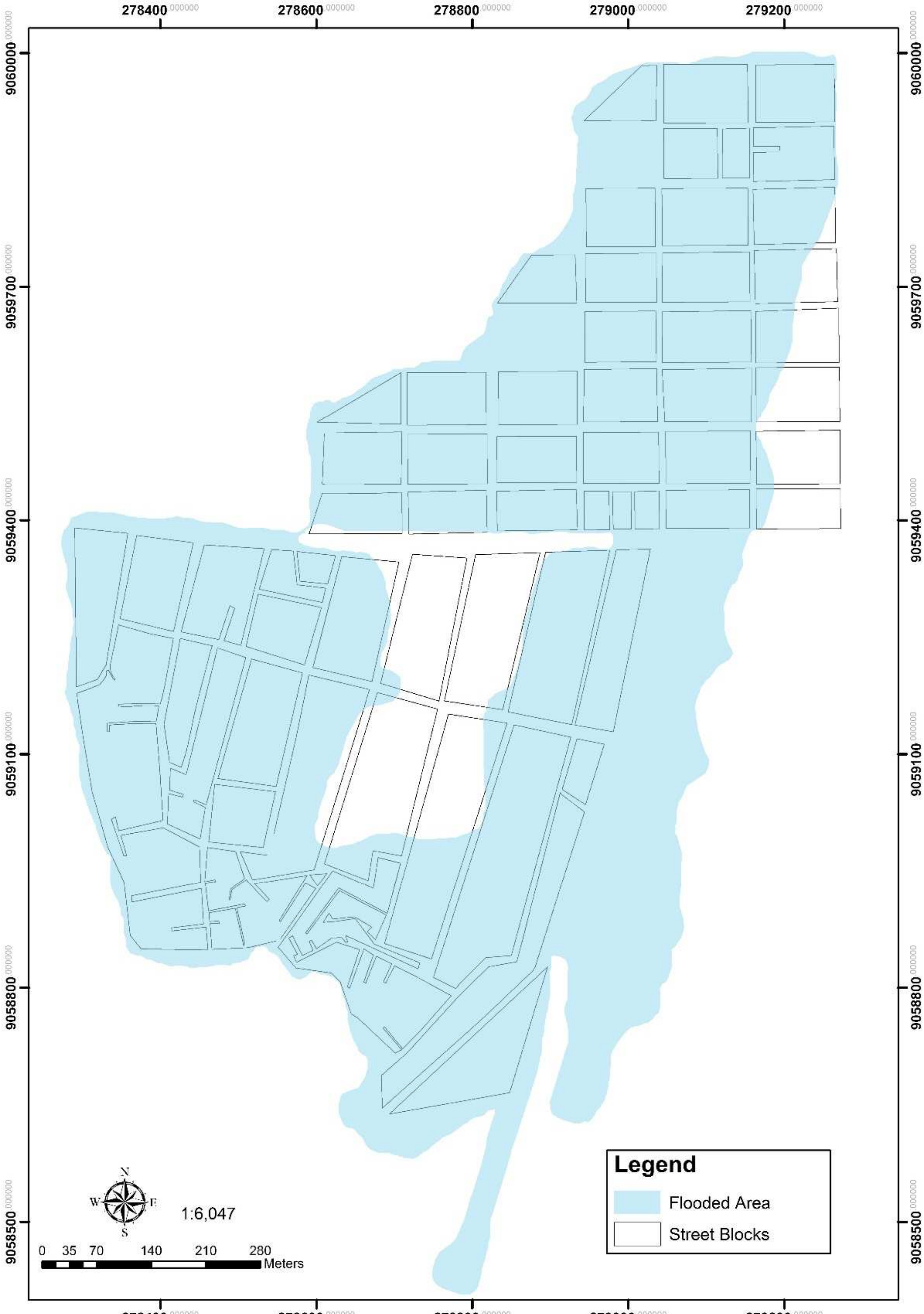

Figure 6.3 - Flooded area during the rainiest month (June) in PG.

6.3.2 Consolidation of scenarios

Our model does not attempt to be precisely predictive, only descriptive. It is quite intricate to predict/assess all the potential events (e.g., meteorological and environmental conditions, numerous control strategies, changes in sanitation quality, rare events) that might occur in the future and influence schistosomiasis transmission in PG. It is possible to construct several models based on scenarios under predefined conditions and compare them against a benchmark scenario such that we can evaluate changes in SM dynamics (and the reduced/added risk) caused by each predefined condition.

The benchmark scenario (Scn-0) is defined as follows.

- No PZQ drug treatment during the simulation period;
- The sanitation level (SL) for each patch in every month of the simulation is equal to 1 minus the proportion of residences with no SWCS in 2012, i.e., $SL_{ME} = 96.3\%$, $SL_{SO} = 94.5\%$, $SL_{PA} = 78.2\%$, $SL_{SA} = 92.8\%$.
- Susceptible snail density for each month of simulation period, $\mathrm{S}_{\mathrm{t}}^{\mathrm{i}}$, will be equal to the observed susceptible snails for each month between July 2010 and June 2011(Figure 6.4).
- Rainfall climatology was used in the simulations, meaning that monthly averaged quantities (1956-2010) were calculated for each month of the simulation period. We model a discrete annually periodic function, r_t, that represents the average rainfall in month *t* (see the rainfall line in Figure 6.5 and Figure 6.6).

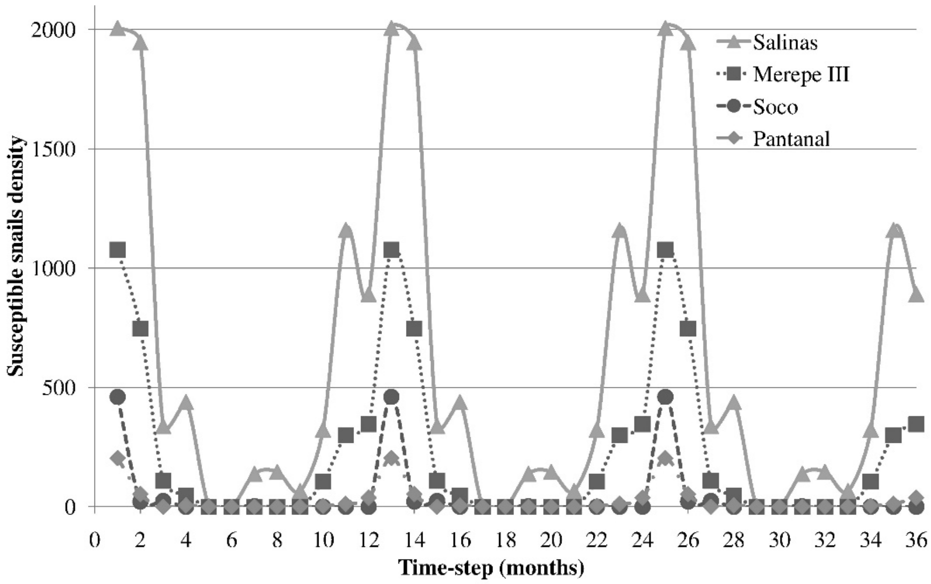

Figure 6.4 - Susceptible snails density (Y) as a function of time-step (X) for each patch i. Time-step 1 represents July/2011. The time-steps here goes until only 36 months for illustration purposes. The function keeps being annually periodic until the end of the simulation at time-step 240.

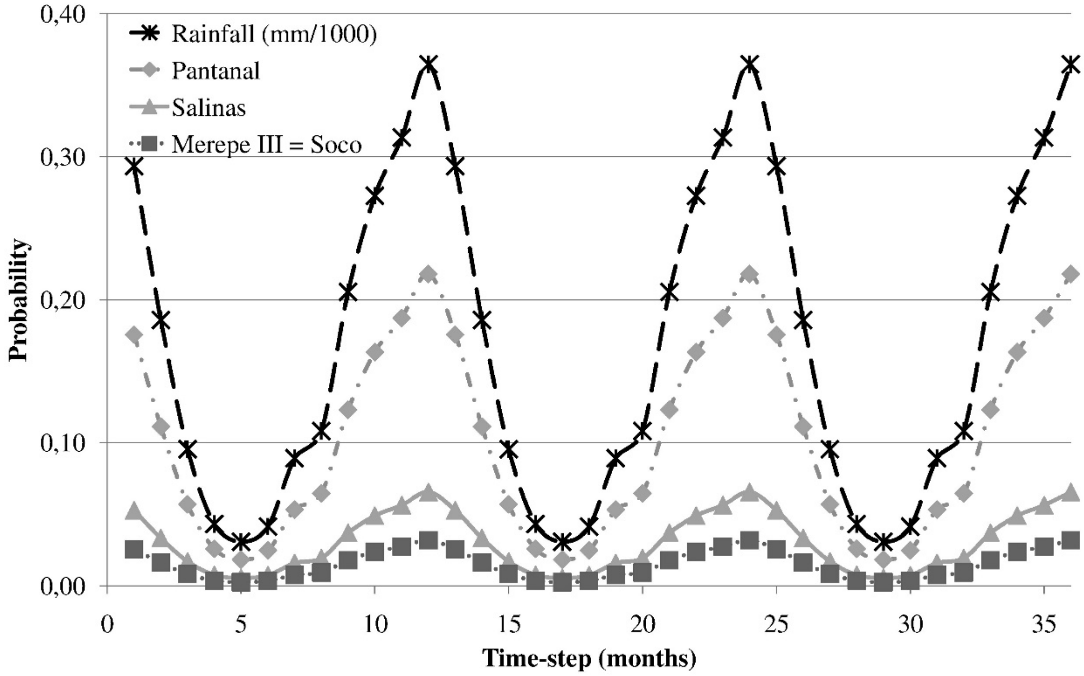

Figure 6.5 - Probability of untreated feces getting into water as a function of time-step, $p_{14}^{i}(t)$, for each patch i. Time-step 1 represents July/2011. The function is annually periodic until the end of the simulation at time-step 240. Here the average month rainfall was divided by 1000 to better illustrate its proportionality to $p_{14}^{i}(t)$.

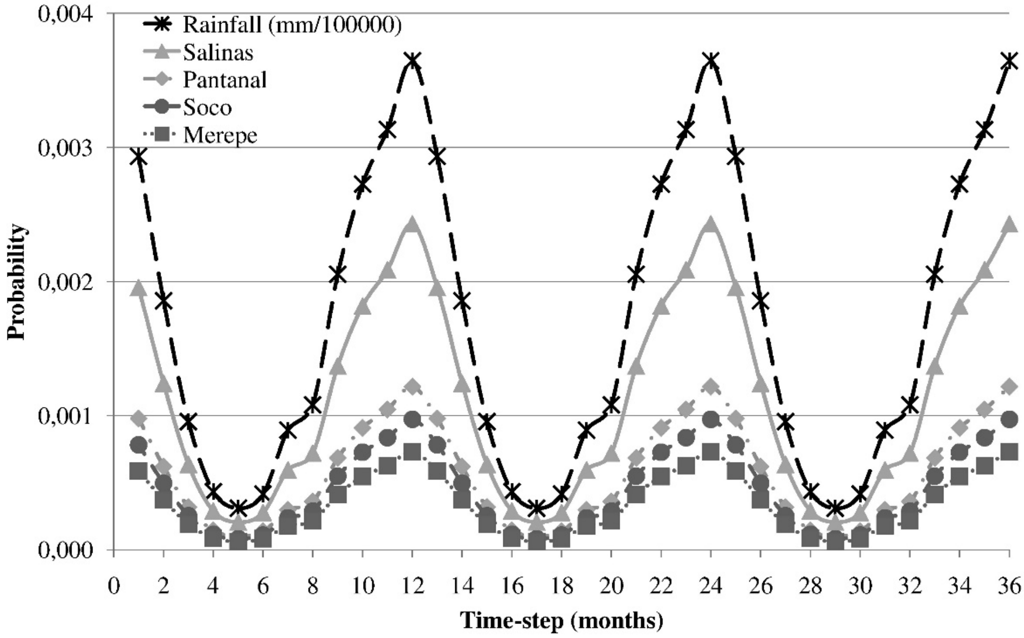

Figure 6.6 - Probability of a cercaria finding a human to infect as a function of time-step, $p_{43}^{i}(t)$,for each patch i. Time-step 1 represents July/2011. The function is annually periodic until the end of the simulation at time-step 240. Here the average month rainfall was divided by 100,000 to better illustrate its proportionality to $p_{43}^{i}(t)$.

To assess the efficiency of BMH's plan [129], we constructed two scenarios: pessimistic, in the sense of not underestimating risks; and optimistic, underestimating risks. The pessimistic PZQ scenario (Scn-1a) assumes that an effective dose of PZQ (i.e., 40-60 mg/kg, divided into two doses [131]) is periodically (every 5 years) given to 70% of infected humans if the prevalence rate is less than 15%, 90% if the rate is greater than 25%, and a linearly adjusted value (from 70% to 90%) as the rate changes from 15% to 25%; the first treatment is in May 2013, and the parasitological cure rate is 80% [131]; all other conditions remain equal to Scn-0. The optimistic PZQ scenario (Scn-1b) assumes that an effective dose is periodically (every 3.5 years) given to 80% of infected humans if the prevalence rate is less than 15%, 100% if the rate is greater than 25%, and a linearly adjusted value (from 80% to 100%) as the rate changes from 15% to 25%; the cure rate is 90% [131]; and the first treatment is in May 2013; all other conditions remain equal to Scn-0.

Using PZQ in 80%-100% of infected humans is an extremely optimistic (almost impossible) assumption because many infected people cannot be treated due to contraindications (pregnancy or impeditive diseases), absences or refusals. By making this assumption, we want to underestimate risks as much as possible and evaluate whether a perfect PZQ mass treatment would be adequate to control disease transmission.

6.3.3 Exposure assessment

6.3.3.1 Snail exposure to Miracidia

Susceptible snails are those living in water, meaning that they are exposed to miracidia throughout the entire month and every month (duration and frequency, respectively). The magnitude of exposure is characterized by the amount of miracidia in water, which is given by the number of miracidia at each time-step through the mathematical expressions in section 6.2. The production of viable miracidia by one adult parasite is calculated as the product of the number of eggs being excreted in the feces by a pair of adult parasites and the probability of feces entering surface water in which susceptible snails live, $\mathrm{p}_{14}^{\mathrm{i}}(\mathrm{t})$. The egg excretion rate has a value of 6000 (lower limit), 7500 (average) and 9000 (upper limit) eggs/month [192, 204]. The probability, $\mathrm{p}_{14}^{\mathrm{i}}(\mathrm{t})$, depends on SL_i and on the proportion of each patch's total area covered by surface water. To calculate an approximation for $\mathrm{p}_{14}^{\mathrm{i}}(\mathrm{t})$ and incorporate variations as a function of time and patch *i*, we proceed as follows.

The proportion of surface water area in each patch, P_i, is estimated by using the definition of SL_i in section 6.3.2, the drawing utilities of Microsoft PowerPoint and ArcMap 10.1 (see Figure 6.3). Field observations support the hypotheses that the flooding area is directly proportional to rainfall in all 4 patches and that no flooding occurs when there is no rainfall. We simply assume that the flooding area is linearly related to rainfall because a better model that relates these variables could not be made due to a lack of data (e.g., figures similar to Figure 6.3 for all months of the year). Because Figure 6.3 represents the maximum flooded area, which occurs in the rainiest month (i.e., June, or $t = 12k,\ \forall\ k\ \in positive\ integers, Z^+$), the probability $p_{14}^i(12k) = P_i \cdot (1 - SL_i)$. The probability of untreated feces entering water for each month in patch *i* is calculated as $p_{14}^i(t) = r_t \cdot p_{14}^i(12k)/r_{12}$, a discrete, annually periodic function with monthly fluctuations, i.e., $p_{14}^i(t) = p_{14}^i(t + 12k),\ \forall\ k\ \in Z^+$. Figure 6.5 illustrates these functions. Note that the maximum flooded area in Figure 6.3 is modeled as an annual event that occurs in June. In the other months of the year, the flooded area is smaller, in accordance with monthly rainfall.

6.3.3.2 Human exposure to cercariae

Humans are exposed to cercariae when a part of their body (frequently the feet) is in water. To quantify exposure, we use measures of both duration and magnitude. We consider the duration per time-step for each patch, E_t^i, as linearly related to the flooding area and to rainfall. Experts at CPqAM provided educated guesses about the duration of human exposure (hours/month) in the rainiest month (June) for the four patches, i.e., $E_{12k}^{ME} = 9, E_{12k}^{SO} = 12, E_{12k}^{PA} = 15, and\ E_{12k}^{SA} = 30$. The function r_t is used to estimate E_t^i for other months, i.e., $E_t^i = r_t \cdot E_{12k}^i / r_{12k}$, a discrete, annually periodic function.

The magnitude of human exposure, given by the number of cercariae at each time-step calculated through the equations in Section 6.2, depends on the production of cercariae by one sporocyst. Literature data provide the production of cercariae by one *B. glabrata* infected with a single miracidium, i.e., 160 (average) and 200 (high emissions) [146]. Because a single successful miracidium becomes a single sporocyst [192], we assume these values to be the same as the production of cercariae by one sporocyst. To incorporate DD effects, we assume that a susceptible snail can carry no more than 2 sporocysts (section 6.2).

6.3.4 Exposure-response assessment

6.3.4.1 Probability of a miracidium successfully infecting a susceptible snail

Miracidia are attracted by chemical cues produced by snails that disperse through the water [192]. We assume that they find a susceptible snail to infect at time-step *t* when they are in water that has susceptible snails. After miracidia find a *B. glabrata* snail, only approximately 30% are able to penetrate and develop, 30% penetrate but do not develop, and 40% are unable to penetrate [192]. We assume that the probability of a miracidium successfully infecting a susceptible snail is 0.3.

6.3.4.2 Probability of a cercaria successfully infecting a human

This parameter is calculated as the product of the probability of a cercaria finding a human to infect, $\mathrm{p}_{43}^{\mathrm{i}}(\mathrm{t})$, the probability that this individual is not immune, and the proportion of cercariae able to penetrate and develop in humans. An approximation to $\mathrm{p}_{43}^{\mathrm{i}}(\mathrm{t})$ is calculated as a function of the frequency per time-step in which a human is exposed ($E_t^i/month$) times the frequency per time-step in which cercariae are active (i.e., for 42 hours after released by a snail

[192]). Then, $\mathrm{p}_{43}^{\mathrm{i}}(\mathrm{t}) = \left(\mathrm{E}_{\mathrm{t}}^{\mathrm{i}}/720\right) \times (42/720)$, assuming that all months have 720 hours and that "human is exposed" and "cercaria is active" are independent events (Figure 6.6).The second and third parameters were provided by expert opinions as 90% and 80%, respectively. The probability of a cercaria successfully infecting a human is equal to $0.9 \times 0.8 \times p_{43}^{i}(t)$.

6.3.5 Model parameterization and initial conditions

Table 6.1 summarizes the model variables, parameters and initial conditions. Some studies from the literature have already estimated parameters governing the transmission dynamics of schistosomiasis, which we use in the proposed model: eggs/day excreted by a pair of adult parasites, time-span of cercarial production, and mean parasite load per human [204]; daily production of cercariae by *B. Glabrata* infected with a single miracidium [146]; and adult parasite lifetime, PZQ-induced death of adult parasites, asymptotic number of Sporocysts per snail, and proportion of viable Miracidia capable of penetrating and growing in *B. glabrata* [192]. On the other hand, the remaining requirements of the model were estimated via conservative educated opinions by experts at CPqAM.

Some parameters were estimated using a mean value and others using a lower limit, mean and upper limit ($\omega_L, \overline{\omega}, \omega_U$). To make the latter stochastic, we consider that they have a truncated normal distribution and that the error ($\max[\overline{\omega} - \omega_L, \omega_U - \overline{\omega}]$) corresponds to a 3σ interval; therefore, such parameters will be randomly selected to fall between their limits in 99,865% of replications. It is believed that one can make good use of a Gaussian approach in vital rates because there is a reasonable reason for random values not to be too far away from the average, i.e., there are biological limitations preventing very large deviations and natural forces of equilibrium bringing vital rates back to their average values [180]. For probabilistic simulation, the software converts the normal distribution of vital rates into a corresponding lognormal distribution. This conversion avoids bias resulting from truncation because $\omega \geq 0$ [202, 205].

With regard to migration, we make some assumptions to model it in a simplistic way. We assume that dispersal of adult parasites in humans is negligible; that migration among patches is stage-specific for sporocysts, which occurs through snails either actively migrating during dry months or being passively transported by tidal streams during rainy months; that snails migrate at the same rate upstream as that downstream; that snails migrate at the same rate in all months of the year (i.e., they migrate actively and passively at the same rate); and that migration barriers are not considered. Overall, we make the migration rates, m_{ij}, dependant on the distance between patches, D_{ij}. We calculate the coordinates of a central breeding point (x_i, y_i) of each patch, *i*, by weighting the x and y, (x_{ib}, y_{ib}), coordinates of each breeding site within *i* by its average number of infected snails per month, n_{ib}, where *b* is the breeding site within *i*(*b* = *1*,…,6 in ME; 1 in SO; 1,2 in PA; and 1,...,27 in SA [16]), i.e., $x_i = \sum_{all\ b} \frac{n_{ib} \times x_{ib}}{nr\ of\ sites\ in\ i}$, and $y_i = \sum_{all\ b} \frac{n_{ib} \times y_{ib}}{nr\ of\ sites\ in\ i}$. Then, $D_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$. We use these data to set a function for S_t^i (Figure 6.4), i.e., S_1^i = sum of observed susceptible snail abundance within patch *i* in July 2011, S_2^i = in August 2011, …,S_{12}^i = in June 2012. Then, S_t^i is made annually periodic, i.e., $S_t^i = S_{t+12k}^i,\ \forall\ k\ \in Z^+$.

Based on the number of infected individuals per patch in PG (section 6.3.1) and on the mean parasite load per human, we estimate the initial abundances of adult parasites, $N_4^i(0)$; the metapopulation explosion threshold, $N_{4,epl}$; and the metapopulation quasi-extinction threshold, $N_{4,ext}$(Table 6.1). The initial abundances of the remaining stages were set at 0 for all patches because field data about such values are scarce and very difficult to collect. Assuming such values is equivalent to making all the initial population abundances concentrated in the adult parasite stage, which is extremely unrealistic. We performed several simulations of Scn-0 to observe how much time is required until the proportion of individuals in each stage of each particular population reaches a more realistic distribution. We observed that at time-step 12, all populations reach approximately the following average distribution: 52.92% miracidia, 0.01% sporocysts, 45.95% cercariae, and 0,13% adult parasites. We use this distribution as the initial conditions and thus exclude the 12 initial time-steps from the risk calculations.

Table 6.1. Definition of variables and parameters. The discrete time-unit is one month.

Variable	**Symbol**	**Description**		
Number of adult parasites in patch *i* at time *t*.	$N_4^i(t)$	Assessment endpoint described as minimum, average and maximum values, with a 95% confidence interval.		
Average monthly rainfall	r_t	Annually periodic function modeled from data on the average monthly rainfall from 1956 to 2010		
Exposure duration and frequency in patch *i* at time *t*.	E_t^i	Annually periodic function dependent on $\mathrm{r_t}$ for human exposure (duration and frequency) in hours/month.		
Magnitude of snail exposure	$N_1^i(t)$	Number of Miracidia in patch *i* at time *t*, predicted as a minimum, average and maximum values, with a 95% confidence interval.		
Magnitude of human exposure	$N_3^i(t)$	Number of cercariae in patch *i* at time *t*, predicted as a minimum, average and maximum values, with a 95% confidence interval.		
Patch-specific sanitation level	SL_i	The proportion of houses that collect their sewage through individual cesspits or another system.		
Snail density at time-step *t* for patch *i*	S_t^i	Assumed equal to the observed susceptible snails for each month between July 2010 and June 2011 (Figure 6.4).		
Parameter	**Symbol**	**Assumptions** $(\omega_L, \overline{\omega}, \omega_U)$ (data source)	**Mean**	**σ**
Transition rate from Adult to Miracidium	$a_{14}^i(t)$	Eggs/month (6000, 7500, 9000)[204]. Probability of untreated feces getting into water, $\mathrm{p_{14}^i(t)}$ (Figure 6.5).	$6000 \cdot \mathrm{p_{14}^i(t)}$	$500 \cdot \sqrt{p_{14}^i(t)}$
Permanence rate from Adult to Adult	a_{44}	Adult life time (0, 5, 30 years) [192].	0.98	0.004
Transition rate from Miracidium to Sporocyst	a_{21}	Probability of a viable miracidium finding a snail *B. Glabrata* to infect (1,if $S_t^i > 0$; 0, if $S_t^i = 0$) [192]. Viable Miracidia capable of penetrating and growing in *B. Glabrata* (30%) [192].	0.3	

Parameter	**Symbol**	**Assumptions** $(\omega_L, \overline{\omega}, \omega_U)$ (data source)	**Mean**	**σ**
Transition rate from Sporocyst to Cercaria	a_{32}	Daily production of Cercariae by one *B. Glabrata* infected with a single Miracidium (70, 160, 200)[146].	4800	400
Permanence rate from Sporocyst to Sporocyst	a_{22}	Time-span (months) of cercarial production (1.17, 2.92, 4.67) [204].	0.66	0.043
Transition rate from Cercaria to Adult	$a_{43}^i(t)$	Human hosts immune to infection (90%) (from CPqAM). Probability of a Cercaria finding a human to infect, $p_{43}^i(t)$ (Figure 6.6). Cercariae capable of penetrating and developing in a human (0.8) (from CPqAM).	$0.72 \cdot p_{43}^i(t)$	
Carrying Capacity	K_t^i	Asymptotic number of Sporocysts per snail (2)[192]. Snail density at time-step t for patch i, S_t^i (Figure 6.4). Immune snails (10%) (from CPqAM).	$K_t^i = 2 \cdot 0{,}9 \cdot S_t^i$	
Migration rates of Sporocysts among patches	m_{ij}	Distance between patches, D_{ij} (from Geographic Information System).	$m_{ij} = \exp(-D_{ij}^{1/100})$	
Periodic PZQ drug treatment	α_t	Frequency at which PZQ is periodically given to infected humans (scenario). Proportion of infected humans that are treated (scenario). PZQ-induced death of Adult Parasites [192].	Varies according to scenario (see section 6.3.2)	
Mean parasite load per human	μ	Total number of individuals in a data set (597) [204]. Total number of parasites in the same data set (67908) [204].	114	
Metapopulation explosion threshold	$N_{4,exp}$	Prevalence rate upper threshold in human population (25%) [129]. Mean parasite load per human (114) [204]. Total of registered people in the four patches (5607) [201].	159799	

Parameter	**Symbol**	**Assumptions** $(\omega_L, \overline{\omega}, \omega_U)$ (data source)	**Mean**	**σ**
Metapopulation quasi-extinction threshold	$N_{4,ext}$	Prevalence rate lower threshold in human population (5%) [129].	31960	
Initial conditions	**Description**		**Mean**	**σ**
$N_4^{ME}(0)$	Initial abundance of Adult Parasites in Merepe III		798	
$N_4^{SA}(0)$	Initial abundance of Adult Parasites in Salinas.		14763	
$N_4^{SO}(0)$	Initial abundance of Adult Parasites in Socó.		5472	
$N_4^{PA}(0)$	Initial abundance of Adult Parasites in Pantanal.		2280	
$N_1^i(0), N_2^i(0), N_3^i(0)$	Initial abundance of the remaining stages for all patches.		0	

6.4 Results and Discussion

6.4.1 Risk quantification and evaluation

Here, we present the main risk results of each scenario and a comparison between each of the results and Scn-0. Table 6.2 shows the metapopulation structure at the final time-step of the Scn-0 simulation to identify the most suitable patches where an SM population might be able to grow. Indeed, Salinas is the most suitable patch for SM to grow and persist, followed by Soco, Pantanal and Merepe III. Patch-specific risk reduction actions would work best if they follow this order of priority.

Table 6.2. Metapopulation structure at final time-step.

Population	Min	-SD	Average	+SD	Max
Salinas	51,259	60,612	64,950	69,288	95,456
Soco	39,211	45,901	48,794	51,687	69,586
Pantanal	31,152	36,842	38,994	41,146	51,505
Merepe III	7,859	11,073	14,414	17,755	76,755

To evaluate the efficiency of drug treatment in disease control, one should examine Figure 6.7 and Figure 6.8, which illustrate a projection of SM metapopulation abundance in PG and time to explosion, respectively, i.e., a cumulative probability distribution for the time to exceed an average prevalence of 25% infected humans in PG. The points between Scn-1a and Scn-1b are a measure of uncertainty for BMH's action plan, which should be compared to Scn-0, which represents a do-nothing plan. According to Figure 6.7, it is useful for BMH's plan to maintain an abundance of approximately 30,000 and 140,000 immediately after and before treatment, respectively. Figure 6.8 shows that BMH's plan significantly reduces the time to explosion.

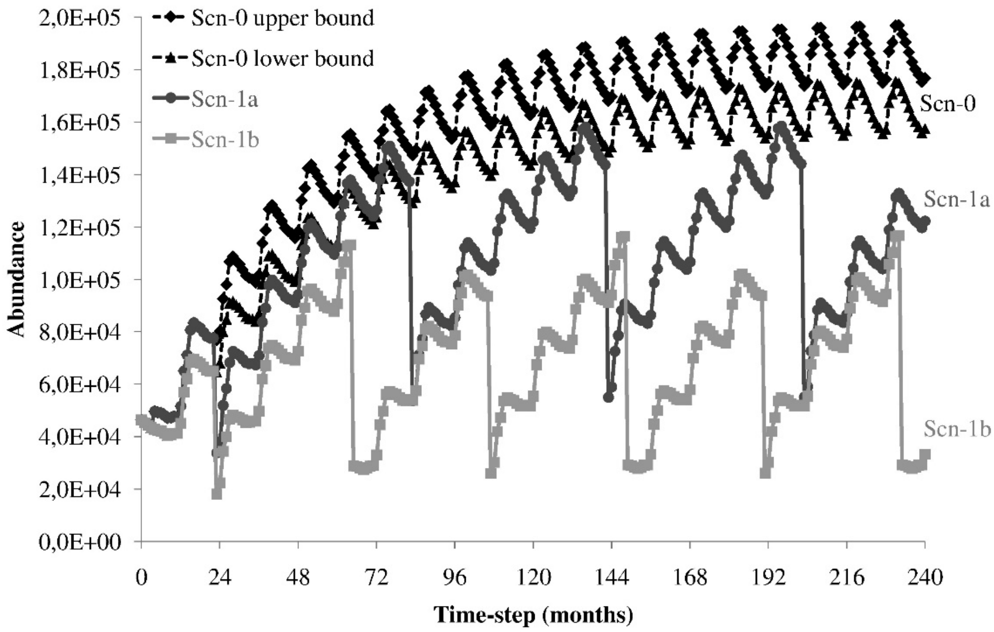

Figure 6.7 - Summary of the abundance of the metapopulation in Porto de Galinhas as it changes over time for the Brazilian Ministry of Health's plan (points between the pessimistic Scn-1a and the optimistic Scn-1b) compared to a do-nothing plan (Scn-0). The area between the dotted lines of Scn-0 represents a measure of uncertainty for a do-nothing plan. The area between the solid lines of Scn-1a and Scn-1b represents a measure of uncertainty for the Brazilian Ministry of Health's plan.

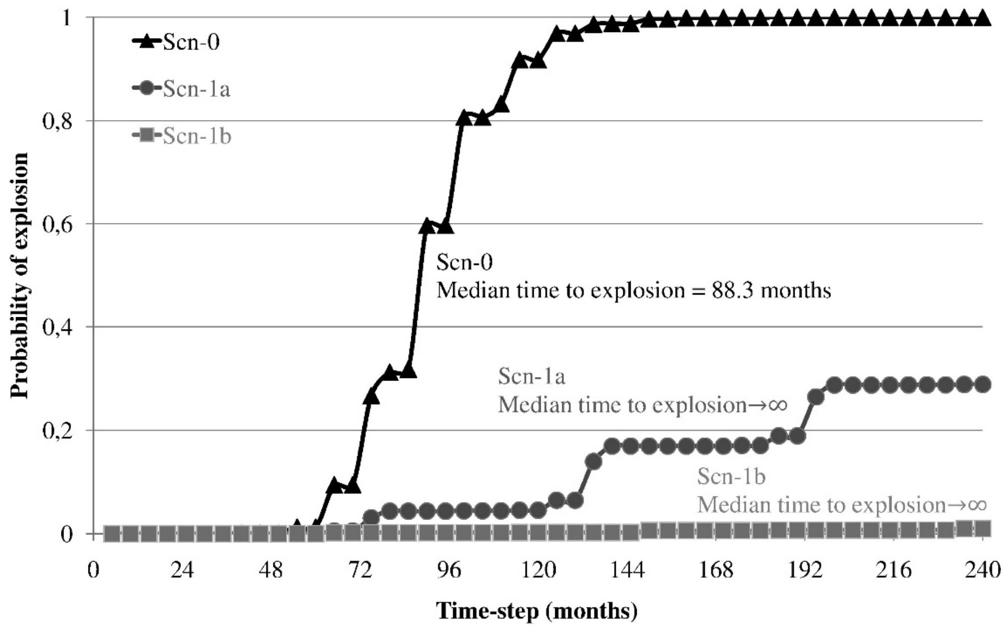

Figure 6.8 - Time to explosion, i.e., cumulative probability distribution for the time that the metapopulation size will exceed the explosion threshold (or 25% prevalence rate in PG). The average (solid lines) and 95% confidence interval (dotted lines) are all output for each scenario. Each point in the solid line of a scenario can be interpreted as "it is expected a Y probability that the metapopulation abundance will exceed 159,799 in or before the time-step X".

Other important results are as follows: Scn-1b causes the explosion risk (i.e., the probability that the prevalence rate will exceed 25% in or before 240 months) to be reduced by 96% when compared to a do-nothing plan; the metapopulation extinction risk is zero for all scenarios; and BMH's action plan alone (i.e., without improvements in SWCSs) is not useful to maintain the prevalence rate under 5%).

A sensitivity analysis of gradual decreases in the proportion of houses with no sewage collection ($1 - SL_i$, for all i) showed that partial improvements in SWCSs for all patches do not cause a significant difference in maintaining the prevalence under 5%, even when in combination with periodic PZQ treatment, i.e., the prevalence decreases below 5% after a mass treatment but rapidly increases again. Such improvements are only significant when fully implemented, i.e., all $SL_i = 100\%$. A simulation of a complete improvement in all SWSs showed that the prevalence would remain under 5% in and after 17.5 months (median time to metapopulation quasi-extinction), with no need for PZQ treatment, although the disease would not be extinct before 240 months. A simulation of a complete improvement in all SWCs integrated with periodic PZQ mass treatments showed that the disease would be completely eliminated between 231 and more than 240 months when considering the median time to metapopulation extinction for an optimistic and pessimistic view of BMH's plan, respectively. A simulation of a complete improvement in SWCs only in Salinas (most suitable patch), with all the SWCs in the other patches left as Scn-0, resulted in risk curves superimposed onto risk curves for Scn-0, showing that it is not efficient to focus limited resources on the most susceptible patch for controlling the metapopulation dynamics.

6.4.2 Discussion

The results show that BMH's plan is useful for significantly reducing the chances of a disease outbreak in PG, even from a pessimistic perspective. Nevertheless, BMH's plan is not useful for controlling SM persistence in the long-term, even from an optimistic perspective. BMH's plan [129] does not objectively state its aim with regard to schistosomiasis. Note that the plan may be efficient if the aim is to maintain the prevalence rate in PG under 6% in the optimistic scenario and 24% in the pessimistic scenario, even though this result does not consider PZQ side effects (nausea, epigastric pain, headache, dizziness, and drowsiness) that would hinder the widespread use of PZQ. If the aim is to maintain the prevalence under 5%, PZQ mass treatments are not useful, but a full improvement in SWCs alone would achieve this aim in approximately 1.5 year. Partial improvements in SWCs proved to be ineffective.

If the aim is to drive the SM metapopulation to total extinction (i.e., zero adult parasites), and thus eliminate schistosomiasis in PG, BMH's plan is equally as efficient as a do-nothing plan. Managers should thus evaluate integrated strategies. A complete improvement in all SWCs integrated with BMH's plan showed to be useful in eliminating schistosomiasis in PG, although this goal would require more than 19 years. We did not quantify the efficiency of other control strategies (vaccination, snail control) because they are still a challenge to science and seldom applied by public managers [192].

6.5 Conclusions

Our model does not attempt to be precisely predictive, only descriptive. It is a tool for describing the dynamics of the system under predefined conditions for the future (PZQ treatment plan, sanitation quality, meteorological conditions, and rare events), for evaluating the role of such conditions, and for producing meaningful conclusions that could be used to drive public health decisions. Hence, the model is useful for decisions under uncertainty, but a careful interpretation of the results is very important.

The output from the proposed model is consistent with the literature description of what occurred after a mass treatment of more than 3 million humans in endemic areas of northeastern Brazil: the prevalence rate is rapidly reduced, but after stopping treatment, it returns to the original value in a few years [192]. The model results are also consistent with our field observations in PG: Salinas is the most suitable patch for SM; drug treatment is not sufficient for eliminating the disease; and sanitation quality improvements are only useful when fully implemented.

Some changes in the model parameters make it applicable to any landscape where *B. glabrata* is the main intermediate host of SM. The data that are currently available were not adequate for completely parameterizing the model for PG. More extensive field surveys and laboratory experiments are required before some parameters can be estimated with more confidence. In particular, the migration rates were estimated based on many simplifications. Field studies are required for estimating more precise migration model parameters that consider the differences between upstream and downstream migration, time-dependent migration, and migration barriers.

The scenarios hold rainfall and sanitation at their initial levels for the entire 20-year projection. An improved rainfall model is being developed using support vector machines (such as those made for the prediction of sea surface temperature [172]) that considers annual shifts in rainfall. This improvement will make our model output for PG more realistic. Gradual shifts in the sanitation parameter are not realistic because real changes in sanitation would require the execution of a 1-year project that will construct water and sanitation facilities, budgeted at approximately 1 billion dollars [206]. If effectively executed, this project would rapidly improve sanitation levels in all four patches from almost 0% to 100%. According to our model output, this measure alone would decrease prevalence rate to less than 5% after approximately 19 months.

7 POPULATION DYNAMICS OF THE SHORTFIN MAKO SHARK IN THE SOUTH ATLANTIC OCEAN: A QUANTITATIVE ECOLOGICAL RISK ASSESSMENT UNDER SEVERAL HARVEST REGIMES

In the date of publication of this thesis, this chapter was being considered as an original research article for publication in the journal PLOS ONE.

Tunas and tuna-like species are an important food source, used mostly for canning and sashimi, and, due to their high economic value and extensive international trade, are an important global commodity. Most of the world's catches of sharks are taken incidentally by tuna fishing gear, constituting bycatch that increases the extinction risk of several species of shark. This not only alters ecosystem functions by removing top predators, but may also hinder the industry production itself due to cutoff measures set by international authorities (i.e., if a bycatch species population declines to less than 20% of its undisturbed abundance, fishing must stop). Thus, risk assessment of bycatch species is of major interest and relevance for both shark conservation and tuna industry production. This paper focusses on a very important bycatch species of worldwide tuna fisheries, i.e., shortfin mako shark. We propose and describe in details a stochastic model to simulate female population abundance of shortfin mako shark over the years under varying harvest regimes and control measures. The flexibility of the model makes it practicable to simulate hundreds of scenarios, pick the most relevant ones, analyze and compare their results (e.g., added risk of population extinction caused by a given harvest regime, median time to extinction, expected minimum biomass, risk of low harvest, risk reduction caused by control measure). This is useful as an aid for rational decisions under uncertainty. Furthermore, we propose risk categories (i.e., Negligible, Vulnerable, Endangered and Critically Endangered), which is useful for easier risk communication to interested parties. The proposed model can be applied to any shortfin mako shark population by changing initial conditions and harvest parameters. We present a case study with the South Atlantic population in order to validate the model and demonstrate that it achieves its intended purpose. The model has proven to be efficient for risk assessment and to drive management decisions for sustainable production.

7.1 Introduction

Fishes represent the only major food source still harvested from wild populations [207]. Tunas and tuna-like species (hereafter referred as tunas) are an important food source, used mostly for canning and sashimi, and, due to their high economic value and extensive international trade, are an important global commodity. The tuna industry is one of the most complex and highly dynamic of the world's seafood industries. Tuna fishing is undertaken by thousands of vessels in the Pacific, Indian and Atlantic oceans, using a range of gear types (e.g., longline) [208-211]. The export value of tuna products in 2004 was US$6.2 billion representing 8.7% of total global fish trade [209].

Most of the world's catches of sharks are taken incidentally by various types of tuna fishing gear, constituting bycatch that is either discarded at sea or landed for sale [212]. Bycatch increases the extinction risk of several species of shark, altering ecosystem functions by removing top predators [213]. In turn, bycatch also causes economical risk to the industry itself because of conservation limits set by the International Commission for the Conservation of Atlantic Tunas (ICCAT), i.e., a cutoff threshold for which fishing should stop, often set at 20% of the unfished equilibrium abundance of relevant species such as the mako shark [214]. In other words, if mako shark population declines more than 80% of its unfished equilibrium abundance, tunas' harvest must be forbidden.

This work aims at developing a stochastic model to evaluate shortfin mako shark (SMA) (*Isurus oxyrinchus*) population dynamics under harvest regimes and control measures for the future. This is useful for both the conservation of mako sharks and the sustainable management of tuna industry.

We focus on a shark species mainly because there has been increasing concern about the status of some shark stocks and the population-level effects caused by their exploitation [212, 213, 215-217]. More specifically, it focuses on the SMA for several reasons [215, 216, 218, 219]: (i) its relatively high abundance and presence in multiple and widespread fisheries; (ii) it is captured in great numbers in all oceans and ranks as one of the most dominant species caught in pelagic longlines and gillnets; (iii) it is considered an apex predator at the top of the marine environment food web; (iv) female SMAs are being caught below the size of maturity; (v) unlike most shark species, the SMA is economically important for both its quality of meat and fins; (vi) it is a valuable product of the pelagic longline swordfish and tuna fisheries; (vii) failures in conservation management of SMA can be significant and costly.

The proposed model considers only females because they are the most relevant to avoid extinction. Females are the one who produce new individuals and keep the life cycle on. An extreme example to explain this is a population of 1 million SMAs composed by too few females and most males. An assessment of the whole population size would say SMA are not under risk of extinction, but an assessment of female population size would say otherwise. Thus, keeping track of females is more effective to evaluate quasi-extinction risk. Furthermore, most available data is given for females only, probably because of the same aforementioned reason. Hereafter, "population", if not specified, refers to "female population".

We propose a model that describes the SMA female abundance for the next 100 years under varying conditions, i.e.: (i) a benchmark scenario (Scn-0) that simulates the natural population dynamics under no harvest and causes background risks; (ii) varying harvest scenarios with different harvest parameters and (iii) harvest scenarios with and without a cutoff threshold for which not harvest occurs if abundance falls below it.

By keeping all other parameters the same (*Ceteris paribus [28, 29]*) as in Scn-0 and varying parameters related to harvest, we aim at assessing the added/reduced ecorisk (i.e., "the probability that ecological adverse effects may occur or are occurring as a result of exposure to one or more stressors" [2, 220]) caused by each harvest scenario. Likewise, by keeping all other parameters the same and varying the cutoff threshold, we aim to assess the reduced ecorisk caused by this threshold that is, in fact, a control measure to satisfy conservation objectives.

In this way, our model is a tool for describing the dynamics of the system under varying conditions for the future (harvest regime and cutoff measure), for evaluating the role of such conditions, and for producing meaningful conclusions that can be used to drive management decisions. The model is thought to be generic, so that it can be applied to any SMA population (e.g., South Atlantic, North Atlantic, North Pacific) by making minor changes in parameters and initial conditions. We conduct a case study with the SMA South Atlantic population and evaluate extinction risk and yield associated with alternative decisions about harvest rates and cutoff threshold. Therefore, the results provided by the simulation of scenarios in the model are:

- probability distribution functions (PDFs) for the proportion of abundance decline within 100 years;

- cumulative distribution functions (CDFs) for the time to quasi-extinction (i.e., 80% population decline) within 100 years;
- point estimates originated from either the PDFs or CDFs, i.e.:
  - year-specific risk of quasi-extinction (i.e., probability of 80% abundance decline);
  - median time to quasi-extinction;
  - expected minimum abundance (i.e., an estimate of the smallest population size that is expected to occur within 100 years).;
  - expected total harvest weight at the end of simulation;
  - and year-specific risk of low harvest (i.e., the probability that the annual harvest will be at or below a threshold measure).
- risk categories and ranking of scenarios for better risk communication to stakeholders;
- reduced risk caused by control measures;
- suggested harvest regime that not only reduces conservation concerns but also achieves maximal benefits by increasing yield over the long term at tolerable risk of low harvest.

The paper is organized as follows. First, we provide a brief review. Second, we propose a model structure to describe the dynamics of the system in any ocean. Third, we parameterize the proposed model and conduct a study case in the South Atlantic, explaining every parameter assumption subsection by subsection. Next, we describe the results and their interpretation. Finally, we conclude the work by presenting the model benefits and shortcomings.

7.1.1 Literature review and an overview of the proposed model

An ecological model is a mathematical expression that can be used to describe ecological processes or endpoints such as population abundance (or density), community species richness, productivity, or distributions of organisms. Ecological modelling can be conducted at all levels within the biological hierarchy (molecule, cell, tissue, organ, individual organism, population, metapopulation, community, ecosystem and landscape). On the one hand, models at individual and lower levels have low ecological relevance and may provide ambiguous results. On the other, models at community and higher levels are too complex for structuring and parameterization in real-world case studies. In this sense, recent research has shown that population-level ecological models achieve the best trade-off between ecological relevance and tractability [20, 22, 27, 32, 33, 153].

First, our model is classified as a population model, i.e., a classification of ecological models, in which mathematical expressions are used to describe the dynamics of a population through population-level endpoints (e.g., abundance) so that one can estimate the risk of adverse effects (e.g., extinction, quasi-extinction) on a population caused by control variables such as industrial activity, toxic accidents, harvesting, management, recovery measures, pesticide use and predatory tourism [8, 20, 22, 27, 31-33, 220-222].

Second, our model is stochastic, since parameters are set as random variables to account for deviations around a central value over time due to: environmental variation, low-frequency events, measurement error and uncertainty. This is based on the following rationale. Harvesting generally accelerates the process of extinction, and an adequate approach, including not only studies of ecology and population status, but also stochasticity and uncertainty, is needed to improve the management of exploited species [223]. Fisheries management and conservation need to include uncertainty in the decision-making process [224].

Third, we consider the effect of model uncertainty not only by using random variables for parameters, but also by making conservative assumptions for uncertain parameters and uncertain initial conditions due to insufficient information; this is suggested by [225]. In accordance, we believe that it is better to be conservative and have the confidence that risks are overestimated than ignoring the unknowns (or to make assumptions based on the most probable estimate) and give a chance for risk results to be underestimated. Thus, we give answers that may error on the high (and, therefore conservative) side. Prevention is better than cure and lot cheaper.

Finally, our model also integrates extreme events, since it accelerates the process of extinction and then should be considered for a conservative assessment. Most population models often ignore the potential occurrence of low probability, high-consequence events (i.e., events, which cannot be easily predicted because of the paucity of data about it; one about which we have to wait too long to collect case-specific data, e.g., overwintering, contemporary warming, cyclones, tornados). Such events may have severe consequences, albeit they are much less likely to occur. However, they do happen at some point in the long-term, so that any attempt to assess accurately long-term ecorisks should consider their potential occurrence. Recent research efforts have shown the importance and feasibility of including improbable large events in model-based ecological risk assessments [31-33, 146].

Regarding similar models in the literature, even though the SMA is physiologically unique, economically important, and exploited in relatively large numbers [218], there are few population models for this species [215, 216]. These aimed at diagnosing the population status over the last 30 years by quantifying measures such as past and current biomass, abundance, and trend in abundance. Conversely, we aim to describe the population dynamics under varying scenarios from the present to the future so that it can be a useful tool for rational decisions under uncertainty.

There are some applications of marine fish stochastic population models for risk assessment [10, 11, 13, 31] that also look to the future, i.e., the modeling aim is to describe the population dynamics under predefined conditions from the present to the future whereas past data are used only for estimating the model parameters and initial conditions. They include stochasticity in parameters and results are given in terms of probability as a measure of uncertainty. To our best knowledge, there is no such modeling applied to shark populations.

Yet, our modelling approach is similar to the two models of herring [10, 13] in the following aspects: it evaluates the extinction risks caused by harvest; includes stochasticity and uncertainty in parameters; has the flexibility to include a cutoff measure; and includes unfrequent events that may cause recruitment failure (i.e., when stage-0 individuals have poor survival due to hypothetical events such as pollution, construction or any human impact in breeding areas on the coast; or environmentally induced recruitment failure such as hurricanes, earthquakes, tsunamis). The exact cause of recruitment failure remains a mystery and there is no research about its effects in SMA, but we suspect that recruitment failure may also occur with SMA as happens with other marine fishes [13, 226]. This is speculative and may overestimate risks, but we prefer to conservatively consider the unknowns than ignore them [94].

Our approach is different in the following aspects: (i) the proposed model describes a population of a shark species, which is the utmost difference because sharks and herrings have remarkably different life histories; (ii) it models females only; (iii) it measures uncertainty about the future harvest regime through a plausible range of scenarios; (iv) it evaluates the risk caused by conservative scenarios of harvest regime [218].

7.2 The proposed model

The equations in the algorithm below constitute a generic model for SMA female abundance that can be parameterized to describe the dynamics of the system in any ocean. Although the proposed model structure is thought to be generic, it can be tailored to incorporate many realistic and case-specific features such as: (i) a stage-structured SMA population (pups, juveniles, mature adults, and post-reproductive adults); (ii) stage-specific initial abundance; (iii) stochasticity and uncertainty in parameters such as survival and fecundity; (iv) density dependence (DD) (i.e., a change in the influence of any factor that affects population growth as the population density changes [8, 27]; (v) unfrequent events that may cause recruitment failure; (vi) stage-specific annual harvest as a proportion of the stage-specific abundance; and (vii) cutoff threshold for which no harvest occurs if abundance is below it. Table 7.1 summarizes the model variables, parameters and initial conditions. The estimate of values for parameters and initial conditions will explained in later sections. For now, it is sufficient for the reader to understand the first and second columns in Table 7.1.

Table 7.1. Definition of variables and parameters. The discrete time unit is 1 year.

Variable	**Symbol**	**Description**			
Number of female SMA at time t	$N(t)$	Assessment endpoint. Population abundance at time t. The sum of the number of females in all stages. It is described as minimum, average and maximum values with a 95% confidence interval.			

Number of female SMA in stage 0 at time *t*	$N_0(t)$	Abundance of female SMA pups. It is described as minimum, average and maximum values with a 95% confidence interval.			
Number of female SMA in stage 1 at time *t*	$N_1(t)$	Abundance of female SMA juveniles. It is described as minimum, average and maximum values with a 95% confidence interval.			
Number of female SMA in stage 2 at time *t*	$N_2(t)$	Abundance of female SMA mature adults. It is described as minimum, average and maximum values with a 95% confidence interval.			
Number of female SMA in stage 3 at time *t*	$N_3(t)$	Abundance of female SMA post-reproductive adults. It is described as minimum, average and maximum values with a 95% confidence interval.			
Parameter	**Symbol**	**Assumptions** $(\boldsymbol{\omega_L}, \boldsymbol{\bar{\omega}}, \boldsymbol{\omega_U})$ **(derived from)**	**Mean**	**Max and/or Min**	**SD**
Transition rate from stage 0 to stage 1 (per year)	a_{10}	Survival of age 0 class (0.87) [215]	0.87		NIL

Permanence rate in stage 1 (per year)	p_1	Annual survival rate for age 1+ (i.e., 1 year or more) is in the range of 0.78-0.97 [215], thus we assume mean = 0.875. Median (50%) age at maturity for females is in the range of 19-21 years [227], thus we assume mean = 20 years.	= 0.875*(20-1)/20 = 0.831	Max = 0.97*(21 - 1)/21 = 0.924; Min = 0.78*(19 -1)/19 = 0.739	= (0.924 – 0.739)/6 = 0.031
Transition rate from stage 1 to stage 2 (per year)	a_{21}	Annual survival rate for age 1+ is in the range of 0.78-0.97, [215], thus we assume mean = 0.785. Median (50%) age at maturity for females is in the range of 19-21 years [227], thus we assume mean = 20.	= 0.875/20 = 0.044	Max = 0.97/19 = 0.051	= (0.051 – 0.044)/3 = 0.002
Permanence rate in stage 2 (per year)	p_2	Annual survival rate for age 1+ is in the range of 0.78-0.97, [215], thus we assume mean = 0.875. Age that female SMA reach sexual mortality is within the range of 25-27 years, [228], thus we assume mean = 26. Average duration in stage 2 = 26 – 20 = 6 years. Max duration in stage 2 = 27 – 19 = 8 years.	= 0.875*(6 – 1)/6 = 0.729	Max = 0.97*(8 – 1)/8 = 0.849;	= (0.849 – 0.729)/3 = 0.04

Fecundity rate from stage 2 to 0 (per year)	f	Litter size ranges from 4 to 27.5 and mean litter size is 12.5 [229]. Reproductive periodicity (3 years) [215]. Probability of producing a female pup = 0.5.	= (12.5/3)* 0.5 = 2.083	Max = (27.5/3)* 0.5 = 4.583	= (4.583 – 2.083)/3 = 0.833
Transition rate from stage 2 to stage 3 (per year)	a_{32}	Annual survival rate for age 1+ is in the range of 0.78-0.97 [215]. Age that female SMA reaches sexual mortality is within the range of 25-27 years [228]. Average duration in stage 2 = 26 – 20 = 6 years. Max duration in stage 2 = 27 – 19.	= 0.875/6 = 0.146	Min = 0.78/8 = 0.098	= (0.146 - 0.098)/3 = 0.016
Permanence rate in stage 3 (per year)	p_3	Annual survival rate for age 1+ is in the range of 0.78-0.97, mean = 0.875 [215].	0.875	Max = 0.97	= (0.970 - 0.875)/3 = 0.032
Carrying Capacity	K	The SMA biomass under virgin conditions (956,777,000 kg) (from S6, Table 19, Anon [215]) Sex ratio in the population (1 female: 1 male) [230] Female SMA mean weight (205.031 kg) (from length-weight correlation and growth function in Parameters, Stochasticity and Error section)	= (956,777, 000/205. 031)*0.5 = 2,333,24 8		

Population cutoff/quasi-extinction threshold	N^{cutoff}	Unfished equilibrium abundance (2,333,248) [215] Cutoff threshold is often set at 20% of unfished equilibrium abundance [214]	= 2,333,248*0.2 = 466,650		
Frequency (per year) of recruitment failure	F^{rf}	Based on population models of other marine fishes [13, 226]	0.1		
Stage 0 abundance multiplier if recruitment failure occurs	M^{rf}	Based on population models of other marine fishes [13, 226]	0.05		
Initial conditions	**Symbol**	**Assumptions**	**Mean**		
Initial abundance of female pups	$N_0(0)$	Refers to Initial Conditions section	381,279		
Initial abundance of female juveniles	$N_1(0)$	Refers to Initial Conditions section	1,431,337		
Initial abundance of female mature adults	$N_2(0)$	Refers to Initial Conditions section	194,529		

Initial abundance of female post-reproductive adults	$N_3(0)$	Refers to Initial Conditions section	151,271		
A harvest weight threshold for which harvest is considered low if bellow this threshold	H_{low}	Estimated catches of SMAs in 2010 (2,496 mt) [215]. Sex selectivity by the fishery (1 female: 1 male) (onboard observers data). Proportion of minimum harvest weight in 2010 to consider that harvest is low (20%) (from expert opinion).	250 mt		

The proposed model is not deterministic; it includes uncertainty. The effect of parameter uncertainty on outcomes can be bounded by fitting a probability distribution function (PDF) (e.g., Normal or Lognormal) to each parameter chosen from their average value, lower and upper ranges of plausibility. By including stochasticity in parameters via Monte Carlo simulation [180] the model is able to account for such sources of uncertainty. We fit a PDF to each parameter using data, literature information, and expert opinion, so parameters are random variables following a PDF. Our model also has the flexibility to include known and/or suspected variations in vital rates (survival and fecundity) caused by low-frequency, high-consequence events such as recruitment failure.

Female individuals in the population are structured in four stages (pups, juveniles, mature adults, and post-reproductive adults) based on characteristics such as their weight, survival, fecundity and harvest rate. A summary of the female SMA life history in our model is as follows (Figure 7.1) [218]. Pups (stage 0) are born age 0. Those who survive until age 1 become juveniles (stage 1). The juveniles who survive until the age of 19-21, reach maturity and become mature adults (stage 2). Mature adults who survive produce new pups until the age of 25-27 years, when they reach sexual mortality and become post-reproductive adults (stage 3). Post-reproductive adults naturally die at an average age of 32 years. By doing so, we can project the stage-specific population abundance using a Lefkovitch matrix (also known as Stage matrix) [231].

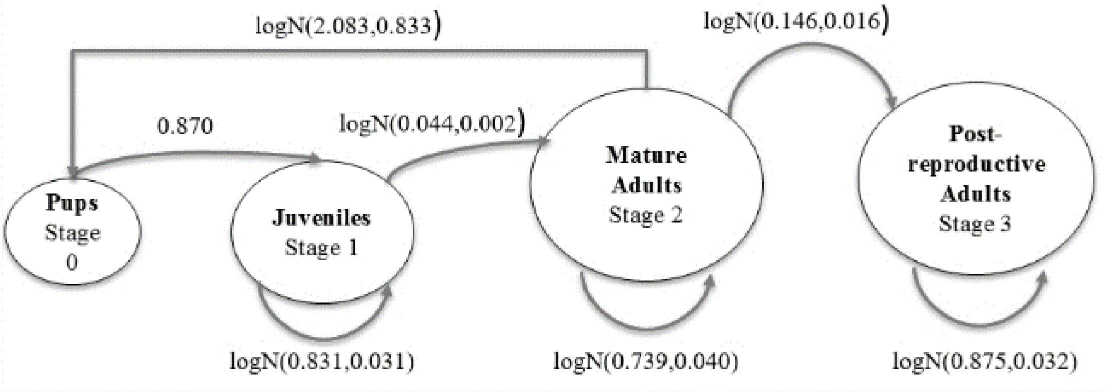

Figure 7.1 - Female SMA life cycle. The values above the arrows are estimates for the transition and permanence rates per year.

The model integrates DD. Authors of fish case studies had difficulty choosing the DD parameters. Most assumed Ceiling-type DD [220] because it is conservative in that productivity is likely underestimated at low density, and, hence, the risk of extinction will be overestimated [221]. This is reasonable because other types of DD increase vital rates at low density. For a conservative approach, we also assume Ceiling-type DD. In the ceiling model, vital rates are not affected until the population reaches the carrying capacity. If the population grows so much that it reaches the carrying capacity, *K*, then it remains at that level until a population decline takes it below this level. In this case, the carrying capacity acts as a population ceiling [220]. These conditions are modeled in the first and second steps of the algorithm below.

Now let $N_i(t)$ be the abundance of females in stage i; N the abundance of female population; s_i the survival rate (per year) of females in stage *i*; p_i the permanence rate (per year) of females in stage *i*; *f* the fecundity rate (pups per year); a_{ij} the transition rate (per year) from stage *j* to stage *i*, where *i* is the line and *j* the column in the matrix; *K* is the carrying capacity (i.e., the level of abundance above which population tends to decline [220]); h_i is the harvest rate for stage i; N^{cutoff} is the abundance threshold for cutoff; and F^{rf} is the frequency per year that recruitment failure occurs. Note that $a_{10} = s_0$; $p_1 = s_1 - a_{21}$; $p_2 = s_2 - a_{32}$; and $p_3 = s_3$.

The following algorithm represents one replication for stochastically simulating the population model. Each equation of the algorithm will be further explained in more details. For each iteration, repeat the following steps for all *i*:

i) If $N < K$, then make:

a. $$\begin{bmatrix} N_0(t+1) \\ N_1(t+1) \\ N_2(t+1) \\ N_3(t+1) \end{bmatrix} = \begin{bmatrix} 0 & 0 & f & 0 \\ a_{10} & p_1 & 0 & 0 \\ 0 & a_{21} & p_2 & 0 \\ 0 & 0 & a_{32} & p_3 \end{bmatrix} \begin{bmatrix} N_0(t) \\ N_1(t) \\ N_2(t) \\ N_3(t) \end{bmatrix} \quad (7.1);$$

b. If $N > N^{cutoff}$, then make $$\begin{bmatrix} N_0(t+1) \\ N_1(t+1) \\ N_2(t+1) \\ N_3(t+1) \end{bmatrix} = \begin{bmatrix} N_0(t+1) \\ N_1(t+1) \\ N_2(t+1) \\ N_3(t+1) \end{bmatrix} * \begin{bmatrix} 1-h_0 \\ 1-h_1 \\ 1-h_2 \\ 1-h_3 \end{bmatrix} \quad (7.2).$$

ii) Otherwise: $$\begin{bmatrix} N_0(t+1) \\ N_1(t+1) \\ N_2(t+1) \\ N_3(t+1) \end{bmatrix} = [K] \begin{bmatrix} 0.169 \\ 0.678 \\ 0.086 \\ 0.068 \end{bmatrix} \quad (7.3).$$

iii) Generate random number *U* from a uniform distribution.

a. If U < F^{rf}, then: $$\begin{bmatrix} N_0(t+1) \\ N_1(t+1) \\ N_2(t+1) \\ N_3(t+1) \end{bmatrix} = \begin{bmatrix} N_0(t+1) \\ N_1(t+1) \\ N_2(t+1) \\ N_3(t+1) \end{bmatrix} * \begin{bmatrix} M^{rf} \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad (7.4).$$

Equation 7.1 is a Lefkovitch matrix [231]. This equation describes the natural dynamics of the population.

Equation 7.2 describes the effect of harvest. Harvest in the simulation was structured to reflect age selectivity by the fishery. For each scenario, harvest was included by removing a certain proportion of the stage-specific population every year, and a cutoff threshold was included to simulate a control measure in which no harvest occurs if the abundance declines bellow this threshold.

Equation 7.3 describes the DD effect. The constants in Equation 3 refer to the stable population distribution (i.e., the proportion of individuals in each stage when the population dynamics reach a stationary state, i.e., 16,9% age 0, 67,8% juveniles, 8,6% mature adults and 6,8% post-reproductive adults). This distribution is based only on the stage matrix for the benchmark scenario. It is the result of matrix analysis (eigen analysis). For more details see references [96, 221, 232].

Equation 7.4 describes unfrequent events that cause recruitment failure. This is modelled via Bernoulli trials [146, 221].

7.3 Case study

We conduct a case study and parameterize the proposed model to the South Atlantic as described in the next subsections.

7.3.1 Materials and Data Sources

Information used in the modeling is derived from several public sources. Estimates of parameters related to the harvest distribution of stages and sex were derived from onboard observers data made available by the Brazilian Ministry of Fisheries and Aquaculture [233]. An onboard observer after each set filled out the logbooks. Data included individual records of 33 vessels in the South Atlantic that registered 241,776 SMAs catches between December/2004 and February/2009. Useful information to this work included: the vessel identification, onboard observer identification, date, location of fishing ground (latitude and longitude), effort (number of hooks), fork length (cm) and sex (male, female or not available).

To translate information given in terms of length into weight or age and the inverse, we use the length-weight correlation [234] (Equation 7.5) and the 3-parameter Gompertz growth function for SMA, [235] (Equation 7.6), which produced the most biologically reasonable estimates for females, i.e., respectively:

$$WT = 5.2432 \times 10^{-6} \times (FL)^{3.1407}, \tag{7.5}$$

where: WT = Total weight; FL = Fork length (i.e., the length of a fish measured from the tip of the snout to the end of the middle caudal fin rays and is used in fishes in which is difficult to tell where the vertebral column ends [106]).

$$L(t) = L_0 e^{G(1-e^{(-kt)})} \text{ and } G = \ln {}^{L_\infty}/_{L_0}, \tag{7.6}$$

where: t is the age (years); L_0 = 88 cm; $L_\infty = 366$ cm; and k = 0.087 $year^{-1}$.

From the female total catches, only 7,359 had their fork length measured, so that we calculate (respectively for age 0, juvenile, mature adult and post-reproductive adult): the annual catch distribution among stages, i.e.: $AC_i = [6.0\%, 92.2\%, 0.4\%, 1.5\%]$ and the average weight of each stage (kg), i.e.: 6.7, 113.9, 329.5, 417.2. Thus, stage-specific harvest rates are estimated for a specific scenario as follows:

$$h_i = \frac{(population\ harvest\ rate\ per\ year\ for\ the\ specific\ scenario) \times \sum_{\forall i} N_i(0) \times AC_i}{N_i(0)} \tag{7.7}$$

A catch time series for the South Atlantic [215] shows that 2,946 metric tons (mt) of SMAs were harvested in 2010. They assume no sex selectivity by the fishery, then half of these catches are considered females (i.e., 1248 mt); this value is not a parameter of the model. It is just an indicator for comparing the total number of SMAs removed from the population in the first time-step of each scenario simulation, assuming that the first time-step is 2010. By doing so, we want that the simulated harvest in the first time-step to be close to the estimated harvest in 2010 according to ICCAT [215], then to estimate the proportion of the population harvested in 2010 and to use this proportion to consolidate harvest scenarios for the future. However, the methods for catch estimates [215] are not clear. We do not know if they consider SMAs that are discarded at sea, then we conservatively assume that real catches are at least greater than catch estimates as follows.

Bycatch of SMAs results in substantial number of SMAs being discarded dead or dying every year. Quantifying total harvest from bycatch is challenging because comprehensive data on these discards are unavailable [219]. We assume that mortality of SMAs is greater than catch estimates [215] for two reasons: estimates are deterministic and may not include uncertainty about (i) post-release mortality [210, 219, 236] and (ii) the catches of sharks that were illegally discarded at sea to make space for tunas in the freezer.

We interviewed an observer and data monitor that worked onboard of the Japanese tuna longline vessel Kinei Maru 108 that had capacity to stock 200 tons of fish meat. This is the same observer in recent news about irregularities of Japanese vessels fishing in Brazilian waters [237, 238]. He stated: "*I do not know how many. We (observers) cannot register that. I just know that many sharks, including the makos, are discarded at sea after they were stocked in the freezer. The Master wants to catch tunas to make more money. If at the end of the voyage there is not enough space for tunas in the freezer, they are going to discard sharks for making space in the freezer for tunas. The same situation happens in most vessels and these sharks are not included in public data.*"

Estimates of initial abundance and carrying capacity were derived from a stock assessment conducted by ICCAT [215]. Estimates of parameters related to the ecology and population dynamics (i.e., natural mortality, age and growth, reproduction, stage-specific life span, age at first maturity, age-weight) were derived from literature. Table 7.1 describes the model parameters and their source of information. For the cases where there is more than one source of information for the same parameter, we assume the one with the wider confidence interval in order to be more conservative. We use the software RAMAS Metapop v.6.0 [96] that is a computational tool for population model construction and probabilistic simulation via Monte Carlo methods [180].

7.3.2 Parameters, Stochasticity and Error

Table 7.1 presents the parameters governing the dynamics of the system. Some parameters were estimated based on a mean value and others on a lower limit, mean and upper limit ($\omega_L, \overline{\omega}, \omega_U$) provided in the literature. To make the latter probabilistic, we consider that they have a truncated normal distribution and that the error ($\max[\overline{\omega} - \omega_L, \omega_U - \overline{\omega}, (\omega_U - \omega_L)/2]$) corresponds to a 3σ interval; therefore, such parameters will be randomly selected to fall between their limits in 99.865% of replications. It is believed that one can make good use of a Gaussian approach in vital rates because there is a reasonable reason for random values not to be too far away from the average, i.e., there are biological limitations preventing very large deviations and natural forces of equilibrium bringing vital rates back to their average values [94]. For probabilistic simulation, the software converts the normal distribution of vital rates into a corresponding lognormal distribution. This conversion avoids bias resulting from truncation because $\omega \geq 0$ [221, 239].

As for improbable large events (Equation 7.4), we assume that the population is exposed each year to a 10% probability of recruitment failure (i.e., $F^{rf} = 0.1/year$) that decreases stage 0 abundance to 5% of the value expected if there had been no such event. Carrying capacity (K) was estimated (Table 7.1) based on the population biomass provided by the stock assessment (i.e., 956,777 mt from Scenario-6 in reference [215]) under virgin conditions (the current population abundance if there was no fishing). Most simulation scenarios included annual harvest that prevented abundance from reaching the ceiling defined by K, thus DD does not influence the results of management strategies.

7.3.3 Initial Conditions

First, we derive the initial population abundance from the stock assessment by ICCAT [215]. They simulated 13 scenarios with varying parameters and provided the SMA biomass in 2010 as result of each simulation. We consider the effect of uncertainty in initial biomass by using the result of the scenario with the lowest value, i.e., 885,085 mt from Scenario-6, Table 19 [215]. Next, we assume that the initial stage distribution is equal to the steady stage distribution in Equation 7.3. This results in the initial conditions in Table 7.1.

7.3.4 Harvest Scenarios

From the proposed model, we simulated hundreds of harvest scenarios by varying catches from zero to thirty-two times greater than catch estimates in 2010.. It would not be practicable to show results of all simulated scenarios, then Table 7.2 presents the parameters of six relevant scenarios in the case study (i.e., zero, one, four, seven, twenty-one and thirty-two times greater than catch estimates in 2010), where the parameter h_i is the harvest annual rate for stage i; N^{cutoff} is the cutoff abundance threshold; total harvest is the proportion of the female population that is removed every year; number of catches at first year (females only) is not a parameter, but a measurement endpoint used to calibrate the proportion of female population that is removed every year.

The number of catches at the initial time-step serves as an indicator to compare scenarios before simulating them. Harvest scenarios are conservative because they assume that initial catches are greater than catch estimates in 2010. Number of catches will increase (decrease) as abundance increases (decreases), since harvest is modeled as a proportion of abundance.

Table 7.2. Harvest parameters.

Harvest scenario	**Scn-0**	**Scn-CE**	**Scn-1**	**Scn-2**	**Scn-3**	**Scn-4**
Total harvest per year	0	0.29%	1%	2%	6%	9%
h_0	0	0.10%	0.34%	0.67%	2.02%	3.03%
h_1	0	0.40%	1.39%	2.87%	8.34%	12.51%
h_2	0	0.01%	0.04%	0.08%	0.25%	0.38%

Harvest scenario	**Scn-0**	**Scn-CE**	**Scn-1**	**Scn-2**	**Scn-3**	**Scn-4**
h_3	0	0.06%	0.21%	0.41%	1.24%	1.87%
Number of female catches at first year	0	6,259	21,584	43,168	129,505	194,257
Number of times that simulated catches are greater than catch estimates [215]	0	1	4	7	21	32

The real number of SMA catches is uncertain. As suggested by [225], the effect of parameter uncertainty on outcomes can be considered by consolidating scenarios with parameters chosen from the lower and upper range of plausibility. From discussions with onboard observer, it is plausible to assume that real catches in 2010 are not smaller than Catch Estimates (CE) and not greater than seven times it. We consolidate two scenarios (Table 7.2) to represent the range of plausibility (i.e., Scn-CE and Scn-2) as well as four other relevant scenarios: no-fishing (Scn-0); an intermediate one within the range of plausibility (Scn-1, i.e., initial catches are four times greater than CE); a pessimistic one above the range of plausibility (Scn-3, i.e., twenty-one times greater than CE); and an extremely pessimistic one (Scn-4, i.e., thirty-two times greater than CE).

By simulating Scn-0, we aim at evaluating the natural population dynamics, quantify its background risks and the added risk caused by all relevant scenarios when compared to background risks. By simulating Scn-CE, Scn-1 and Scn-2, we aim to propagate the effect of uncertainty about real catches. It is improbable that real catches will be out of the assumed range of plausibility between Scn-CE and Scn-2. However, a conservative manager may think it is necessary to evaluate the improbable. Thus, by simulating Scn-3 and Scn-4, we intend to meet the needs of conservative risk managers and evaluate if such heavy harvest regimes are sustainable.

We simulate all harvest scenarios with and without cutoff to evaluate the maximum reduced risk caused by this management threshold that is, in fact, a control measure to satisfy conservation objectives. The quantified number is based on two-sample Kolmogorov-Smirnov test [96].

7.3.5 Proposed Risk Categories

We aim to categorize risks so that results can be better interpreted by risk managers, society, and other interested parties. We make some changes to the categories of risks assigned by the International Union for the Conservation of Nature (IUCN) [127] in order to adapt them to our case, i.e.,: undesirable consequence “quasi-extinction” instead of “extinction”; and additional risk instead of absolute risk. It is important to note that the proposed categories are more conservative than the IUCN categories. The latter are used to classify species affected by a whole range of environmental changes and human disturbance at regional [181] or global-levels, whereas the former is proposed to classify risks caused by a single stressor (harvest) to a single population, which is our case. Then, we propose the following risk categories:

- CRITICALLY ENDANGERED (CR): more than 50% additional probability of quasi-extinction within 3 generations (i.e., median time to quasi-extinction is shorter than 3 generations);
- ENDANGERED (EN): more than 20% additional probability of quasi-extinction within 5 generations;
- VULNERABLE (VU): more than 10% additional probability of quasi-extinction within 5 generations;
- NEGLIGIBLE (NE): less than 10% additional probability of quasi-extinction within 5 generations.

We assume that female SMAs have a generation time of 20 years [106] and harvest scenarios that cause NE risks are considered sustainable.

7.4 Results and Discussion

Figure 7.2 illustrates a projection of female SMA average abundance in the South Atlanticas it changes over time for several harvest scenarios (Scn-0, Scn-CE, Scn-1, Scn-2, Scn-3 and Scn-4, respectively, 0%, 0.29%, 1%, 2%, 6% and 9% of the population removed every year).

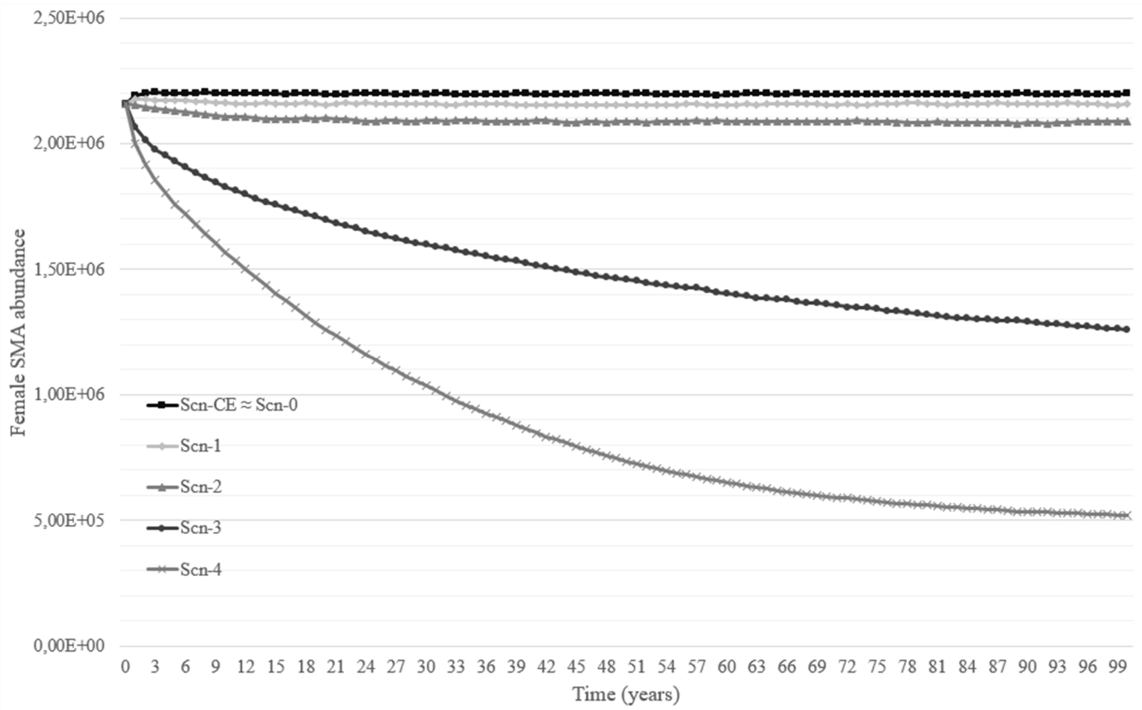

Figure 7.2 - Female SMA average abundance for relevant scenarios.

The Scn-0 curve represents the population dynamics if no fishing occurs. Scn-0 curve is superimposed on Scn-CE, which shows the population dynamics if real catches were as described by landing data. The abundance reaches a dynamic equilibrium at the carrying capacity.

The range between Scn-CE and Scn-2 (2% annual harvest) curves is a measure of the effect of uncertainty about real catches. An annual harvest between 0.29% and 2% would cause the expected population abundance in 100 years to terminate between 2,198,456 (biomass = 450,752 mt) and 2,089,189 females (428,349 mt). Scn-1 (1% annual harvest) is an intermediate scenario within the plausible range of uncertainty, while Scn-3 and Scn-4 (6% and 9% annual harvest, respectively) are improbable scenarios, which show rapid population decrease in case of heavy harvest regimes.

Table 7.3 summarizes the main risk results, i.e.: probability and time to quasi-extinction (80% decline) within 100 years, and expected minimum abundance. Values with a + or – symbol mean that they are being compared to the benchmark Scn-0, except for the maximum effect of cutoff measure, which is being compared to the same scenario without cutoff. The maximum effect of cutoff is measured as the maximum reduced risk of a scenario with and without cutoff. The reported number is the Kolmogorov-Smirnov test statistic D (which is the maximum vertical difference between risk curves), based on a two sample Kolmogorov-Smirnov test [96]. The approximate location (point X at which maximum reduced risk occurs, i.e., percentage of decline) is also given.

The risk of harvest scenarios are indicated both as additional risk of quasi-extinction compared to the benchmark (Scn-0) and as reduced expected minimum abundance compared to Scn-0. The median time to quasi-extinction is calculated from the CDF for the time that the population size will fall bellow the quasi-extinction threshold. Only Scn-4 had the median of its distribution shorter than 100 years, i.e., 50% probability of quasi-extinction within 56 years. All other scenarios had less than 50% probability of quasi-extinction within 100 years.

Table 7.3. Summary of risk results.

Harvest scenario	**Scn-0**	**Scn-CE**	**Scn-1**	**Scn-2**	**Scn-3**	**Scn-4**
Risk of quasi-extinction	0	0	0	0	+0.106	+0.878
Risk category	NE	NE	NE	NE	VU	CR
Median time (years) to quasi-extinction	>100	>100	>100	>100	>100	56
Expected minimum biomass (mt)	332,785	-5,007	-16,704	-35,012	-162,308	-252,054
Maximum effect of cutoff measure	Not applicable	Not significant	Not significant	Not significant	-0.057 risk of 83% population decline	-0.721 risk of 87% population decline

Expected yield (total harvest weight (mt))	Not applicable	73,660	241,554	469,821	1,000,000	886,045
Risk of low harvest (≤ 250 mt)	Not applicable	0	0	0	0.132	0.887

The Scn-3 and Scn-4 curves (Figure 7.2) represent improbable scenarios, but are useful to describe an overfishing situation in which the population rapidly declines to, respectively, 1,260,764 (258,496 mt) and 519,322 (106,477 mt) females. Scn-3 causes an additional 10.6% risk of quasi-extinction within 5 generations, then it is classified as VU. Scn-4 causes 56.2% probability of quasi-extinction within 3 generations, so it is categorized as CR.

7.4.1 The effect of the cutoff threshold measure

We quantify the maximum effect caused by the cutoff management threshold. We simulate all harvest scenarios with and without cutoff, compare their risk of population decline and measure the maximum reduced risk and the point at which it occurs (Table 7.3). For Scn-4, the cutoff measure reduces by 72% the risk of 87% population decline. For Scn-3, it reduces by 5.7% the risk of 83% population decline. For all other scenarios, risk reduction is insignificant.

7.4.2 Harvest Results

These results are useful to yield management. The yield of SMA is not only important as a secondary product, but also as an indicator for yield of tuna, since SMA are bycatched by various types of tuna and tuna-like fishing gear. Thus, changes in SMA harvest means proportional changes in tuna harvest. The number of SMA catches as a proportion of tuna catches depends on several specific factors such as the vessel fishing gear and fishing grounds. Thus, the vessel interested in how the presented SMA harvest results impact their yield of tuna should make their own estimates.

Scn-0 is not applicable here since it is not a yielding scenario. Figure 7.3 shows, for each harvest scenario, the expected total weight of harvest as a function of time. The harvest is calculated based on the average weight of each stage (Materials and Data Sources section). Total harvest for the 100 years of simulation and risk of low harvest are presented in Table 7.3.

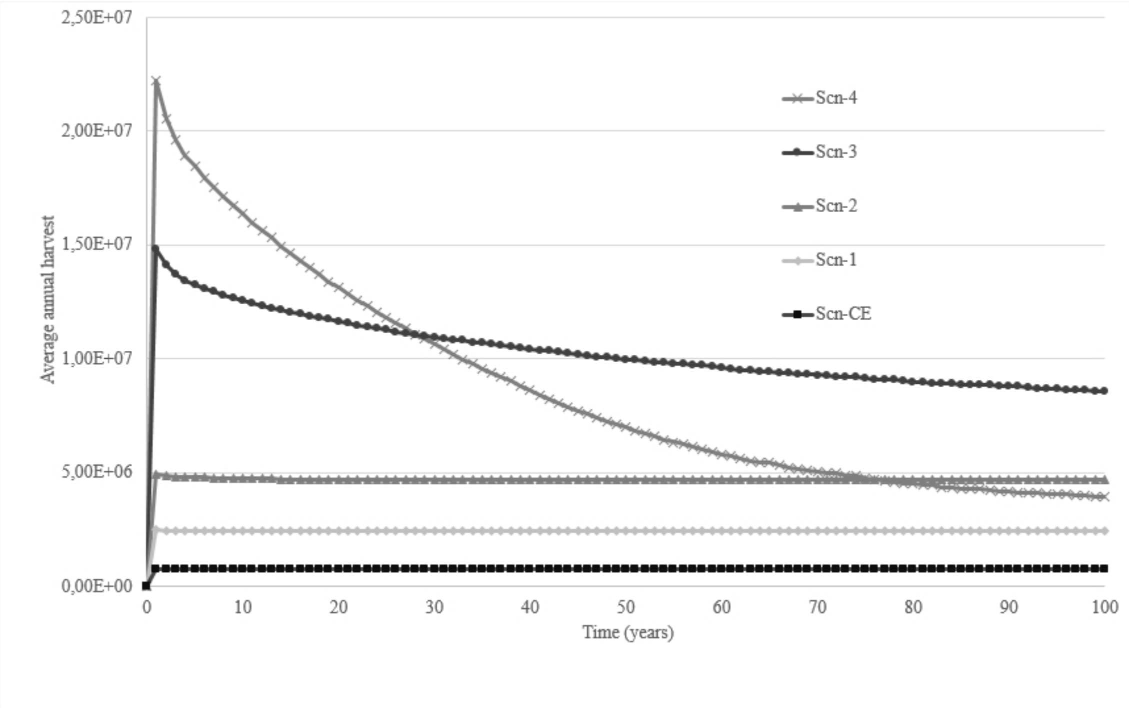

Figure 7.3 - Average weight of female SMA harvest as a function of time for each harvest scenario (Scn-CE, Scn-1, Scn-2, Scn-3 and Scn-4).

At the beginning of the 100 years simulation, it is expected that Scn-4 yields the most, but the population rapidly drops (Figure 7.2) and then harvest decreases (Figure 7.3) until it is lighter than Scn-3 at year 25 and than Scn-2 at year 79. The results suggest that harvesting 6% of the population every year (Scn-3) is the regime that causes the heaviest yield, with significant risk of low harvest (13.2%). Harvesting 2% every year (Scn-2) causes a good and consistent yield every year and no risk of low harvest.

Therefore, it is suggested a harvest regime that corresponds to remove 2% of the population per year (Scn-2), thus providing maximum expected yield at negligible risk (sustainable production) and no risk of low harvest. Scn-CE and Scn-1 are also sustainable, but yields are low and might not satisfy the demand. Scn-3 and Scn-4 are not good for both conservation and production because: (i) they are not sustainable, i.e., Scn-3 is categorized as VE and Scn-4 as CR; (ii) although Scn-3 maximizes yield, it causes a considerable risk of low harvest (13%); and (iii) Scn-4 does not provide maximum yield and risk of low harvest is high (89%).

7.5 Conclusions

This paper deals with a very important bycatch species of worldwide tuna fisheries. Its capture is of major conservation concern, thus this subject is of major interest and relevance for pelagic fisheries and for their management. Yet, the methodology to approach the problem is innovative.

The proposed model can be applied to any SMA population by changing initial conditions and harvest parameters. We conducted a case study with the SMA South Atlantic population in order to test the model and found consistent results.

The model is most useful for risk managers as an aid for rational decisions about harvest regimes under uncertainty. The flexibility of the model makes it practicable to simulate and evaluate hundreds of scenarios and analyze their results. The risk results of relevant scenarios can be translated into risk categories for easier communication to stakeholders. The model flexibility also allows for update of parameters as new data becomes available every year. Private companies interested in sustainable production can thus register data of SMA bycatch and use them as an input in the model, which is much more reliable given that the public data used in our study provide SMA landings (i.e., they do not show SMAs discarded at sea).

It is very difficult to discuss our model advantages or improvements relatively to others already proposed and accepted in previous ICCAT stock assessment of the species [215, 216] because their model structure and parameterization is not clearly described. Thus, one advantage of this work is that we present a clear methodology to build and parameterize the model. We provide a detailed step-by-step procedure to replicate the model.

It is important to note that the proposed model itself is the main contribution of this work, not the case study. By means of the case study, in which we use limited public data, we calibrate and validate the model. It is not our aim neither to predict the real SMA population abundance in the South Atlantic nor to conclude whether they are really endangered by tuna fishing or not. The results of the case study prove that the model is able to generate consistent results and that is all. However, the model is clearly described and can be used in future works together with more data gathering for quantifying the real risk of SMA extinction implied by tuna fishing.

This work focused on a single species, thus it fails to address more complicated problems that involve environmental variability, spatial structure, and changes in productivity due to habitat modification. A multi-species model at ecosystem-level that includes tuna, tuna-like fishes and other shark species would better represent reality. However, there is no such model applied to pelagic fisheries management, mainly because of limited information in the field of Ecology to quantify the interaction among these species.

8 CONCLUSIONS

It was proposed a methodology capable of quantifying risks in systems where the biological environment (plants, animals, microbes) are involved and susceptible to human disturbance. By means of probabilistic ecological modeling, risk could be quantified as a measure of probability and undesirable consequence over time. The main goal was to provide a systematic way of conducting either an ecological or microbial risk assessment based on ecological modeling and proving its efficiency by applying it to four case studies in different Brazilian problems (chapters 4, 5, 6 and 7). As to the case studies, each one of them had its specific conclusions (see sections 4.4, 5.4, 6.5 and 7.5).

As to the theoretical background (chapter 2), it was provided a detailed review on the basic concepts of ecology, risks, risk assessment, quantitative risk assessment and QERA. This is mostly useful for engineers, biologists, oceanographers and researchers starting in this field of study. It was given several basic references, which will probably save lots of time of new researchers conducting a bibliographic review in this field.

As to the proposed methodology (chapter 3), it has specific goals such as:

- It can integrate reliability analysis for estimating frequencies of occurrence of accidental scenarios caused by equipment failure or human error.
- It can integrate meteorology and oceanography for estimating frequencies of occurrence of environmental extreme events.
- It can use fate and transport modeling to predict individual-level exposure in case of a particular toxic spill scenario.
- It can use dose-response modeling and hazard quotient to estimate individual-level adverse effects.
- It uses population modeling to translate individual-level into population-level adverse effects.
- It provides results that allows for the comparison of the added risk caused by varying impact scenarios as well as the reduced risk caused by varying control measures, as a basis for prioritizing risk management measures under limited resources.

- It is capable of presenting the total ecological risks of an establishment in a single risk measure (i.e. FN risk curve), as a simple way to communicate risks to stakeholders.
- It deals with environmental variability in time and space.
- It can point out further work that can effectively improve results via a sensitivity analysis.
- It can deal with uncertainty, measuring it and communicating it to risk managers on a quantitative basis.
- It is flexible in terms of data needs, i.e., can use several types of data.
- It is flexible in terms of application, i.e., can be adapted for application to any system where the extinction/explosion, quasi-extinction/explosion or decline/increase of a population of a certain species is an undesirable consequence.
- It uses objective criteria throughout the second, third and fourth steps in order to rule out accidental scenarios that will not contribute to the final ecological risk, avoiding waste of cost and time.
- It was tested and validated by applying it to four case studies in different Brazilian problems, proving that the methodology is efficient, flexible and applicable in practice.

Additional benefits of the methodology are described step by step as follows. The first step of the methodology allows for an improved knowledge about dangerous installations or activities, chemicals of concern and characteristics of the ecological environments possibly affected. It also encourages interaction of the risk assessor with other professionals such as risk managers, environmental managers, ecologists, technical managers and operators. The second step allows to systematically identify the existing hazards and their possible damage, causing an improved level of preparation to emergencies.

The third step provides a screening assessment of the ecological damage possibly caused by the identified hazards. It provides methods to predict individual-level exposure. Most of these methods are deterministic and some uncertainty in the results of the risk assessment is originated from their predictions. Uncertainty can be reduced by identifying the most influent meteorological conditions and creating meteorological scenarios.

The frequencies of extreme events are estimated in the fourth step. Also, some uncertainty in the results of the risk assessment is originated from frequency estimates. This can be minimized by conducting a detailed case-specific reliability analysis.

The fifth step of the methodology uses mathematical modeling applied to ecology (i.e. population modeling) to translate individual-level exposure (predicted in the third step) into population-level effects. Population modeling proved to be an efficient approach to quantify ecological risks caused by human impact, providing results in more relevant units than individual-level effects. The iterative process in implementing a population model was presented in a comprehensive scheme.

Some uncertainty in the final results of the QERA is originated from uncertainty in the population model, which is originated from: difficulties in data gathering; difficulties in parameter estimation; weak ability to validate population models; effects of alternative model structures. Nonetheless, uncertainty is an indelible characteristic of any future prediction. It does not make population modeling unfeasible as long as it is evaluated and communicated to decision makers. To make this claim, one needs to correctly represent uncertainty in the results. In this sense, the methodology measures uncertainty by estimating a range (lower bound and upper bound) to risk measures based on the best and worst case of impact scenarios.

Besides being useful to a QERA for industrial accidents, the population model built in the fifth step provides relevant information to tackle many key gaps in environmental management, such as: optimal resource allocation for monitoring affected areas, optimal management of threatened and endangered species, optimum control of undesirable species, and spatial planning for landscape restoration and management.

The ecological risks originating from accidents in an establishment are quantified in the sixth step. Risks can be assessed in a comparative approach, in which ecological risks related to each impact scenario are compared with ecological risks in the absence of any disturbance (i.e. a no-impact scenario). Thus, the decision maker can evaluate different alternatives of risk reduction via a cost-benefit analysis. It is important to note again that the proposed methodology is interactive, so that revaluation may occur during any part of the assessment or new information can be incorporated to improve results.

It is worth mentioning that the methodology usually requires more than one person to perform it. In other words, the methodology demands team work because specific knowledge on several different fields of studies is necessary. In most cases, team should be composed by a risk assessor, a biologist, a fate and transport modeler (e.g., an oceanographer, if toxic disperses through the ocean), a reliability analyst and a system engineer.

8.1 Limitations

- There are more complex and accurate ways of measuring and communicating uncertainty than the approach used in the methodology (i.e. based on the difference between the best and worst case of accidental scenarios).
- There are more complex and accurate ways of estimating frequency of maritime accidents than the approach used in the case studies in chapters 4 and 5.
- In order to avoid waste of resources, we propose the hazard quotient (PEC/PNEC) in the third step of the proposed methodology (section 3.3) as a first criterion to screen out risk scenarios that are clearly not a problem. This is based on other studies, which have found that PEC/PNEC < 0.01 is a very conservative criterion. However, this criterion may be not conservative enough for extremely conservative risk assessments.
- As a second criterion, in the fourth step of the methodology (section 3.4), we screen out scenarios that are clearly not a problem if their estimated frequency of occurrence is lower that 10^{-8} per year. Unlike the first criterion, this may be too conservative, since generic accidents have frequencies lower than 10^{-7}.
- The severity classes in Table 3.3 are subjective.

8.2 Future studies

In order to tackle the limitations aforementioned, it is proposed the following future studies:

- to study the several concepts and techniques of uncertainty analysis in population models, compare their performances, determine the best way to estimate and communicate uncertainty in a QERA for industrial accidents, and incorporate it into the methodology;
- to study maritime waterway quantitative risk assessment models [163, 164, 240], compare their performance, determine the best way to estimate frequency of maritime accidents in the case studies in chapter 4 and 5 and incorporate it into the case studies.

- to propose ecological risk criteria for acceptability in terms of the results provided by the FN risk curve;
- to investigate the role of expert opinion (i.e. ecologists) in order to improve the parameterization of a population model, focusing on the study of Bayesian methods to do so;
- to incorporate expert opinion in the fifth step (i.e. population modeling) of the methodology using Bayesian methods.
- In the case of the criterion PEC/PNEC < 0.01 (section 3.3) being not conservative enough to screen out scenarios for a specific risk assessment, we suggest either using an even lower PEC/PNEC criterion (e.g., 0.001) or not using it at all, at the chance of having to model and simulate irrelevant risk scenarios.
- In the case of the frequency of occurrence < 10^{-8} per year (section 3.4) being over conservative to screen out scenarios for a specific risk assessment, we suggest using a higher criterion (e.g., 10^{-7}) at the chance of ignoring relevant risk scenarios.
- to propose more objective severity classes (Table 3.3).

8.2.1 Future applications

The proposed methodology can be applied to any system where humans (e.g., industry, turism, fishing, urban environment), materials (e.g., pollutants, drugs), physical environment (e.g., soil, ocean, river, lake, atmosphere) and biological environment (e.g., plants, animals, microbes) interact with each other. It is useful to guide many other applications in any region of the world. As follows we suggest high relevant problems that the proposed methodology can assist:

- Quantifying zika virus risk of explosion in a specific region and the reduced risk implied by control measures.
- Quantifying dengue virus risk of explosion in a specific region and the reduced risk implied by control measures.
- More development on the space-time evolution of oil in the ocean, exploring its evolution in the long-term (decades).
- More development on the schistosomiasis model, exploring the risks caused by events of extreme rain.

- More development on the coral reef model, exploring the risks caused by global warming and coastal erosion.

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GLOSSARY

Abundance: the total number or density (number per unit area or unit volume) of organisms in a given location.

Acute toxicity: the ability of a chemical to cause a toxic response in organisms immediately or shortly after exposure.

Adverse ecological effects: Changes that are considered undesirable because they alter valued structural or functional characteristics of ecosystems or their components. An evaluation of adversity may consider the type, intensity, and scale of the effect as well as the potential for recovery.

Age Class: a category comprising individuals of a given age within a population.

Agent: Any physical, chemical, or biological entity that can induce an adverse response (synonymous with stressor).

Age-specific fecundity: the number of eggs or offspring produced per unit time by an individual of a specified age.

Age-specific survival: the proportion of individuals of age *x* alive at time *t* who will be alive at time *t*+1.

Assessment endpoint: environmental characteristic or value that is to be protected (e.g. population abundance, species diversity, or ecosystem productivity).

Biodegradation: a process by which microbial organisms transform or alter (through metabolic or enzymatic action) the structure of chemicals introduced into the environment.

Biomarkers: measures of body fluids, cells, tissues or measures taken on the whole organism, indicating, in terms biochemical, cellular, physiological, compartmental or energetic, the presence of contaminants substances or the magnitude of the response of the target organism.

Biota: living groups of organisms or species.

Biotic: living organisms, usually referring to the biological components of an ecosystem.

Chronic toxicity: the ability of a chemical to produce a toxic response when an organism is exposed over a long period of time.

Community: an assemblage of populations of different species within a specified location in space and time. Sometimes, a particular subgrouping may be specified, such as the fish community in a lake or the soil arthropod community in a forest.

Conceptual model: A conceptual model in problem formulation is a written description and visual representation of predicted relationships between ecological entities and the stressors to which they may be exposed.

Density dependence: a change in the influence of any factor (a density-dependent factor) that affects population growth as population density changes. Density-dependent factors tend to retard population growth by increasing mortality or emigration or decreasing fecundity as population density increases. They enhance population growth by decreasing mortality or increasing fecundity as population density decreases.

Dose: the amount of chemical taken into an organism per unit of time.

Deadweight tonnage: a measure of how much weight a ship is carrying or can safely carry. It is the sum of the weights of cargo, fuel, fresh water, ballast water, provisions, passengers, and crew.

EC_{50}: the toxicant concentration at which 50% of the test organisms show effects (e.g. mortality).

Ecological entity: A general term that may refer to a species, a group of species, an ecosystem function or characteristic, or a specific habitat. An ecological entity is one component of an assessment endpoint.

Ecological model: a mathematical expression that can be used to describe or predict ecological processes or endpoints such as population abundance (or density), community species richness, productivity, or distributions of organisms.

Ecological relevance: One of the three criteria for assessment endpoint selection. Ecologically relevant endpoints reflect important characteristics of the system and are functionally related to other endpoints.

Ecological risk assessment: The process that evaluates the likelihood that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors.

Ecosystem: the interacting system of a biological community and its non-living environmental surroundings.

Ecotoxicology: the branch of toxicology concerned with the study of toxic effects, caused by natural or synthetic pollutants, to the constituents of ecosystems, animal (including human), vegetable and microbial, in an integral context.

Emigration: the movement of an individual or group out of an area or population.

Endpoint: the biological or ecological unit or variable being measured or assessed.

Environmental Impact Statement (EIS): Environmental impact statements are prepared under the national environmental policy act by federal agencies as they evaluate the environmental consequences of proposed actions. EISs describe baseline environmental conditions; the purpose of, need for, and consequences of a proposed action; the no-action alternative; and the consequences of a reasonable range of alternative actions. A separate risk assessment could be prepared for each alternative, or a comparative risk assessment might be developed. However, risk assessment is not the only approach used in EISs.

Exposure: The contact or co-occurrence of a stressor with a receptor.

Exposure-response assessment: a description of the relationship between the concentration (or dose) of the chemical that causes adverse effects and the magnitude of the response of the receptor.

Fate and transport model: a description of how a chemical is carried through the environment. This may include transport through biological as well as physical parts of the environment.

Fecundity: the number of live offspring per individual in a given age class that will survive to be counted in the first age class.

Fish measurement: Standard Length (SL) refers to the length of a fish measured from the tip of the snout to the posterior end of the last vertebra or to the posterior end of the midlateral portion of the hypural plate. Simply put, this measurement excludes the length of the caudal fin; **Total length (TL)** refers to the length from the tip of the snout to the tip of the longer lobe of the caudal fin, usually measured with the lobes compressed along the midline. It is a straight-line measure, not measured over the curve of the body; **Fork length (FL)** refers to the length from the tip of the snout to the end of the middle caudal fin rays.

Geographic information system (GIS): software that combines a database and mapping capability; often used in spatially explicit modeling.

Grow rate: the rate of change of population abundance. Depending on the context, growth rate could also refer to the rate of change in mass or size of an organism.

Habitat: the place where animals and plants normally live, often characterized by a dominant plant form or physical characteristic.

Hazard quotient: the ratio of an estimated exposure concentration (or dose) to a toxicity threshold expressed in the same units.

Immigration: the movement of an individual or group into a new population or geographical region.

Indicator species: species thought to be more sensitive and therefore serve as an early warning indicator of ecological effects.

Key species: species strategically chosen to represent ecological effects in the risk assessment. Key species can be, for example, indicator species that are thought to be more sensitive and therefore serve as an early warning indicator of ecological effects, species of scientific and economic importance, rare and endangered species, or any species to be protected.

Landscape: the traits, patterns, and structure of a specific geographic area, including its biological composition, its physical environment, and its anthropogenic or social patterns. An area where interacting ecosystems are grouped and repeated in similar form.

Life stage: a developmental stage of an organism (for example, juvenile, adult, egg, pupa, larva).

Life story: the temporal pattern and habitat association of life stages (e.g. egg, larva, pupa and adult in an insect or egg, fry, smolt, juvenile, and adult in a salmon) and the schedule of births and deaths for a species.

Lowest-observed-effect-level (LOEL): the lowest concentration or amount of a substance, found by experiment or observation under the same defined conditions of exposure, that causes any alteration in morphology, functional capacity, growth, development, or life span of target organisms.

Measurement endpoints: quantitative expressions of an observed or measured biological response, such as the effects of a toxic chemical on survivorship or fecundity, related to the valued environmental characteristic chosen as the assessment endpoint.

Microbial risk assessment: the process that evaluates the likelihood that adverse effects on humans may occur or are occurring as a result of exposure to one or more microbial pathogens.

Migration: the movement of an individual or group into or out of an area or population.

Mortality: the number of individuals of a population that died in a given period of time.

Neap tide: when the tide's range is at its minimum.

No-observed-effect-level (NOEL): the greatest concentration or amount of a substance, found by experiment or observation under the same defined conditions of exposure, that causes no alterations of morphology, functional capacity, growth, development, or life span of target organisms.

Organism: any form of animal or plant life.

Population growth rate: the rate at which numbers of individuals are added to the population over time.

Population: a group of interbreeding organisms occupying a particular space.

Predicted Environmental Concentration (PEC): the local maximum of a predicted concentration function $C(x,y,z,t)$ related to an accidental scenario.

Predicted No Effect Concentration (PNEC): the concentration below which exposure to a substance is not expected to cause adverse effects.

Productivity: the rate of production of living biomass in a population or community.

Receptor: The ecological entity that might be exposed to a stressor.

Recovery: The rate and extent of return of a population or community to some aspect(s) of its previous condition. Because of the dynamic nature of ecological systems, the attributes of a "recovered" system should be carefully defined.

Recovery measures: mitigation actions which could reduce the magnitude of the consequences of an accidental scenario, and so reduce the risk.

Remedial action goals: a subset of remedial action objectives consisting of medium-specific chemical concentrations that are protective of human health and the ecological environment.

Spatially explicit model: a model that tracks spatial information (e.g. the locations of organisms or the pattern of a landscape).

Species: An organism belonging to such a category, represented in binomial nomenclature by an uncapitalized Latin adjective or noun following a capitalized genus name, as in *Ananas comosus*, the pineapple, and *Equus caballus*, the horse.

Species richness: the total number of species in a location or the number per unit area or volume.

Spring tide: when the tide's range is at its maximum. It is not named after the season (i.e. spring) but, like that word, derives from an earlier meaning of jump, burst forth, rise as in a natural spring.

Stressor: any physical, chemical, or biological entity that can induce an adverse response in an organism.

Survival: the number of individuals of a population that are alive after a given period of time.

Threshold: the chemical concentration (or dose) at which physical or biological effects begin to be produced.

Toxicity extrapolation model: any mathematical expression for extrapolating toxicity data between species, endpoints, exposure durations, and so forth. Also includes uncertainty factors.

Toxicity test: a test in which organisms are exposed to chemicals in a test medium (for example, waste, sediment, soil) to determine the effects of exposure.