Development of Ocean Acidification Endpoint Characterization Model for Life Cycle Assessment

MSc Industrial Ecology
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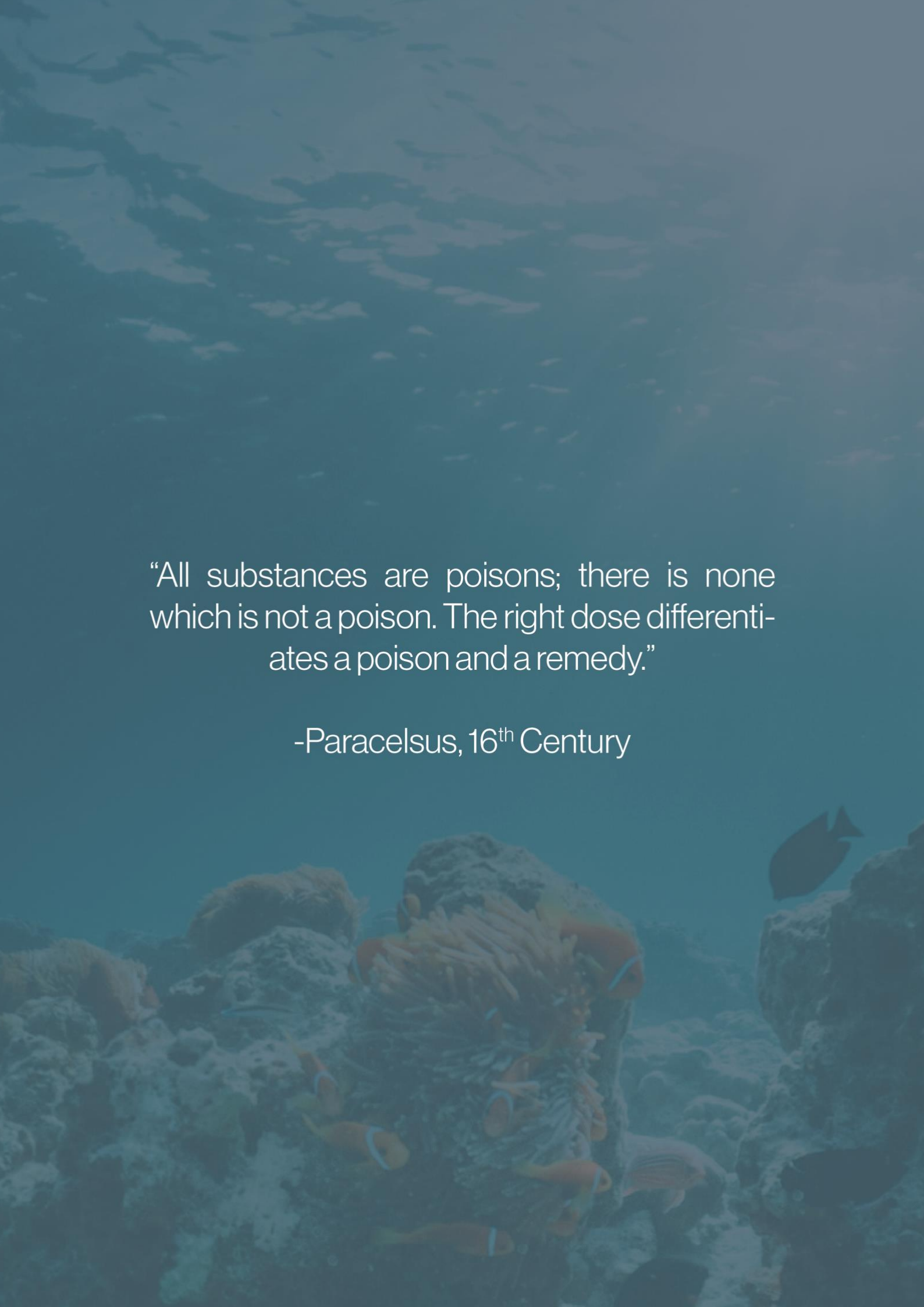

"All substances are poisons; there is none which is not a poison. The right dose differentiates a poison and a remedy."

-Paracelsus, 16th Century

Development of Ocean Acidification Endpoint Characterization Model for Life Cycle Assessment

Quantification of the impacts of GHG emissions on marine biodiversity loss through ocean acidification

İrem Gürdal

MSc Industrial Ecology Master Thesis

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Executive Summary

Ocean acidification, also referred to as the evil twin of global warming, occurs due to the CO_2 absorption of the oceans from the atmosphere. Both the pH and carbonate saturations are altered with this absorption process. The optimal operating conditions of the biological systems in the marine environment are therefore no longer maintained. The marine species are reacting in various ways to this change, eventually leading to a loss in biodiversity. With the current trend in emissions, the pH levels of the oceans are expected to decrease from 8.1 to 7.8 by the end of the century. In combination with the other stressors, it is projected that OA will have a wide range of impacts on marine life and its services to humanity. The representation of these implications is limited in environmental assessment tools such as Life Cycle Assessment.

This research explores the relationship between the changing acidity of the oceans and marine biodiversity loss. This relation is quantified through utilizing the ecotoxicology impact assessment approach for LCA. Following this approach, an endpoint characterization model is developed for ocean acidification. The approach consists of the development and integration of fate, exposure, effect and damage models. The fate model, expressing the relation between the GHG emissions (CO_2, CO, CH_4) and change in acidity of the ocean is based on the work of Bach et al. (2016). The effect model has been developed by constructing species sensitivity distributions utilizing species response data from 5 taxonomic groups (mollusca, echinodermata, fish, cnidaria, crustacea) to obtain the potentially affected fraction of species with changing pH. Furthermore, 3 different categorizations (climate zones, calcification, exposure duration) were made to assess their effects on species responses. The results revealed that there is no significant difference in responses based on different exposure durations or climate zones. Calcifying species on the other hand is found to have a higher sensitivity to ocean acidification as the change in carbonate chemistry directly influences the shell and skeleton formation of these organisms. Lastly, these models were integrated into an endpoint characterization model for ocean acidification. From the 3 GHG emissions included within the scope of this research, CO_2 has the highest ($CF_{CO2} = 4.883 \times 10^4 (PDF) m^3/kg_{GHG}$) and CH_4 has the lowest ($CF_{CH4} = 4.072 \times 10^4 (PDF) m^3/kg_{GHG}$) impact on marine biodiversity loss due to OA. These ecosystem damage indicators can be utilized in the impact assessment phase of the Life Cycle Assessment to translate the inventory results into impact on marine biodiversity.

Through the quantification of the impacts of ocean acidification, the effects of this major stressor on marine life can be better understood and targeted strategies can be developed. However, more research is required to increase the robustness of these models through expanding the species scope and incorporating temporal and geographical aspects into the models. Furthermore, the cascading effects of the changing ocean pH are still unknown and its consequences on ecosystems and socio-economic structures are unprecedented. To establish science-based targets and strategies to conserve the species richness in marine life, the extent of our understanding of the damage caused by anthropogenic actions needs to be further explored and estimated for the future.

Acknowledgements

Writing a master thesis has been a process very much resembling a roller coaster, especially during pandemic times. Besides learning about this interesting research topic (and how to carry out a research project), I got introduced to many facets of myself that I haven't met before. Though challenging at times, I learnt a lot and am feeling very grateful for it.

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I want to give my thanks to Dr Katja Mintenbeck for generously and kindly sharing the dataset of her research with me. This extensive collection of data provided me with a great foundation on to build my research upon.

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İrem Gürdal
August, 2021

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List of Abbreviations

- **OA:** Ocean Acidification
- **GHG:** Greenhouse gases
- **OAP:** Ocean Acidification Potential
- **IPCC:** Intergovernmental Panel on Climate Change
- **LCA**: Life Cycle Assessment
- **LCIA**: Life Cycle Impact Assessment
- **SETAC:** Society of Environmental Toxicology and Chemistry
- **PAF:** Potentially Affected Fraction of Species
- **PDF:** Potentially Disappeared Fraction of Species
- **p_{CO_2} :** Partial pressure of carbon dioxide
- **CO_2:** Carbon dioxide
- **$CaCO_3$**: Calcium carbonate
- **H_2CO_3:** Carbonic Acid
- **H^+:** Hydrogen ion
- **HCO_3^-**: Bicarbonate ion
- **Ca^{2+}:** Calcium ion
- **CH_4:** Methane
- **CO:** Carbon Monoxide

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Introduction

Chapter 1. Introduction

1.1. Ocean Acidification

Atmospheric carbon dioxide (CO_2) levels have increased up to 47% since the industrial revolution, reaching 412 ppm in 2019 (Buis, 2019). According to the global measurements of several scientific institutes, this concentration is going to continue rising due to the increasing global energy consumption and deforestation (Figure 1) (Buis, 2019). This long-term trend will escalate the severity of climate change impacts through the complex interactions of the climate system. The climate system is composed of different components of planet earth such as the atmosphere and the land surface, as well as the biogeochemical cycles (Ahmed, 2020). The impacts of climate change are therefore observed and expected both within and across these components, leading to a large variety of emerging outcomes. Some of these outcomes can be listed as extreme weather conditions, water scarcity, and disruption of marine and terrestrial ecosystems (IPCC, 2014).

The consequences of the changing climate and the impact of anthropogenic activities are observed and measured for global ecosystems in various forms. Global warming is the most well-known and discussed impact of climate change. Global warming is a predictable consequence of heat-trapping greenhouse gas (GHG) emissions released to the atmosphere, primarily due to the combustion of fossil fuels. Through the increased human interference due to industrialization, the planet is warming much faster compared to the previous centuries. With its current rate, the warming is expected to reach 1.5 °C within the two centuries after 2030 (IPCC, 2018).

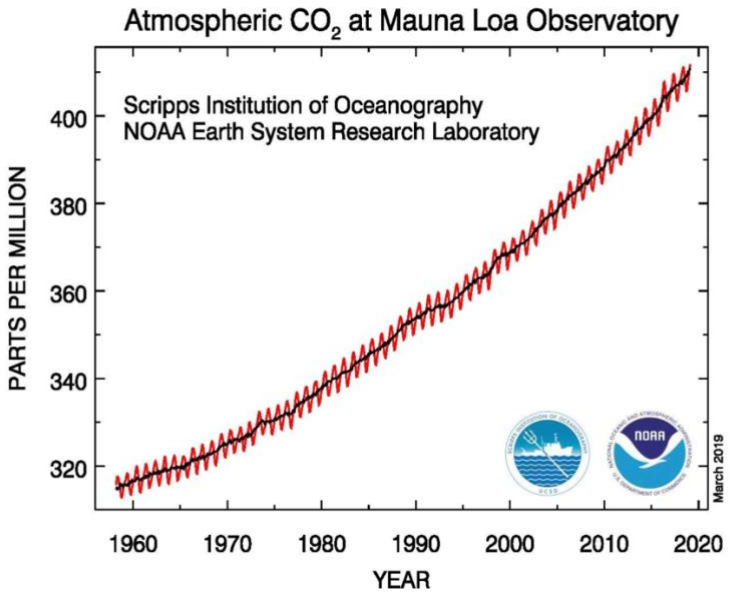


Figure 1 Concentration of CO_2 in the atmosphere in ppm over the course of 60 years (Buis, 2019)

Being the primary carbon sink of the earth, oceans have tempered this rise by absorbing up to 40% of the anthropogenic GHG emissions during the last 200 years (Woods et al., 2016). Approximately 525 billion tons of CO_2 have dissolved in the oceans since the beginning of the industrial revolution (Fabry et al., 2008). This flow of carbon is beneficial for mitigating global warming by reducing the GHG concentration in the atmosphere. However, the large quantities of dissolved CO_2 also imply a shift in the chemical balance, eventually lowering the pH of the oceans (Doney et al, 2009). This phenomenon is called ocean acidification, commonly referred to as the "evil twin of global warming" (Cooke et al., 2019).

Ocean pH levels have shifted from 8.2 to 8.1 while the carbonate ion concentration within the ocean has been reduced by 16% within the Anthropocene (Bach et al., 2016). IPCC (2014) scenarios estimate that the ocean acidity will fall to 1.5 times lower than its current value and that the carbonate ion concentration will decrease by 50% by 2100 (Bach et al., 2016). The low emission scenarios suggest a shift of the ocean pH from 8.1 to 7.95, whereas the high emission scenarios suggest 8.1 to 7.8 (Azevedo et al., 2015). Considering the volume of the oceans and the logarithmic measurement of the pH scale, the impacts of such variation in acidity is detrimental, especially on marine organisms and ecosystems (Woods et al., 2016).

The alterations within the biogeochemical cycles in the oceans have significant effects on the marine species and ecosystems (Doney et al., 2009). According to Bach et al. (2016), these effects can be categorized as primary, secondary and tertiary effects. The primary effects represent the changes in water chemistry. The more acidic the water gets, the fewer carbonate ions (CO_3^{2-}) will be present in the water. Secondary effects are described in terms of the reaction of organisms to OA. Secondary effects of OA are classified based on the distinctive biophysical reactions of the organisms such as acidosis, reduced larval survival and decreased calcification. Decreased calcification especially is the most well-known effect of OA and it implies the reducing ability of calcifying organisms to form shells and skeletons due to the reduction in CO_3^{2-} (Figure 2). Because of the complex interconnectedness of marine organisms, the secondary effects have the potential to disrupt the marine food web and life on an ecosystem level. This disruption causes a loss in marine biodiversity, which is described as the tertiary effects.

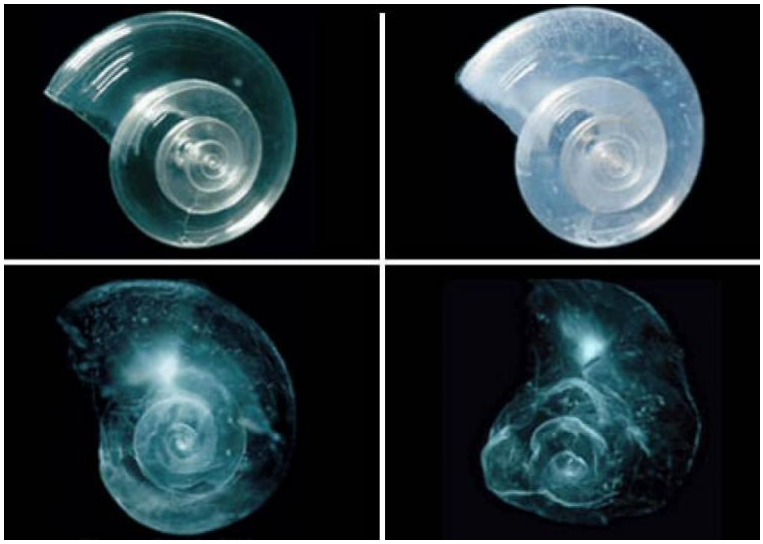


Figure 2 Time sequence of shell dissolution of the Antarctic pteropod Limacina helicina due to OA (exposure times; top left = 0 days, top right = 15 days, bottom left = 30 days, bottom right = 45 days) Photo credit: David Liittschwager/National Geographic Stock

Bach et al. (2016) express that the IPCC 2014 report evidenced the necessity and importance of OA research and discussions, which lead to an increase in scientific research on the topic. The majority of research results confirm that marine ecosystems will be significantly influenced. Nevertheless, these results do not currently represent realistic gradual alterations in habitats and biodiversity. This is because the research is mostly based on short-term laboratory and mesocosm experiments to gather species responses to acidification. Therefore, it does not reflect the cascading of impacts due to the interactions between species within ecosystems. Moreover, data availability is a major concern considering the vast number of species within marine life and requires enhancements through further research (Woods et al., 2016). Overall, the extent of the impact of OA on marine biodiversity is largely unknown and underrepresented in the environmental assessment tools, which is hampering the capability of taking both adaptive and mitigative action with regards to the conservation of marine species. Further research and model developments are required to understand and mitigate its impacts.

1.2. Ocean Carbonate System and Calcification Process

Ocean Carbonate System

When atmospheric CO_2 dissolves on the surface of the ocean, a near-equilibrium reversible reaction between CO_2 and H_2O takes place (Bach et al., 2016) (see Eq 1.2.1). The first chemical compound formed from the CO_2 and H_2O reaction is carbonic acid (H_2CO_3). H_2CO_3 further dissolves into bicarbonate (HCO_3^-) and hydrogen ions (H^+). Eventually, the remaining H^+ dissociates from HCO_3^-, which results in 2 H^+ and a carbonate ion (CO_3^{-2}). The rates of disassociation of aqueous CO_2 and HCO_3^- are dependent on the pH levels of the ocean. Despite this fact, estimates of global averages of these rates are provided in the scientific literature (Royal Society Great Britain, 2005; Doney et al., 2009). Being an unstable acid, up to 90% of the H_2CO_3 dissociates rapidly into HCO_3^- and hydrogen ions (H^+). Following this conversion, 9% of the HCO_3^- further dissolves into CO_3^{-2} and H^+.

$$CO_{2(aq.)} + H_2O \leftrightarrow H_2CO_3 \leftrightarrow HCO_3^- + H^+ \leftrightarrow CO_3^{-2} + 2H^+ \quad (1.2.1)$$

This alteration in seawater chemistry has two interpretations that are interconnected. First of all, as described above, when the aqueous CO_2 increases, the H^+ concentration increases. As pH represents the negative logarithm of the H^+ concentration, an increase in H^+ concentration means a lower pH value (Doney et al., 2009). Secondly, H^+ released from the reaction binds with already existing CO_3^{2-}, which decreases the overall available CO_3^{2-} in the surface waters. In other words, the more dissolved CO_2, the higher H^+ and lower CO_3^{2-} in terms of bioavailability. This balance can be observed from the Bjerrum plot (see Figure 3).

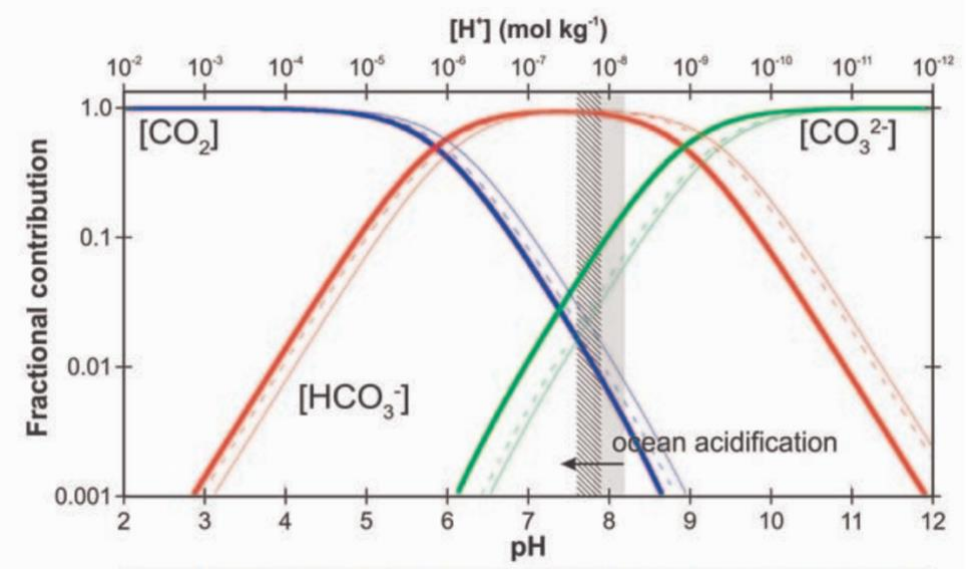


Figure 3 Bjerrum plot showing the change in seawater chemistry due to OA (Barker & Ridgwell, 2012)

Calcification Process of Marine Species

The inorganic carbon equilibrium in Eq. 1.2.1 takes place on the surface of the ocean with a timescale of one year. In longer time scales, CO_2 absorption potential of the surface waters becomes dependent on the dissolved calcium carbonate ($CaCO_3$) in the ocean (Doney et al., 2009). $CaCO_3$ dissolves from the sediments in the ocean into CO_3^{2-} and calcium ions (Ca^{2+}). In time, CO_3^{2-} ions move through pelagic zones of the ocean and react with available Ca^{2+} (see Eq. 1.2.2) to form the shells or skeletons of the calcifying marine species and organisms such as corals, crustaceans and echinoderms. However, as the concentration of H^+ originated from aqueous CO_2 is higher compared to CO_3^{2-}, H^+ bind with both the previously existing and CO_2 based CO_3^{2-} in the ocean, which lowers the $CaCO_3$ formation rate (called calcification) of the marine organisms.

$$CaCO_3 \leftrightarrow CO_3^{2-} + Ca^{2+} \quad (1.2.2)$$

The rate of this calcification process is dependent on the saturation state, denoted as **Ω** (see Eq.1.2.3). The saturation state is calculated using Ca^{+2} and CO_3^{2-} concentrations and the solubility product Ksp'. Temperature, pressure, salinity and mineral phase are the parameters that affect the solubility product value (Doney et al., 2009). Therefore, Ksp' values change depending on the location of the ocean. For instance, as solubility is lower in higher water temperatures, warm waters in the tropics and subtropics have a higher saturation state compared to polar regions. The same reasoning applies to the vertically differentiated zones within the ocean. At greater depths, solubility is higher and saturation is lower due to high water pressure. The mineral states are classified into two: aragonite and calcite. Compared to aragonite, calcite is a more stable mineral form, which makes it approximately 50% less soluble (Mucci, 1983). When the saturation state is lower than 1 ($\mathbf{\Omega} < 1$) Eq 1.2.2 can shift towards the side of CO_3^{-2} and Ca^{+2}. When $\mathbf{\Omega} > 1$, calcification occurs through formation of $CaCO_3$. Being highly dependent on carbonate ion concentration, saturation state and the calcification ability of organisms are estimated to be negatively affected by increasing levels of aqueous CO_2.

$$\mathbf{\Omega} = [Ca^{+2}][CO_3^{2-}] / Ksp' \quad (1.2.3)$$

1.3. Scientific Knowledge Gap

The impact of anthropogenic activities on marine ecosystems and biodiversity is currently underrepresented in impact assessment methods. According to Woods et al. (2016), there are 7 major drivers of marine biodiversity loss: climate change, seabed damage, overexploitation, invasive species, eutrophication induced hypoxia and lastly, ocean acidification. In combination with these other stressors, it is projected that OA will have a wide range of impacts on marine life and its services to humanity (Fallis., 2013). Overall, OA is expected to influence 3 areas of protection: the natural environment, natural resources and human health (Bach et al., 2010).

In order to be able to establish effective ecosystem-based protection and management systems for the ocean, first, the impacts of OA should be quantitatively modelled and anticipated (Olsen et al., 2018). The cascade of impacts of the changing pH is currently unknown. Understanding such unprecedented consequences of OA in the near future is essential for protection of ecosystems. Life Cycle Assessment (LCA) is one of the core analytical tools utilized to quantify the environmental impacts of all of the life stages of product and service systems. LCA allows for impacts to be tangible through quantification of effects with impact indicators (Rosenbaum, 2016). However, the focus of impact assessments in LCA has been mainly directed towards terrestrial and freshwater ecosystems. While a fate model has been constructed for OA by Bach et al., (2016), an endpoint characterization model is not yet developed. Thus, a comprehensive impact indicator for OA in LCA is currently missing (Woods et al., 2016).

Development of in-depth cause-effect chains regarding the species responses to OA is necessary to provide a foundation for modelling the cascading effects of OA (Woods et al., 2016). Such mechanistic understandings of marine ecosystems, especially spatially explicit ones are currently lacking in the scientific literature. Furthermore, there are limitations in terms of the development of modelling methodologies for marine impacts (Woods et al., 2016). The global representation of the marine species as well as a consistent interpretation of changes in acidity is lacking (Olsen et al., 2018). Furthermore, a limited number of published scientific resources are available to reflect the extent of marine biodiversity loss induced by acidification. The scope of these publications mostly covers calcifying species, like Azevedo et al. (2015), or warm water species. The representation of non-calcifying species as well as colder region species are limited (Bach et al., 2016), as well as the consequences of longer durations of exposure to a gradual decrease in acidity (Doney et al., 2009).

1.4. Aim of Research

The objective of this thesis research is to address these gaps in knowledge described in *Chapter 1.3*. The overarching goal is to quantify the link between GHG emissions and loss of biodiversity in marine life. The initial aim is to quantify the first section of the impact pathway through understanding the ocean acidification potential of the emitted GHG (SQ1). The secondary aim is to understanding the negative effects of this pH change on the species richness. Hence, SQ2 is formulated. To shed light on the missing aspects in literature such as the limitations in inclusion of non-calcifying species and the effects of geographical and temporal variations separate models will be developed and analysed. The tertiary aim is to link the quantify the impact relations obtained by answering the first two questions through developing a comprehensive impact indicator to be used in LCA.

The main research question and the 3 sub-research questions of this thesis are:

Main RQ: How do GHG emissions affect marine biodiversity loss through ocean acidification?

- ***SQ1:*** How do GHG emissions affect ocean acidification?
- ***SQ2:*** How does the change in ocean acidity affect species richness?
- ***SQ3:*** What is the OA endpoint characterization model for LCA that describes the relation between GHG emissions and marine biodiversity loss?

2

Methods

Chapter 2. Methods

2.1. Life Cycle Assessment

Life Cycle Assessment (LCA) is an analytical method commonly used by industrial ecologists. Its purpose is to understand and assess the impacts of a product or process from cradle-to-grave (Muralikrishna et al., 2017). Cradle-to-grave implies all of the stages from raw material extraction to waste management. The inputs (resources and energy) and the resulting outputs (pollutants and waste) are determined for each of these stages and translated into the extent of their impact on categories such as sustainable resources, biodiversity and climate change (Muralikrishna et al., 2017). LCA is an enabler in terms of choosing the products with life cycles with minimal impact on the environment and society.

Application of LCA

LCA is a systemic approach with four main phases (Brusseau, 2019). The first phase is the goal and scope in which the object of the study is specified. When the object of the study is determined, the following step is data collection and modelling, known as the inventory phase. The third phase is the impact assessment, referred to as LCIA. The purpose of LCIA is to quantify and evaluating the contributions to the impact categories selected in stage one. The fourth and final phase is the interpretation. This phase is aimed at translating the quantitative results into meaningful outcomes based on the objectives of the researchers and stakeholders involved throughout the life cycle. In the interpretation phase, the impact results are compared with the expectations and with other products, processes or services.

Development of LCA

The research on the environmental impacts of products began around the 1960s. The initial studies had a relatively narrow focus, involving impact categories based on energy analysis and pollution (Guinee et al., 2011). Before long, the context of analysis became comparative and it was realized that the impacts of most of the products are not predominantly from the use, but rather in life stages such as transport and production (see Figure 4). With these developments, systems perspective and cradle-to-grave analysis were integrated into the assessment of the environmental impact of the consumer products.

Figure 4 Cradle-to-grave stages used in LCA

Guinee et al. (2011) categorize the development of LCA in decades. The two decades from 1970 to 1990 are identified as “Decades of Conception”. This period is characterized by the broadening scope of LCA through the additions of emissions, waste and resource requirements of products. Moreover, the first impact assessment method was introduced by the Swiss Federal Laboratories for Materials and Testing in 1984. Throughout the decades of conception, LCA was mainly applied by firms who had diverging interests in performing the assessment, without any standard methodological framework. In order to resolve this challenge, the succeeding decade from 1990 to 2000 became the “Decade of Standardization” (Guinee et al., 2011). Within this decade, “The Code of Practice " established by the Society of Environmental Toxicology and Chemistry (SETAC) and international standards developed by the International Organization for Standardizations (ISO). These two associations covered two facets of the standardization requisite of LCA within the given time period. While SETAC focused on harmonizing and optimizing the methods, ISO created international guidelines on how to approach the procedural aspects of the assessment. Impact assessments methods such as endpoint and damage approaches and CML 1992 also developed within this time frame.

Despite the main focus of standardization, ISO 14044, (2006) highlights that “there is no single method for conducting LCA” due to the wide scope of the assessment both in terms of the products and goals of the assessment. With the increasing attention and broadening scope of LCA, the necessity to diversify in methodologies arose. This encompasses the optimization of supporting tools for LCA, development of databases and indicators, and prioritization of transparency and reliability of the assessments. Several institutions such as UNEP and SETAC launched initiatives and partnerships to focus on these improvements and LCA evolved into becoming one of the primary analytical tools for decision-making regarding sustainable development (Brusseau, 2019). To understand the unprecedented impacts of anthropogenic

actions, LCA methodologies are under continuous development. The temporal and spatial specifications of the impacts are researched, impact categories are improved and novel indicators are developed.

2.2. Ecotoxicology Impact Assessment Approach for LCA

The methodological framework of this thesis was formulated based on the ecotoxicology impact assessment approach for LCA, as described by Rosenbaum (2016).

Methodologies for including ecotoxicity as an indicator category in LCA originate from the field of environmental hazard and risk assessments. Within the last decade, the maturity of these approaches became sufficient to be widely used in the application of impact assessments. The ecotoxicological approach aims to quantify the effects of environmental alterations caused by chemicals on biological systems. These effects are measured for specific chemicals in a specific environment. For OA, these chemicals are the GHG emissions and the environment is the ocean. This cause and effect process begins from the source of emission and ends in the response of biological systems. To assess the effects, toxicological tests are utilized. These tests estimate the relationship between the concentration and the effect of the chemicals on certain species. The level of toxicity of the given chemical, the characteristics of the exposed environment and the biological systems within this environment are key variables in determining the extent of the effect. Another variable is the duration and intensity of exposure of the life forms in that medium to the chemical. Understanding the variables and the interaction between them along the impact path can be rather complex. Thus, cause-effect pathways are utilized to understand and analyse these environmental impact mechanisms.

Cause-effect pathways establish the causal relationship between the environmental interventions and their effects, from the release of the chemicals to the environment to their impact on ecosystems (see Figure 5). Once this pathway is established for a chemical, different category indicators can be chosen for application by practitioners. A category indicator is “a quantifiable representation of an impact category” (ISO 14040, 2006). This choice is commonly made considering the goal of the assessment and the type of input data, and it depends on the availability of a mature methodology for that category indicator.

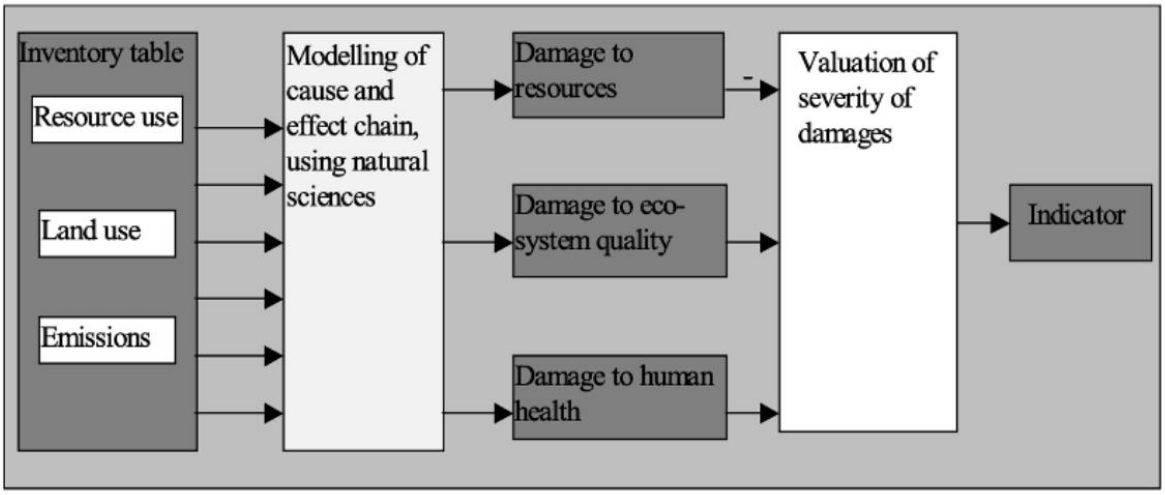


Figure 5 Structure of the endpoint-oriented model based on Eco-Indicator 99 methodology (Goedkoop, M., & Spriensma, R., 2001)

Cause-effect pathways in the ecotoxicological approach can be translated into impact indicators for LCIA through 2 different methods. These two methods are referred as midpoint and endpoint models which represent the impact in different stages of the chain (Bare et al., 2000). Midpoint indicators focus on the effects that are earlier in the cause-effect chain, relatively closer to the interventions (Goedkoop, M., & Spriensma, R., 2001). The uncertainty of the results increases as one moves further in the causal chain, so the midpoint models commonly have the advantage of relying on robust data and scientific information with a higher degree of reliability (Bare et al., 2000). Endpoint indicators, on the other hand, present the results closer to the actual effect that represents greater relevancy to decision-makers (Bare et al., 2000). In the case of OA, the change in the acidity of the ocean is reflected by the midpoint indicator. This environmental mechanism has a higher level of certainty and robustness. Although the level of uncertainty increases with increasing complexity further along the chain, the endpoint indicator provides the actual effect of this mechanism on an ecosystem by quantifying the loss of marine biodiversity (see Figure 6). Endpoint modelling is the selected approach for this thesis to be able to communicate the effects of OA on biodiversity.

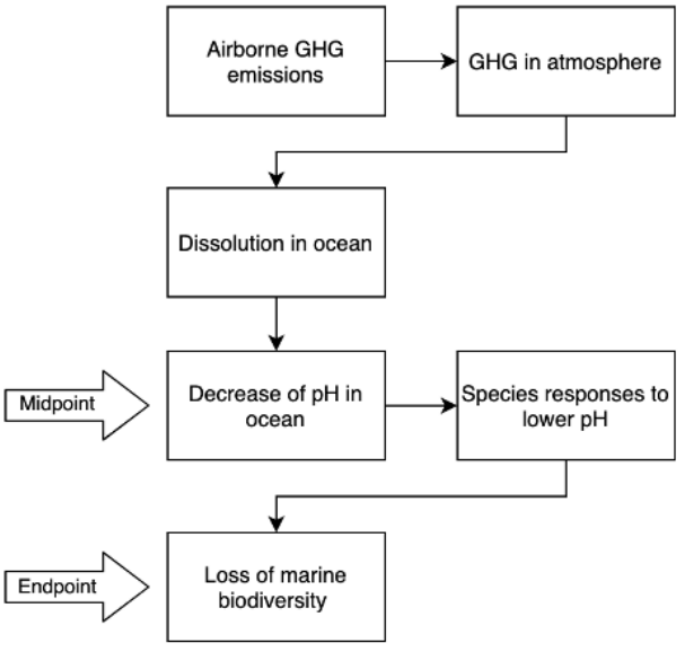


Figure 6 Simplified version of the cause-effect chain for OA including midpoint and endpoint indicators, based on Bach et al. (2016)

To construct the endpoint model for OA with a mechanistic approach, the cause-effect chain is evaluated in separate sections. As explained above, the midpoint model reflects the change in pH of the ocean due to airborne GHG emissions (Figure 6). This requires the modelling of the fate of the emissions from source to dissolution in the ocean. For the endpoint model, this factor needs to be complemented with the extent of exposure and responses of the marine species. This way, the extent of damage on marine biodiversity can be established in relation to the GHG emissions (Figure 6). According to Rosenbaum et al. (2016), these sections of the cause-effect chain are reflected in 4 distinct models for toxic chemicals (in this case, GHG emissions);

(1) The fate model,

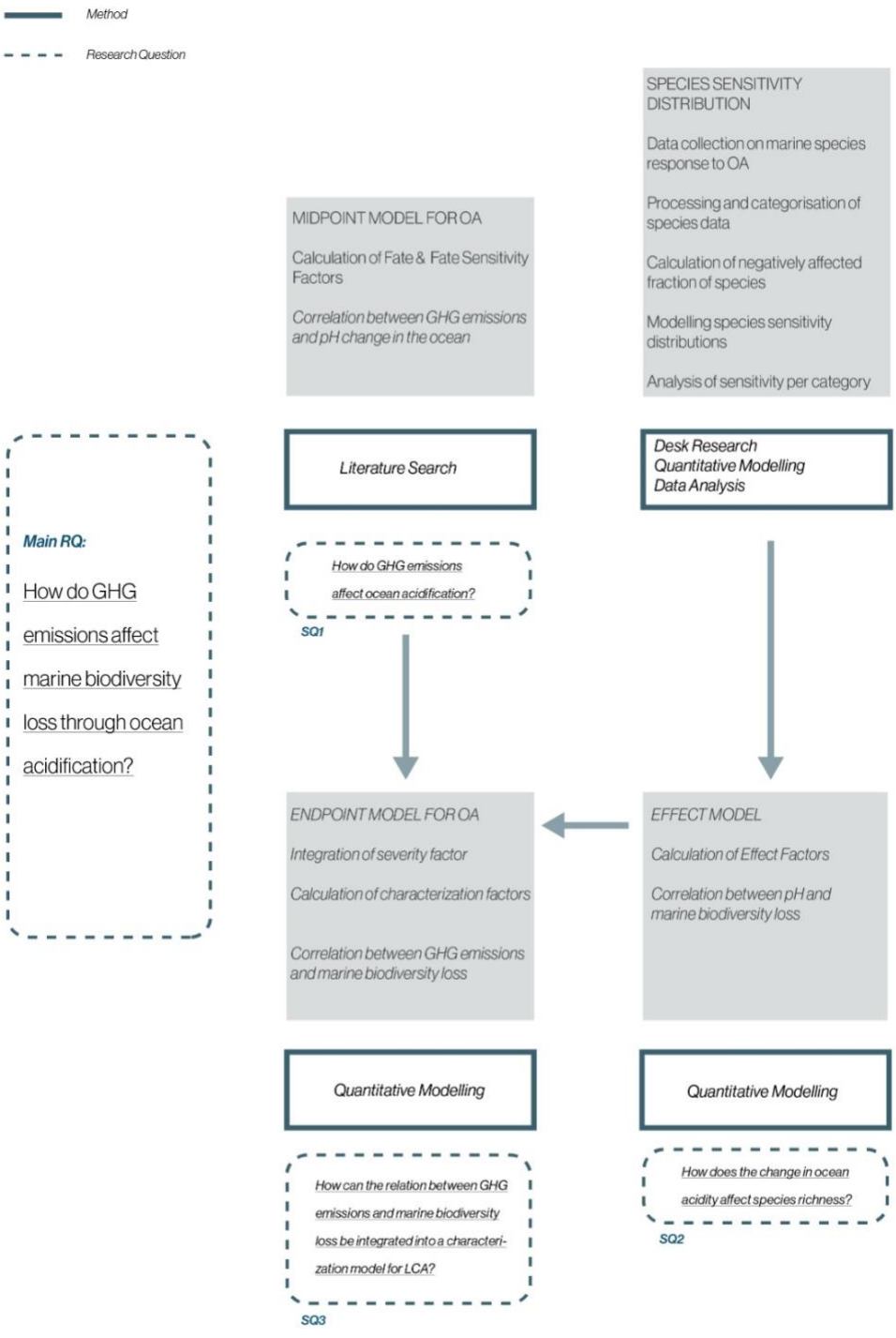
(2) The exposure model,

(3) The effect model,

(4) The damage model.

The definitions and modelling approaches are explained further under the *Chapters 2.3, 2.4* and *2.5*. These models are used as factors to calculate an endpoint characterization factor for OA. This approach is elaborated in *Chapter 2.6.* Data is categorized to further understand whether there are geographic, taxonomic or time-based differences in species responses.

Research Flow Diagram



2.3. Fate and Exposure Models

The objective of the fate model method is to explore the effect of GHG emissions on the OA. The fate model expresses the probability of a substance entering a specific environment. It is the initial step of modelling the mechanisms of ecotoxicity impacts of a substance for LCA (Rosenbaum, 2015). The type of the medium and the geography of the source of the emissions affect the behaviour of the chemicals. For the case of OA, the emissions are released directly into the air and then a certain percentage of them dissolve in the ocean, altering the acidity levels of the water. The fate model for OA is intended to denote the extent of this change in water chemistry on a global level.

The exposure model on the other hand expresses the contact between a target species and the pollutant, which is elucidated by the concept of bioavailability (Rosenbaum, 2015). It covers the duration and frequency of exposure to a substance and is influenced by the amount of chemical available within the given medium. In the case of OA, the probability of the partial reactions in Eq. 1.2.1 is taken into consideration to account for bioavailability. Homogeneity is assumed in terms of exposure of the organisms to chemical composition change along the global ocean surface area. The reason for this assumption is that the airborne emissions dissolve in the ocean surface and it is not within the scope of this research to account for the changes in the bioavailability of the dissolved hydrogen ions in different geographical locations and along the different depths of the ocean.

The chemical behaviour of CO_2 in ocean water is well-known and denoted by Eq. 1.2.1, as previously described in *Chapter 1.2*. Moreover, the current ocean carbon cycle models enable the estimation of variations in ocean carbonate chemistry in relation to atmospheric CO_2 concentrations (Doney et al., 2009). Having established quantitative models that operate on a global scale makes it possible to construct a fate model for OA that is aligned with the LCA method. In the paper "Characterization model to assess ocean acidification within life cycle assessment", Bach et al. (2016) develop a midpoint characterization model based on the cause-effect chain. The midpoint model utilizes the fate model to calculate the characterization factor for OA. In this thesis, the methodological steps of Bach et al. (2016) were followed to construct the fate model, in order to quantify the impacts of GHG emissions on ocean chemistry. The midpoint characterization factor in this model is Ocean Acidification Potential (OAP), which is the product of the fate factor (per elementary flow *i*) and the fate sensitivity factor (see Eq. 2.3.1). The fate sensitivity factor as denoted by Bach et al. (2016) is reflective of the exposure model described by Rosenbaum (2015). The exposure model was therefore included as the fate sensitivity factor within this modelling approach.

$$\text{Ocean Acidification Potential}_i = \text{Fate Factor}_i \times \text{Fate Sensitivity Factor}_i \quad (2.3.1)$$

The fate factor represents the portion of the substances ending up in the ocean and is calculated by Eq. 2.3.2. To answer SQ1, the first step is to identify the elementary flows in terms of their relevance to this impact category. In the case of OA, CO_2, CH_4 and CO were determined as the most significant emissions (Bach et al., 2016) and therefore selected as the elementary flows.

CO_2 can directly dissolve in the water, however, CH_4 and CO need to be converted into CO_2 before entering the ocean. The conversion factor in Eq. 2.3.2 represents the share of these substances (CH_4 and CO) that are converted to CO_2. The conversion reactions occur in the troposphere through OH^- ions (Wuebbles and Hayhoe, 2002). This induces the need to start by calculating the percentage of substances entering the troposphere, which is expressed by the distribution factor. This calculation was done using the values obtained from the literature. The unit of the conversion factor is g_{CO2}/g_i.

$$\text{Fate Factor}_i = \text{Distribution}_i \times \text{Conversion}_i \times \text{Dissolution}_i \quad (2.3.2)$$

Ultimately, the dissolution factor was computed to account for the fact that the environmental compartment within the model is water. Only 25-30% of the atmospheric CO_2 dissolves in the ocean and the rest remains in the atmosphere as GHGs, contributing to global warming (IPCC, 2013). The dissolution factor integrates this dissolving percentage of the substance into the fate factor and was calculated by the ratio of the overall amount of dissolved CO_2 over the overall share of CO_2 able to be dissolved (see Eq. 2.3.3). The latter is equal to the sum of shares of the 3 elementary flow that are able to dissolve (see Eq. 2.3.4). The shares of substances able to dissolve are the product of distribution and conversion factors for the given substance.

$$\text{Dissolution Factor}_i = \text{Overall amount of dissolved } CO_2 \text{ / Overall share of } CO_2 \text{ able to be dissolved} \quad (2.3.3)$$

$$\text{The overall share of } CO_2 \text{ able to be dissolved} = \text{share of CO able to dissolve} + \text{share of } CO_2 \text{ able to dissolve} + \text{share of } CH_4 \text{ able to dissolve} \quad (2.3.4)$$

The dissolution factor is the same for all the substances because CO_2 is the only chemical composition from the 3 elementary flows that can directly dissolve in the ocean. Thus, the dissolution factor can be calculated after knowing the share of CO_2 available in the troposphere, including the CO_2 converted from CO and CH_4. However, the conversion and distribution factors are different per substance. Consequently, after determining the common dissolution factor, fate factors for CO, CO_2 and CH_4 were calculated separately. Unit of the fate factors is g_{CO2}/g_i as the distribution and dissolution factors are unitless whereas the unit of the conversion factor is g_{CO2}/g_i.

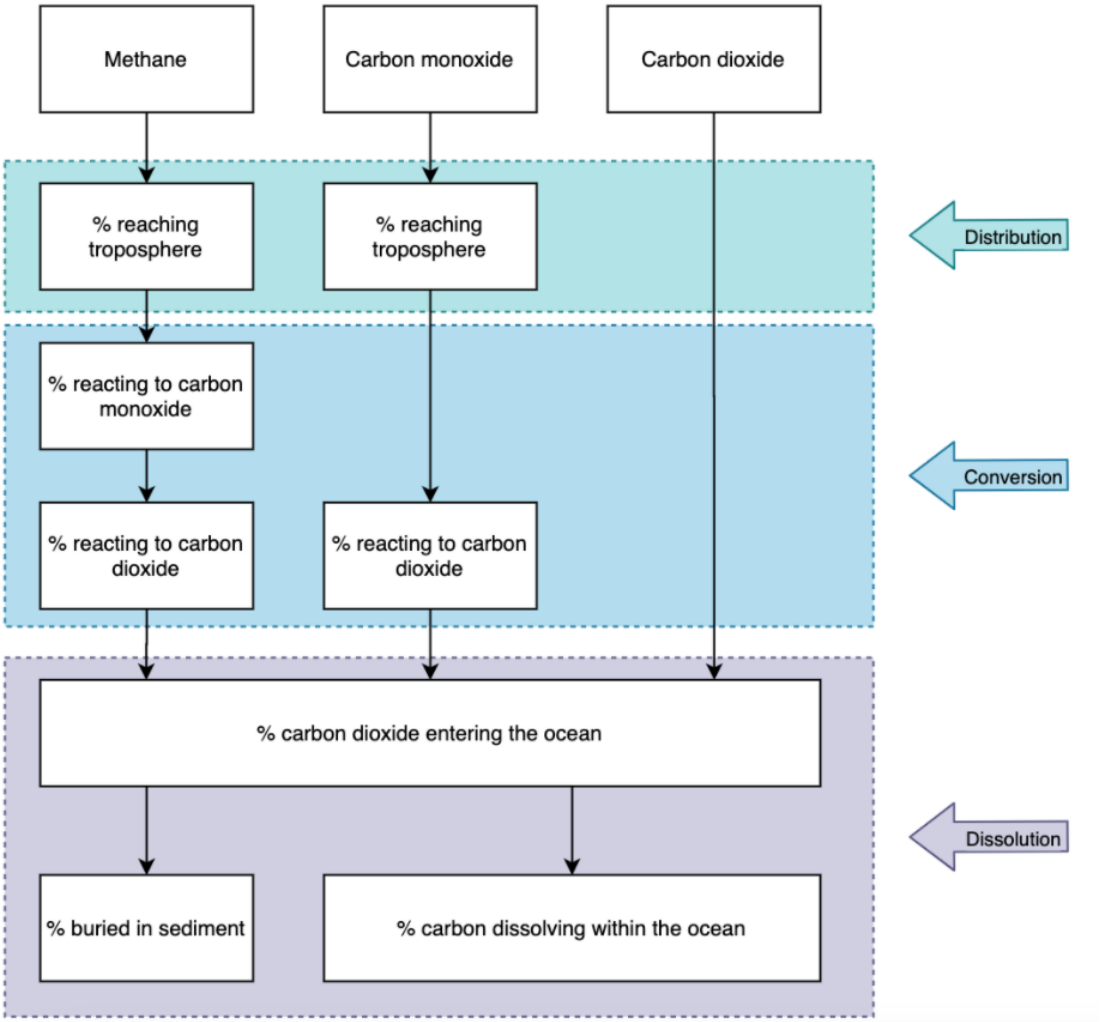


Figure 7 Distribution, conversion and dissolution pathways of CO2, CO and CH4 based on Bach et al. (2016)

Fate sensitivity factor denotes the alterations in the ocean chemistry due to the dissolution of the substances. The approach of Heijungs et al. (1992) for terrestrial and freshwater acidification was utilized to determine the fate sensitivity factor. The primary effect from the cause-effect chain (the amount of H^+ released per gram of substance) was selected as the category indicator as recommended by Bach et al. (2016).

The probability of each reaction taking place is different within the chemical balance denoted by Eq. 1.2.1. Accordingly, to determine the fate sensitivity factor, the number of released H+ ions was calculated per reaction, incorporating the probability of that reaction taking place. Then this number was divided by the molar mass (g/mol) of CO_2, which leads to the fate sensitivity factor with the unit of mol/g_{CO2}. Similar to the dissolution factor, the fate sensitivity factor is the same for all 3 substances as the focal point is dissolution, which always occurs in the form of CO_2. Having computed the fate sensitivity factor and the fate factors for each substance, the OAP can now be calculated by Eq. 2.3.2 to conclude the fate model and exposure models. Through the multiplication of the fate (g_{CO2}/g_i) and fate sensitivity factors (mol/g_{CO2}), the OAP has the unit of mol/g_i, where i = CO_2, CO, CH_4.

2.4. Effect Model

The effect model denotes the percentage of species that become affected by the exposure of the chemical in the given environment (Rosenbaum, 2015). The function of the effect factor is to link and translate the pH change in the ocean into an ecosystem damage indicator; marine biodiversity loss. The effects are typically measured by standardized lab tests and "effect" can have many meanings such as reduced growth, calcification, mortality and oxygen consumption rates. The results of these lab tests are commonly reported with dose-response curves which denote the response of the species to chemical exposure as a function of the concentration of the chemical in the environment (Spurgeon et al., 2020). USEtox model, which is endorsed by Rosenbaum (2015), calculates the effect factor by looking at the hazardous concentration (HC_{50}) values. HC_{50} stands for the concentration level at which 50% of the species in the ecosystem that are negatively affected and can be determined from the species sensitivity distributions. An SSD is a probabilistic model that reflects the sensitivity of an ecosystem or a collection of species in response to being exposed to a substance (Rosenbaum, 2015).

While the overarching approach remains to be based on the chapter by Rosenbaum (2015), several methods were tested and combined in order to develop an effect model. The main reason for this approach is the issue of data availability. Regardless of the choice of method, the initial step was data collection on species responses to OA. The aim is to calculate a global effect factor that would be used in LCIA, thus the data should be representative of marine species on a global scale. However, due to the vast variety of marine species and ecosystems, it is not currently possible to find and include species response data with full taxon coverage. In order to collect data and ensure representativeness per taxon and geographical area, key meta-analyses were identified through a literature search.

In the article "Towards a meaningful assessment of marine ecological impacts of LCA", Woods et al. (2016) provide an overview of the cause-effect based methods related to the drivers of marine biodiversity loss, including OA. In this study, the authors provide a list of quantitative approaches (Zeebe et al., 2008, Doney et al., 2009, Azevedo et al., 2015) that are recognized by the scientific community. From this list, the most recent study is Azevedo et al. (2015), which is also referred to by Bulle et al. (2019) as the "first LCA compliant model covering marine acidification". Therefore, the method of Azevedo et al. (2015) was initially chosen as the framework for constructing the effect model. In their method, the authors focus on observing the effects of OA on calcifying species through constructing SSDs. The initial approach was to expand the dataset to increase the species scope. However, due to data unavailability, the approach of Azevedo et al. (2015) is not utilized further to construct the effect model. The modelling approach of Azevedo et al. (2015) can be found in Appendix H.

Data Collection

The next attempt at data acquisition was to construct a list of potential sources of raw data collection. The authors of several key meta-analyses such as Hendriks et al. (2010), Kroeker et al. (2013) and Wittmann et al. (2013) were contacted to gain access to the raw data collections they used to perform these analyses. The datasets acquired from these meta-analyses were analysed in terms of compatibility with the data requirements of the ecotoxicological approach and being the most suitable, the dataset of Wittmann et al. (2013) was selected. The study by Wittman et al. (2013) is a meta-analysis that studies the effects of altered seawater carbonate chemistry on various marine species. Consequently, their analysis approach was adopted in order to be able to work with the data format of the provided dataset. In this dataset, responses of the species to OA are not expressed in terms of effect size, which is the common approach in meta-analyses in this field of research. Instead, the authors collected the species responses from multiple experiments and then categorized these responses as none, negative or positive. The effects are not quantified and there is no distinction between life processes. Non-calcifying species are included within the scope and there are 5 different animal taxa: cnidaria, echinoderms, molluscs, crustaceans and fish. Physiological performance of the species such as growth, morphology, fertilization, behavioural changes, immune response and metabolic rate are collected. Overall, there are 153 species included in the analysis which are further categorized based on the duration of the experiments.

The species responses were analysed across different p_{CO2} ranges which were determined using representative concentration pathways (RCPs) based on the work of Meinshausen et al. (2011). The p_{CO2} bins range from 500-651, 651 - 850, 851 - 1370, 1371 - 2900, 2901 - 10000 and above 10000 µatm (Wittmann et al., 2013). Most of the experimental data include the response measurements for 2 to 3 different p_{CO2} values. To compensate for the missing data for the rest of the p_{CO2} bins, the authors employed 2 main assumptions. The first assumption indicates that if a species shows negative effects at low p_{CO2} levels, then it will also be negatively affected at the higher p_{CO2} levels. The second assumption is that if a species has the same effect at a high and a low p_{CO2} levels, then that effect will be the same for the p_{CO2} levels in between those high and low values. The interpretation of negative, positive and none was done by comparing the results to the effects observed in the control treatments. In most of the studies, the control treatment is approximately around 380 µatm and only the studies before February 2012 were included.

Expansion and Processing of the Dataset

For this thesis research, the dataset of Wittmann et al. (2013) was expanded with the purpose of including more data points from the recent scientific literature and to be able to conduct analysis based on different categorizations of data. Pangaea is an Open Access Library for data related to earth system research (Data Publisher for Earth & Environmental Science, 2021). This data source was identified from the paper "Data compilation on biological response to Ocean Acidification: An update" (Yang et. al, 2016) and was used as the data platform to collect more species response data. As previously mentioned, the format of the database requires the responses to be categorized into positive, negative and none. It is claimed by the authors that this categorization is based on expert opinions. In order to be aligned with this approach, only the papers with clear declarations on the trend of the impact - as significantly negative or positive - were added to the dataset, leaving the interpretation to the authors of the articles. This limits the number of studies that can be included in the expansion of the current dataset. If there are multiple experimental data available for a single species and the effects are different from each other for the same p_{CO2} bins, then priority was given to the experiments with the longest duration and then to the results indicating a negative effect.

The additional data collection was performed based on the underrepresented data categories. The data available for the fish species as well as the species that live in polar regions are limited within the dataset from the meta-analysis of Wittmann et al. (2013). The keywords "fish" and "ocean acidification" were used to initiate the literature search within Pangaea in order to collect more responses of fish species. The experiment results between the years 2014 and 2021 were scanned and selected depending on their relevance and their alignment with the criteria explained above. Response types such as metabolic and behavioural effects are included in the fish data. 17 new studies on fish species are added to the dataset (see Appendix A). In order to enlarge the scope of the polar species, two rounds of search were executed. The keyword "OA" was coupled with "arctic" and "antarctic" respectively. The search included studies from 2013 to 2021, which resulted in the addition of 10 new studies from the polar region (see Appendix A).

Overall, the number of scientific studies within the given time frame is larger than the number of data points added to the dataset. There are several reasons for this selective addition. First of all, some species such as Amphiprion percula, Godus morhua and Acanthochromis polyacanthus are repetitively present in the experiments in OA research. For Amphiprion percula, 7 different studies were already included within the dataset for the given species, indicating a negative response across all of the p_{CO2} bins. Therefore, an addition of a new study with a shorter duration did not alter the response results in the dataset. Moreover, some researchers such as Mccormick et al. (2018) or Nagelkerken et al. (2016) examined the effect of OA on the interaction between prey-predators, the symbiotic relationships between different species or the combined effects of OA and temperature change. These types of studies were also excluded due to the multitude of independent variables within the experiments. Another example is the type of studies that looked into the effects of fluctuating aquatic CO_2 as the independent variable is the change in CO_2 pressure rather than a distinct p_{CO2} value. Last but

not least, most of the OA experiments focus on highly abundant species such as various algae types, which were not included in the scope of this research.

Categorizations

Information on both the experiment variables (temperature, duration, type and number of variables, control pressures) and species characteristics (class, habitat) were recorded in the dataset because the response of the marine species to the acidifying ocean is dependent on various factors. Temperature, for instance, is one of these factors and a prominent one. The temperature of the water affects the solubility of aragonite and the saturation state, therefore influences the bioavailability. The effect of temperature on the chemical states and reactions can lead to diverse outcomes in terms of species response. Another variable is the duration of the experiments that were conducted to measure the responses. Longer durations of exposure to a less alkaline environment are expected to increase the rate and extent of the changes occurring within the biological systems. While this remains true, the possibility of adaptation of species over longer durations also remains a valid possibility. In order to understand the impact of some of these variables on the results, the data were categorized into certain sections.

The core categorizations of the species response analysis were geographical zones (temperate, tropical, polar), duration of experiments (acute, sub-acute, chronic) and calcification capability of the taxons (strongly calcifying, slightly calcifying). The reasoning behind the geographical classification is that the rate of OA is different in different latitudes. Polar oceans are considered the most vulnerable regions due to the different saturation states induced by lower temperatures (Schmutter et al., 2017). In terms of calcification, the strongly calcifying taxa were considered as molluscs, echinoderms and cnidaria, whereas the slightly calcifying taxa were grouped as fish and crustaceans based on the approach of Wittmann et al. (2013). The strongly calcifying species have lower metabolic rates, are relatively more sedentary and build heavier skeletons through calcification. Crustaceans and fish, on the other hand, have significantly lower intensity in calcification, higher mobility and better acid-base regulation (Wittmann et al., 2013). Last but not least, the boundaries of categorization in terms of the duration of the experiments are dependent on whether the species is a vertebrate or an invertebrate. From the 5 taxa, fish is vertebrate while the remainder are invertebrates. The distinction was made based on the work of Rosenbaum (2015). Acute duration indicates brief periods of exposure and is measured in relation to the lifetime of the species. Acute exposure duration is <7 days, which is the same for both vertebrates and invertebrates. Chronic experiment duration indicates longer periods of time that would be equivalent to one or more life cycles or sensitive periods of the given species. Sensitive periods describe specific time thresholds at which the species groups become more vulnerable towards negative influences from the environment (Bodin et al., 2011). The chronic period is >32 days for vertebrates and >21 days for invertebrates. The period between acute and chronic was classified as sub-chronic duration.

Modelling Approach

Following the data collection and processing stages, the effect of OA was modelled. The SSDs were constructed that indicate the relationship between PAF and pH. The data under each category was grouped based on their taxon. To account for the global relative species richness of each taxonomic group, global normalization factors were calculated. The number of extant number of species were obtained from the literature (see Appendix C). These factors represent the ratio of the number of extant species per taxon to the total number of extant species for the 5 taxa (see Appendix C). The total number of global extant species for the taxonomic groups included in this study is calculated as 132,000. For instance, the number of extant species for Echinodermata is found to be 7000. The global normalization factor for this taxon is therefore 7,000/132,000 = 0.053. Weighted averages of the negatively affected fractions per each taxonomic group were obtained using the global normalization factors. In this way, the negatively affected fraction of species per each p_{CO2} range for each category were obtained.

Due to the assumptions explained in the dataset acquisition section, there are different numbers of responses per each p_{CO2} bin. In order to account for this, weighing factors were determined as the ratio of the number of species responses within a bin to the total number of responses in that category. Then, the averages of the upper and lower limits of the bins were calculated to have one partial pressure value per PAF. The responses of the control group were recorded as zero because the control groups function as a reference to measure the extent of change. The control pressures of the categories on the other hand are calculated by taking the average of the control pressures of the experiments within the categories. These control values were then used as the initial data point of the regressions.

The ecotoxicological models use the concentration of the chemicals as the independent variable. However, the independent variable for the model at this stage was represented by the p_{CO2}, which is partial pressure rather than concentration. Therefore, the mean p_{CO2} values were converted to pH (see Appendix B). Eq. 2.4.4 expresses the relationship between pH and p_{CO2} on a global scale and was utilized for this conversion (Feely et al., 2009) (see Figure 8). The negatively affected fraction of species and their associated pH values were then fitted into a non-linear regression using Eq. 2.4.5 to construct the SSDs. Eq. 2.4.5 denotes a species sensitivity curve with a variable slope called hillslope, where A is equal to $\log_{10}HC_{50}$. HC_{50} represents the hazardous concentration level at which 50% of the species are affected.

$$pH = -0.38 \times \ln(p_{co2}) + 10.32 \quad (2.4.4)$$

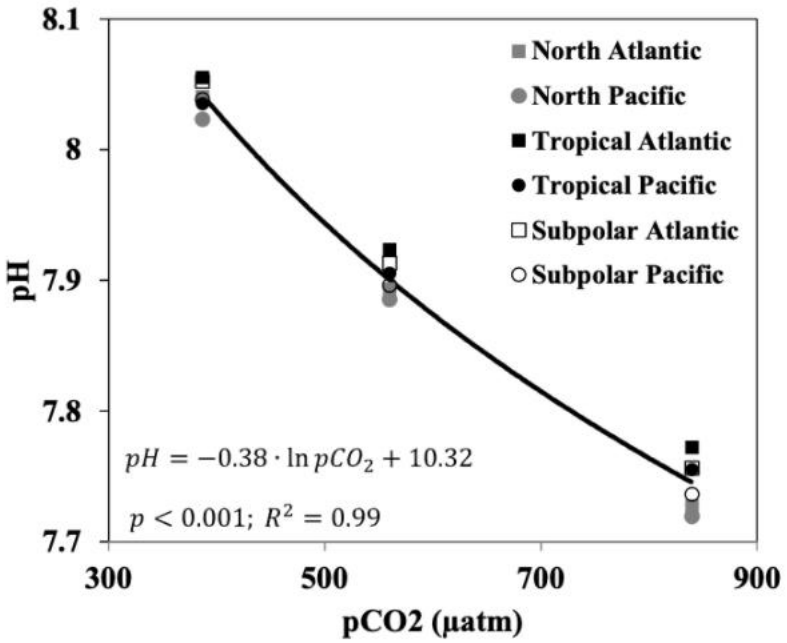


Figure 8 p_{CO2} - pH relationship on a global scale (Feely et al., 2009)

$$Y = \frac{100}{1+10^{(A-x)\times B}} \tag{2.4.5}$$

The original hillslope equation (see Eq. 2.4.6) is a commonly used 4 parameter logistic model for dose-response analysis (Gadakgar et al., 2015). The 4 parameters in this equation are; bottom response, top response, HC_{50} and hillslope coefficient. "x" represents the logarithm of dose or concentration, whereas "y" represents the response in a normalized form. Bottom and top values indicate the asymptotes of the non-linear regression. As the response values are represented in percentages, the bottom value was set as 0 and the top as 100. Setting these values as such reveals that Eq. 2.4.5 is a form of Eq. 2.4.6; that the variable "B" in Eq. 2.4.5 is equal to the Hillslope coefficient in Eq. 2.4.6. Hillslope coefficient, also known as the slope factor, is unitless and quantifies the steepness of the curve (Gadakgar et al., 2015). The higher the slope factor, the steeper the slope of the regression (see Figure 9). The slope of the model is indicative of the sensitivity of the species as it denotes the rate of change of the effect with changing pH. In other words, having a steeper slope indicates higher sensitivity to a change in concentration.

$$Y = Bottom + \frac{Top-Bottom}{1+(\frac{10^{LogHC50}}{10^{x}})^{Hillslope}} \tag{2.4.6}$$

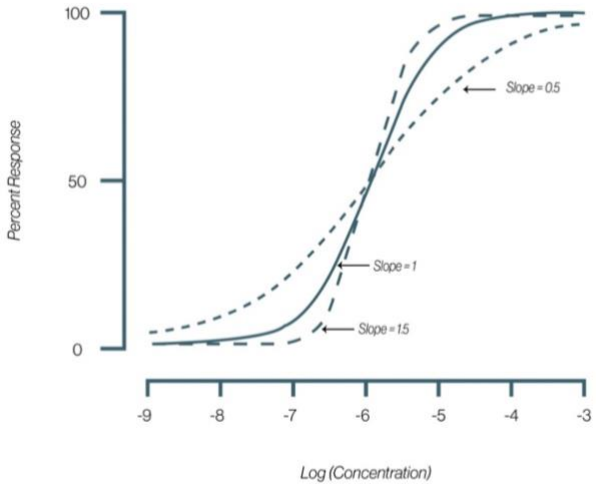


Figure 9 Hillslope curves indicating different slope values

The models were constructed and analysed in R (see Appendix I). The nls() function, which stands for "nonlinear least squares", was used for finding the two variables (A and B) in Eq. 2.4.5. The function of nls() is to determine the parameter values of nonlinear fits (Baty et al., 2015). The slope factor and pH_{50} values (pH value at which 50% of the species are negatively affected) were used to analyse the sensitivity of the species within each category to the change in acidity of the ocean. In ecotoxicology, the SSDs tend to express the increasing effect with increasing concentration. In the case of pH, this is reversed as pH is equal to the negative logarithm of H^+ ions. Therefore, the absolute value of the b value was considered while comparing the slopes of the regressions.

For assessing the goodness of fit of the models, pseudo R^2 values were calculated per SSD. In linear regression, the goodness of fit is generally expressed as R^2. However, in a non-linear regression, R^2 is considered an inadequate measure (Spiess & Neumeyer, 2010). Instead, modified versions of R^2 such as Cox-Snell, Efron or Nagelkerke R^2 are suggested by the literature for the non-linear models (Smith & McKenna, 2013). Being one of the most commonly utilized Pseudo R^2 versions for non-linear regressions, Nagelkerke R^2 was selected as the statistic for SSDs. The second statistic chosen for analysing the goodness of fit is the residual standard error, which is the standard deviation of the residuals of the regression. Smaller residual standard error values imply better fits.

Once the strength of the models was assessed by obtaining these two statistics, they were compared to each other to evaluate the species response data in different categories. The selected approach for this comparison is the introduction of interaction variables to the free parameters of the models (A and B) (Karaca-Mandic et al., 2012). These variables were added to Eq. 2.4.5 in a way that can move the parameter values up or down and tested against 0. M is the interaction variable for parameter A and N is for parameter B (see Eq. 2.4.7). To account for the different categories within the datasets, (for example, polar species versus tropical

species) a binary indicator variable (ind) was also included in the equation. Both the estimations for the interaction variables and their p values were utilized to analyze whether the difference between model parameters is statistically meaningful enough to calculate individual effect factors. Effect factors were then calculated for the statistically meaningful categorizations and for the SSD constructed using all of the data points.

$$y = \frac{100}{1+10^{(A+M\times ind-x)\cdot(B+N\times ind)}} \quad (2.4.7)$$

According to Rosenbaum (2015), the effect factor typically has the dimension of PAF and the unit of m^3/kg. The effect factor is the ratio of 50% change in PAF to the corresponding change in hydrogen ion concentration (see Eq. 2.4.10). The pH values at 0% and 50% PAF values are converted to hydrogen ion concentrations using Eq. 2.4.8. The difference between these two concentrations were calculated using Eq. 2.4.9, which indicates the HC_{50} values. The litre in the unit of $\Delta[H^+]$ is then converted to m^3. The effect factor for OA was calculated using Eq. 2.4.10 and has the unit of (PAF) m^3/mol.

$$At\ PAF\ 50\%, [H^+] = 10^{-pH50}$$

$$At\ PAF\ 0\%, [H^+] = 10^{-pH0} \quad (2.4.8)$$

$$10^{-pH50} - 10^{-pH0} = \Delta[H^+] \quad (2.4.9)$$

$$EF = \frac{0.5\ PAF}{\Delta[H^+]} \quad (2.4.10)$$

2.5. Damage Model

The last model in characterization modelling is the damage. This is also called the severity model and it incorporates the furthest section of the ecotoxicity impact pathway into the endpoint model (see Figure 10). After knowing the effects of a toxic chemical on the biological systems within an environment, the damage model can be constructed by transforming the potentially affected fraction (PAF) of species to the potentially disappeared fraction (PDF) of species, reflecting the damage on ecosystem quality. However, there is no consensus from the scientific community on how to determine PDF (Rosenbaum, 2015). One of the current approaches in LCA, as also utilized in ReCiPe, is assuming that 50 % of the potentially affected fraction of species will disappear from the ecosystem (Rosenbaum, 2015). Therefore, the damage factor was calculated using Eq. 2.5.1.

$$PDF = PAF\ /2 \tag{2.5.1}$$

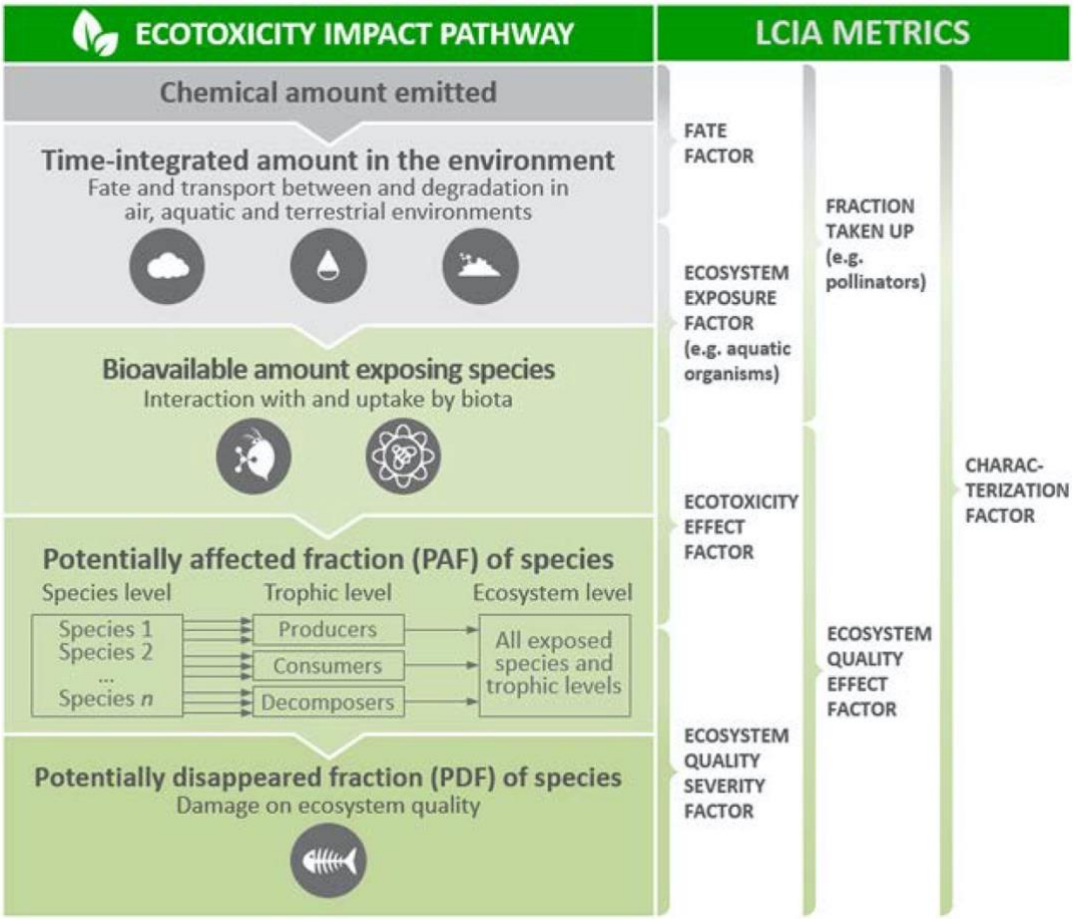


Figure 10 Conceptual representation of ecotoxicity impact pathway in life cycle impact assessment (LCIA) (Angeler et al., 2019)

2.6. Characterization Model

The characterization model indicates the relation between an elementary flow and its impact through the characterization factor (see Figure 10). The ISO 14040 (2006) definition of the characterization factor is: "a factor derived from a characterisation model which is applied to convert the assigned LCI results of the common unit of the category indicator". The model is constructed in relation to a specific category indicator. As discussed previously, for OA, the midpoint category indicator was selected as OAP and the endpoint indicator as the loss of marine biodiversity. The third sub-research question was answered by employing the results of the first two sub-questions. Fate, exposure, effect and damage factors were calculated to answer these questions. As explained in *Chapters 2.3 and 2.5*, the exposure factor was already integrated into the fate model and the severity factor was obtained by translating PAF to PDF by multiplying with 0.5. Consequently, the characterization factor for the endpoint environmental mechanism of OA was determined by multiplying the fate, exposure, effect and damage factors (see Eq.2.6.1), which links the OAP at the midpoint to marine biodiversity loss at the endpoint. The unit of the endpoint characterization factor is (PDF) m^3/kg-GHG emitted.

$$Characterization\ Factor = Fate\ Factor \times Exposure\ Factor \times Effect\ Factor \times Damage\ Factor \quad (2.6.1)$$

3

Results

Chapter 3. Results

3.1. Fate and Exposure Model Results

In this chapter, the results of the fate and exposure models are provided to answer the first sub-question; *"How do GHG emissions affect ocean acidification?".*

The fate and exposure model results are based on the work of Bach et al. (2016). As can be seen in Table 1, there are 3 different OAPs, each for a different GHG emission. CO_2 is the chemical that dissolves in the ocean; therefore, the distribution and conversion factors are equal to 1. Thus, CO_2 has the highest potential for changing the pH of the ocean compared to CO and CH_4 ($OAP_{CO2} = 2.47 \times 10^{-3}$ mol H^+/g_{GHG}). Though having similar values with CH_4, CO has the lowest distribution factor compared to the other two substances (0.871). However, due to having a lower conversion factor compared to CO, CH_4 has the lowest acidification potential ($OAP_{CH4} = 2.05 \times 10^{-3}$ mol H^+/ g_{GHG}). The fate sensitivity factors are representative of the exposure factors and are equal for all of the emission types (2.45×10^{-2} mol H^+/g_{CO2}). Further explanations and calculations to obtain the results in Table 1 can be found in Appendix D.

Table 1 Results of the Fate and Exposure Model for the 3 elementary flows

	CO	**CH_4**	**CO_2**
Distribution Factor	0.871	0.878	1
Conversion Factor (g_{CO2}/g_{GHG})	1	0.95	1
Dissolution Factor	0.1008	0.1008	0.1008
Fate Sensitivity Factor (mol H^+/g_{CO2})	2.45×10^{-2}	2.45×10^{-2}	2.45×10^{-2}
OAP (mol H^+/ g_{GHG})	2.15×10^{-3}	2.06×10^{-3}	2.47×10^{-3}

3.2. Effect Model Results

In this chapter, the results of the effect model are provided to answer the second sub-question; *"How does the change in ocean acidity affect the marine species richness?".* The effect of the alterations of ocean carbonate chemistry on species richness is analysed. Within each categorical comparison, model parameters, the goodness of fit results and statistical significance of the difference between groups are presented.

Calcification Category Results

There are two groups in this categorization: "(strongly) calcifying species" and "slightly calcifying species". The calcifying species consist of 3 taxonomic groups: mollusca, echinodermata and cnidaria, overall including 96 species responses. The slightly calcifying species consist of 80 species responses from 2 taxonomic groups: fish and crustacea. As explained in *Chapter 2*, the calcifying species are expected to be affected more by OA than the remainder of the species groups. This assumption is tested by constructing SSDs, which is shown in Figure 11.

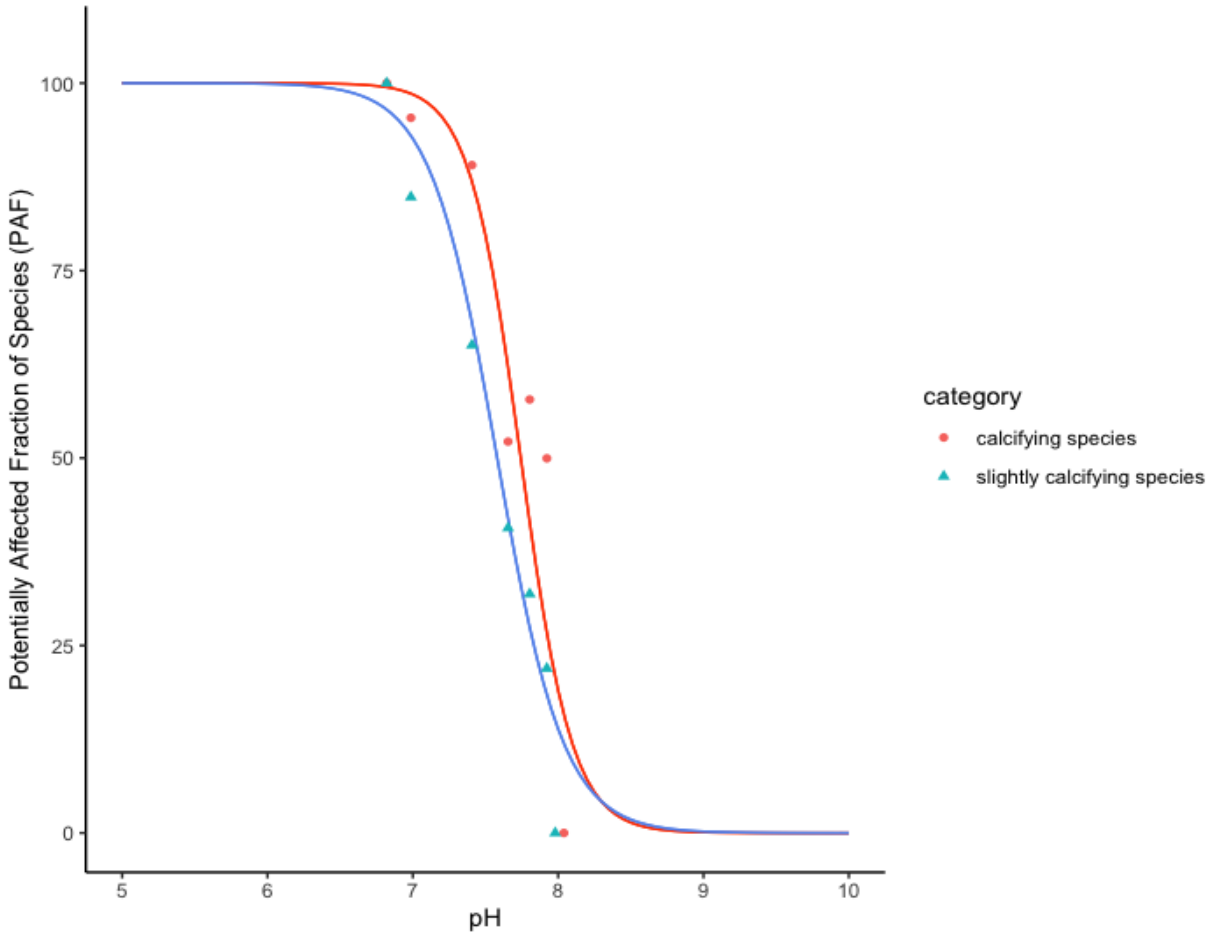


Figure 11 SSDs of calcifying and slightly calcifying species

The goodness of fit of these regressions are analysed by looking at the Pseudo R^2 and RSE values. Although the R^2s are quite similar for these two groups, slightly calcifying species SSD has a slightly better fit compared to calcifying species ($R^2_{scal} = 0.898 > R^2_{cal} = 0.870$). This is also endorsed by the higher RSE of the calcifying SSD ($RSE_{cal} = 11.90$), indicating a larger error compared to the other regression ($RSE_{scal} = 9.52$).

Table 2 Model parameters, number of species, average control pH values (pH_0) and goodness of fit results for category "calcification"

Category	pH_{50}	Hillslope	Number of Species	Average pH_0	ΔpH	Pseudo R^2	RSE
Calcifying species	7.743	-2.447	96	8.046	0.303	0.870	11.90
Slightly calcifying species	7.581	-1.891	80	7.983	0.402	0.898	9.52

By looking at the graphs (see Figure 11), it can be seen that there is a difference in the predicted values, especially at lower pH levels. The gap between the two regression lines is narrowing down with the increasing pH. Beyond this visual interpretation, the difference between the SSDs of calcifying and slightly calcifying species is assessed by utilizing the estimated model parameters. The calcifying species have a higher pH_{50} value (7.743) compared to the slightly calcifying species (7.581). This implies that 50% of the calcifying species are already negatively affected at higher pH values (lower CO_2 pressure). Furthermore, the calcifying species also have a higher rate of change (2.447) compared to slightly calcifying species (1.891), highlighting a higher sensitivity. The percentage of the negative responses changes more rapidly by increasing acidity when the slope is higher. The difference between the control and pH_{50} values endorse this trend as well. At control pH (pH_0), the negatively affected percentage of species is equal to zero for all categories. A pH change of 0.303 is required for 50% of the calcifying species to be affected. This value is higher for slightly calcifying species (0.402). To sum up, all of the indicators of sensitivity (pH_{50}, slope and ΔpH) confirm that the calcifying species are indeed more sensitive to OA.

Table 3 Interaction term test results for calcification category, including the estimated values for the differences between the model parameters and their p-values

	Estimation	**p-value**
M	0.199	0.031
N	-0.501	0.576

The statistical significance of the difference between the categories is tested to validate the decision to calculate separate effect factors for this category. It is assumed that the p-value at 0.05 for the estimation of the interaction terms is significant. The difference between the pH_{50} values (M) is estimated to be 0.199 with a p-value of 0.031. This error rate is lower than the selected significance threshold and therefore considered acceptable. The p-value for the differences in slopes of the regressions (N) is not significant enough with a p-value of 0.576. However, the test results are considered to confirm the hypothesis on the difference between categories as one of the model parameters is statistically significant. Therefore, the effect factors are calculated for both groups within this category.

Effect factor for calcifying species:

$$At\ PAF\ 50\%, [H^+] = \ 10^{-7.743} = 1.807 \times 10^{-8}\ mol/L$$
$$At\ PAF\ 0\%, [H^+] = \ 10^{-8.046} = 8.994 \times 10^{-9}\ mol/L$$
$$\Delta[H^+] = 9.077 \times 10^{-9} \frac{\text{mol}}{\text{L}} * \left(\frac{1000\text{L}}{1m^3}\right) = \ 9.077 \times 10^{-6} \text{mol}/m_3$$

$$EF_{cal} = \frac{0.5\ PAF}{9.077 \times 10^{-6}\ mol/m^3} \ = \ 5.508 \times 10^4\ (PAF)\ m^3/\ mol$$

Effect factor for slightly calcifying species:

$$At\ PAF\ 50\%, [H^+] = \ 10^{-7.581} = 2.624 \times 10^{-8}\ mol/L$$
$$At\ PAF\ 0\%, [H^+] = \ 10^{-7.983} = 1.039 \times 10^{-8}\ mol/L$$
$$\Delta[H^+] = 1.584 \times 10^{-8} \frac{\text{mol}}{\text{L}} \times \left(\frac{1000\text{L}}{1m^3}\right) = \ 1.584 \times 10^{-5} \text{mol}/m^3$$

$$EF_{scal} = \frac{0.5\ PAF}{1.584 \times 10^{-5}\ mol/m^3} \ = 3.165 \times 10^4\ (PAF)\ m^3/\ mol$$

The fraction of the potentially affected species is higher for calcifying species (EF_{cal} = $5.508 \times 10^4\ (PAF)\ m^3/\ mol$) compared to slightly calcifying species (EF_{scal} = 3.165×10^4 *(PAF)* m^3/ mol).

Climate Zones Category Results

There are three groups in this categorization: "polar species", "temperate species" and "tropical species". The polar species category includes 21 species, which is the least amount of data points compared to the other two categories. The temperate region with 73 species and the tropical region with 82 species are close to each other in terms of the number of data points. SSDs of the species from these 3 regions are constructed to explore whether there are differences in the effect of OA on species based on geographical differences (see Figure 12). The goodness of fit of the polar region SSD is the lowest amongst the 3 groups (R^2_{polar} = 0.837, RSE = 14.30). Both the temperate and tropical categories have R^2 values higher than 0.9, indicating better fits of models. Tropical region SSD has a better fit compared to the other groups by having both the lowest RSE (8.67) and highest R^2 (0.959).

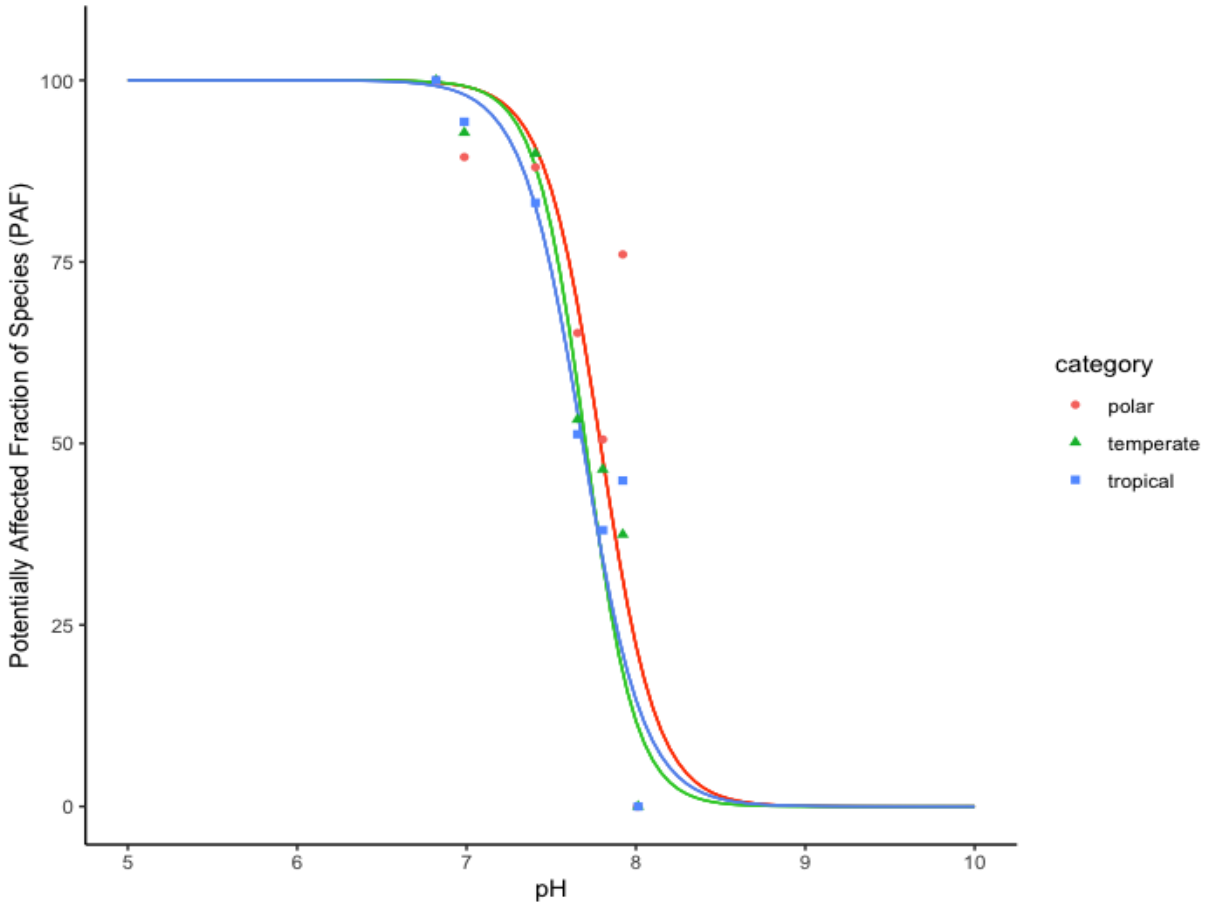


Figure 12 SSDs of species from polar, temperate and tropical regions

Even though the difference is not large between the 3 groups, the SSDs show that the most sensitive group is the species from the polar region. The temperate and tropical SSDs are overlapping, especially within the pH range between 7 and 8. Polar SSD is positioned more towards the right side of the graph (see Figure 12) with a higher pH_{50} value (7.790) compared

to the temperate (7.703) and tropical (7.686) regions, which are almost the same. The temperate region has the highest slope value (2.943) in comparison to the other two regions. The difference between the control pH and pH_{50} (ΔpH) for the polar species group is equal to 0.264, which is the smallest value amongst the 3 groups.

Table 4 Model parameters, number of species, average control pH values and goodness of fit results for category "climate zones"

Category	***pH_{50}***	***Hillslope***	***Number of Species***	***Average pH_0***	***ΔpH***	***Pseudo R^2***	***RSE***
Polar	7.790	-2.593	21	8.055	0.264	0.837	14.30
Temperate	7.703	-2.943	73	7.986	0.283	0.916	9.35
Tropical	7.686	-2.429	82	8.043	0.357	0.959	8.67

To understand if the model parameters statistically differ between the 3 groups, interaction variables are introduced and tested. As the indicator variable is selected as binary in the interaction term test, 2 groups are tested against each other at a time. The p-values of all of the tests show that there is no statistically significant ($p > 0.05$) difference between the 3 SSDs (see Table 5). The small difference between the temperate and tropical SSDs is also seen from the high p-value of the test between the groups (0.823). Consequently, no separate effect factors are calculated for the climate zones category.

Table 5 Interaction term test results for climate zones category, including the estimated values for the differences between the model parameters and their p-values

Test		***Estimation***	***p-value***
Polar vs. Temperate	***M***	0.072	0.378
	N	0.102	0.944
Polar vs. Tropical	***M***	0.097	0.259
	N	-0.239	0.860
Temperate vs. Tropical	***M***	0.025	0.680
	N	-0.342	0.731

Duration Category Results

The exposure lengths of the marine species to acidic environments are different in each experiment. To test whether there is a difference in responses to shorter and longer exposure durations, the data is divided into 3 groups. The first group is "acute responses" which includes the experiments that are less than 7 days of exposure. 58 of the experiments belong to this category. Another one of these 3 groups is "chronic responses". This group has the highest number of species responses (78). Chronic indicates longer exposure to an acidic environment. The third group is the "sub-chronic responses" with 40 experiments.

When a species is exposed to a substance for longer durations, the primary assumption is that the effects will be more severe. However, there is also the possibility of adaptation and alterations in behaviour throughout those longer exposure times. With the purpose of assessing the impact of this time variable on the species response, SSDs are constructed per group (see Figure 12). The acute SSD has the lowest RSE (6.34) amongst the 3 groups ($RSE_{chronic}$ = 10.40, $RSE_{subchronic}$ = 10.60). Even though this is the case, all 3 SSDs are considered good fits due to having R^2 value higher than 0.9.

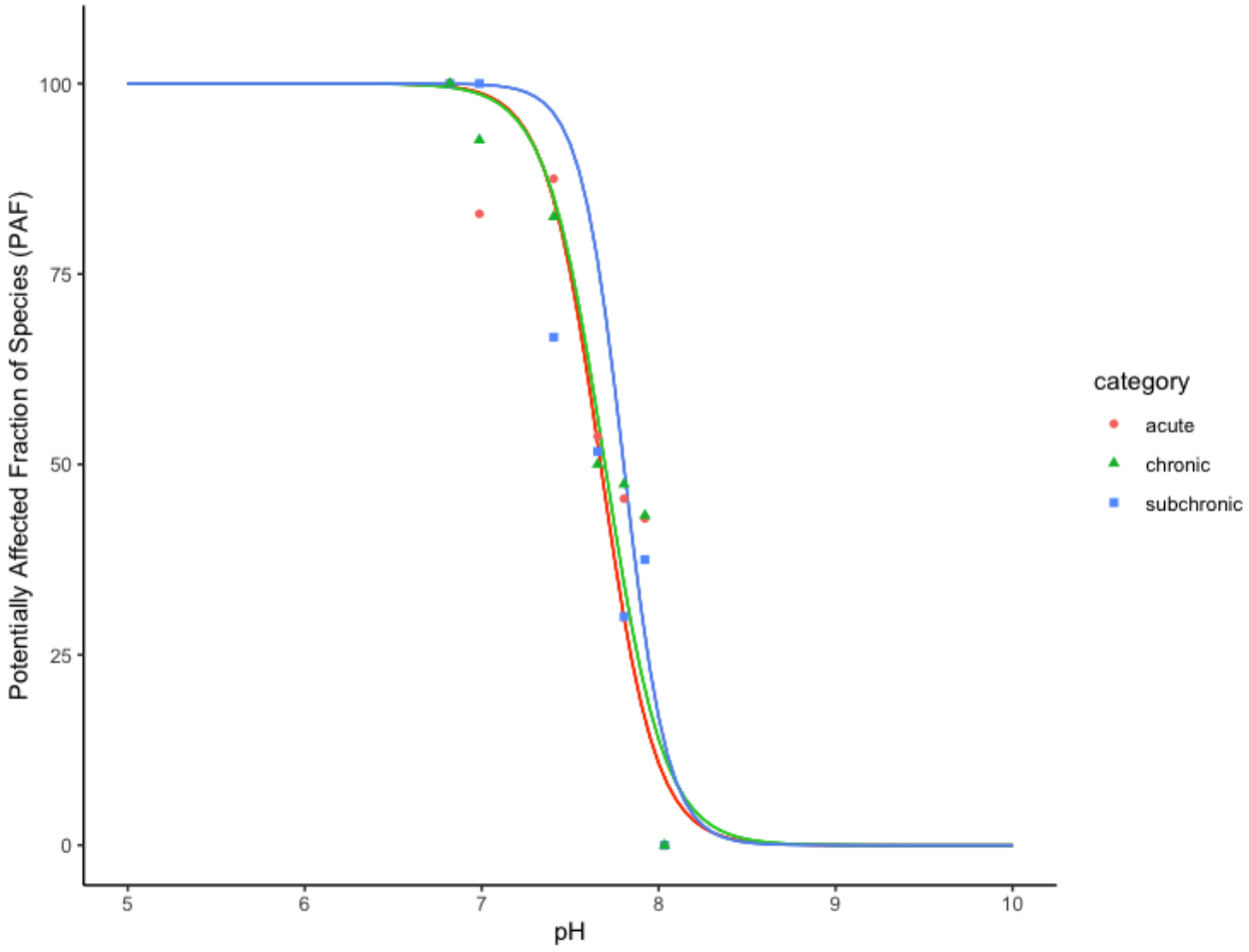


Figure 13 SSDs of species groups with different groups of experiment durations (acute, chronic, sub-chronic)

The highest pH_{50} value (7.805), as well as the steepest slope (3.454), belong to the sub-chronic group. This shows that the sub-chronic responses have a high sensitivity in terms of responding to acidification. It is visible in Figure 13, acute and chronic models are eminently similar. The pH_{50} of the chronic group (7.698) is very close to the value of the acute group (7.674); the difference between the pH_{50} of these two models is as low as 0.024. A pH change of 0.359 is required for 50% of the species to get affected for the acute group whereas this difference is equal to 0.312 for the chronic group.

Table 6 Model parameters, number of species, average control pH values and goodness of fit results for category "duration"

Category	***pH_{50}***	***Hillslope***	***Number of Species***	***Average pH_0***	***ΔpH***	***Pseudo R^2***	***RSE***
Acute	7.674	-2.738	58	8.033	0.359	0.921	6.34
Sub-chronic	7.805	-3.454	40	8.023	0.218	0.912	10.60
Chronic	7.698	-2.585	78	8.010	0.312	0.935	10.40

The significance of the difference between the SSDs is tested by the introduction of the interaction terms (see Table 7). The similarity between the acute and chronic SSDs are confirmed with the high p-values for both parameter estimations (Mp-value = 0.891, Np-value = 0.826). As none of the p values for the model parameters reveal statistical significance ($p < 0.05$), these SSDs are not utilized for calculation of separate effect factors.

Table 7 Interaction term test results for duration category, including the estimated values for the differences between the model parameters and their p-values

Test		***Estimation***	***p-value***
Acute vs. Subchronic	***M***	0.074	0.337
	N	-0.570	0.056
Acute vs. Chronic	***M***	0.010	0.891
	N	-0.239	0.826
Chronic vs. Subchronic	***M***	0.064	0.393
	N	-0.332	0.694

Main SSD Results & Effect Factor

All of the species response data (in total 176 species) is utilized to construct the main SSD (see Figure 14). There are 5 different taxonomic groups within the dataset which include varying numbers of extant species. The model parameters obtained from this SSD (see Table 8) are utilized to calculate the global effect factor for the endpoint characterization model. The SSD has a good fit with the Pseudo R^2 value of 0.961.

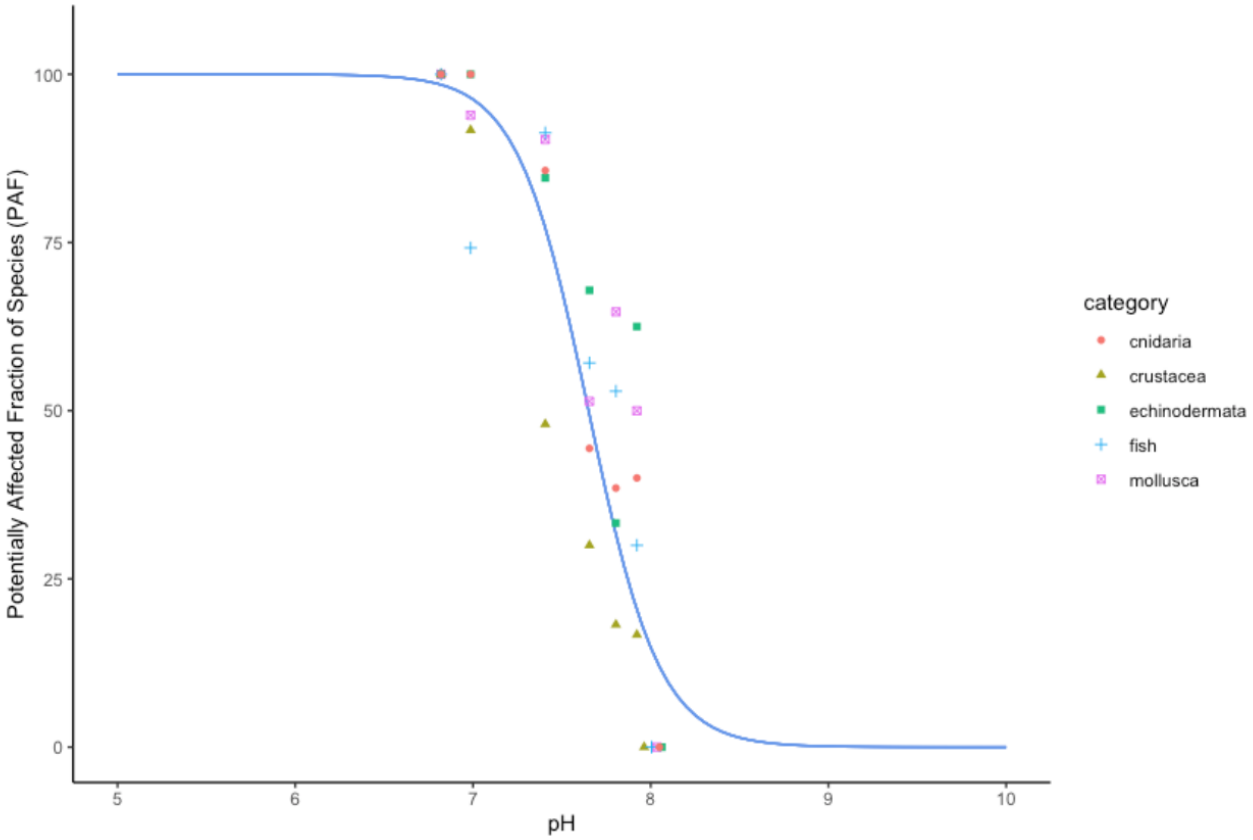


Figure 14 Main SSD including species response data from the 5 taxonomic groups

Table 8 Model parameters, number of species, average control pH values and goodness of fit results for the main SSD

Category	*pH_{50}*	*Hillslope*	*Number of Species*	*Average pH_0*	*ΔpH*	*Pseudo R^2*	*RSE*
All species	7.649	-2.167	176	8.009	0.360	0.961	9.409

The main SSD has a pH_{50} value of 7.649 and the hillslope of 2.167. The pH difference required for the percentage of affected species to become 50% is 0.360. The effect factor for the global characterization model is calculated using the pH_{50} value of this SSD. First the hydrogen ion concentration at PAF = 0 and PAF = 0.5 are calculated from the pH values obtained from the SSD to calculate HC_{50}.

$At\ PAF\ 50\%, [H^+] = \ 10^{-7.649} = 2.243 \times 10^{-8}\ mol/L$
$At\ PAF\ 0\%, [H^+] = \ 10^{-8.009} = 9.795 \times 10^{-9}\ mol/L$

The difference between these two concentrations is calculated as:

$$\Delta[H^+] = 1.264 \times 10^{-8} \frac{\text{mol}}{\text{L}} \times \left(\frac{1000\text{L}}{1m^3}\right) = \ 1.264 \times 10^{-5} \text{mol}/m_3$$

The ratio of ΔPAF and Δconcentration gives the effect factor as:

$$EF = \frac{0.5\ PAF}{1.264 \times 10^{-5}\ mol/m^3} \ = \ 3.954 \times 10^4\ (PAF)\ m^3/\ mol$$

3.3. Characterization Model Results

Characterization factors are calculated and presented in this chapter to answer the third sub-question: *"What is the OA endpoint characterization model for LCA that describes the relation between GHG emissions and marine biodiversity loss?"* Additionally, characterization factors for the calcifying and slightly calcifying species are provided based on the effect factors calculated in *Chapter 3.2*.

Main Characterization Factors

The fate factors, effect and damage factors are utilized to calculate the characterization factors using Eq. 2.6.1. The g_{GHG} in the unit of the OAP is converted to kg_{GHG} by multiplying the results with 1000. Furthermore, the damage factor is incorporated into the characterization model by converting PAF to PDF using Eq. 2.5.1. The calculations for obtaining the characterization factor for the main SSD can be found below (see Eqs. 3.3.1, 3.3.2, 3.3.3.):

$$CF_{CH4} = \left(\frac{2.06 \times 10^{-3}\ mol}{g_{GHG}}\right) \times \left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right) \times \left(\frac{3.954 \times 10^{4} (PAF) m^3}{mol}\right) \times \frac{1\ (PDF)}{2\ (PAF)}$$
$$= 4.072 \times 10^{4} (PDF) m^3 / kg_{GHG} \quad (3.3.1)$$

$$CF_{CO} = \left(\frac{2.15 \times 10^{-3}\ mol}{g_{GHG}}\right) \times \left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right) \times \left(\frac{3.954 \times 10^{4} (PAF) m^3}{mol}\right) \times \frac{1\ (PDF)}{2\ (PAF)}$$
$$= 4.251 \times 10^{4} (PDF) m^3 / kg_{GHG} \quad (3.3.2)$$

$$CF_{CO2} = \left(\frac{2.47 \times 10^{-3}\ mol}{g_{GHG}}\right) \times \left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right) \times \left(\frac{3.954 \times 10^{4} (PAF) m^3}{mol}\right) \times \frac{1\ (PDF)}{2\ (PAF)}$$
$$= 4.883 \times 10^{4} (PDF) m^3 / kg_{GHG} \quad (3.3.2)$$

OAPs of the 3 elementary flows are linked to marine biodiversity loss through PDF within the characterization model. CO_2 has the highest characterization factor ($4.883 \times 10^{4} (PDF) m^3 / kg_{GHG}$) due to having the highest OAP. CF for CO_2 indicates that for each kg of CO_2 emitted, the relative species loss will be higher compared to CO and CH_4.

Table 9 Endpoint characterization factor results for OA for the 3 elementary flows (CO, CO_2, CH_4)

$CF_{CH4}\ (PDF) m^3 / kg_{GHG}$	$CF_{CO}\ (PDF) m^3 / kg_{GHG}$	$CF_{CO2}\ (PDF) m^3 / kg_{GHG}$
$\mathbf{4.072 \times 10^{4}}$	4.251×10^{4}	4.883×10^{4}

Calcification Category Characterization Factors

The results for the calcifying and slightly calcifying species are calculated (see Appendix F for calculations) using the same method as the main SSD of calculations. Due to having a higher effect factor both in comparison to the main SSD and the slightly calcifying group, calcifying species have the highest characterization factor values.

Table 10 Endpoint characterization factor results for OA for calcifying species and slightly calcifying species, for the 3 elementary flows (CO, CO2, CH4)

	$CF_{CH4}\ (PDF)m^3/kg_{GHG}$	$CF_{CO}\ (PDF)m^3/kg_{GHG}$	$CF_{CO2}\ (PDF)m^3/kg_{GHG}$
Calcifying species	5.673×10^4	5.921×10^4	6.802×10^4
Slightly calcifying species	3.260×10^4	3.402×10^4	3.909×10^4

4

Discussion

Chapter 4. Discussion

4.1. Relevance of Research

It is of vital importance to develop a new paradigm to guide policymakers in integrating the development of societies and maintaining ecosystem stability (Steffen et al., 2015). The planetary boundaries framework is constructed by an international group of scientists to support such development, exploring the limits of reversibility of the changes imposed on planet earth by humanity. OA and biosphere integrity (expresses the loss of biodiversity) are two of the nine planetary boundaries within this framework that are related to this research. OA is currently below the safe boundary (see Figure 15). On the other hand, the rate of change in the ecosystems and biodiversity, especially in terms of genetic diversity, is already in the zone of high risk with serious impacts (Steffen et al., 2015) (see Figure 15). To tackle this rapid decline in global biodiversity, strategic targets are being determined by associations like the Convention on Biological Diversity (CBD). Aichi targets were set until 2020, including strategic goals of to reduce the pressure on biodiversity (4 of them were found relevant to marine biodiversity) (Carr et al., 2020). Following the Aichi targets, new strategic goals were set for the next 10 years and nations began uniting with the aim of reversing the loss of biodiversity. One example of this is the Leaders Pledge for Nature, which involves 10 different commitment areas that are expected to be translated into meaningful actions (United Nations, 2020). To sum up, the awareness on marine acidification and biodiversity is increasing and more research is urgently needed to understand, minimize and tackle the impacts of OA (Fallis, 2013).

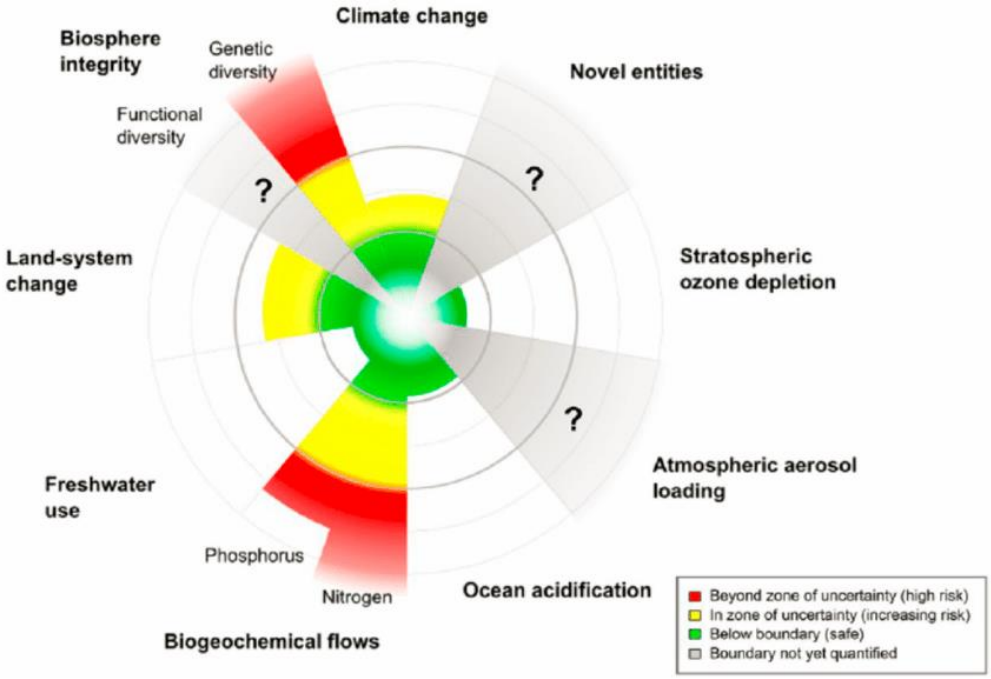


Figure 15 Planetary Boundaries diagram (Mahaffy et al., 2019)

The discipline of industrial ecology applies a systematic approach using multiple perspectives from societal, economic and environmental spheres to create a holistic understanding around the anthropogenic impacts. Even though it is currently highly underrecognized, the effects of ecosystem and biodiversity loss cascade through all these spheres. A reduction of biodiversity in marine life implies a reduction of biotic resources for humanity. This is especially visible for corals. Within the 100 km range of coral reefs, the population of people is estimated to be around 400 million. This population mainly rely on aquatic resources to maintain their livelihoods, thus are directly affected by the marine ecological shifts causing issues in food security and safety (Schmutter et al., 2016). Both the fishing and tourism sectors are influenced through the decreased abundance and productivity of marine species (Gascuel & Cheung, 2019). Due to the high complexity of the balances and processes within the ecosystems, unprecedented consequences of rapid marine biodiversity loss beyond these known socio-economic implications are expected in the future.

OA is an environmental stressor that causes a significant threat to marine biodiversity (Gascuel & Cheung, 2019). Therefore, exploration and incorporation of the extent of this threat is highly relevant to the field of IE. LCA is one of the core analytical tools of IE that can represent this threat in a quantitative way. In this thesis research, this quantitative model is established to create a basis of research for exploring further implications of OA and loss of biodiversity.

4.2. Reflections on the results of the research

The SSDs modelled for the 3 categories revealed that the calcifying and slightly calcifying species respond to OA differently, whereas there is no difference in effect in different climate zones or experiment durations. Furthermore, the characterization model results indicate that CO_2 is the GHG with the highest impact on marine biodiversity loss through OA when compared to CO and CH_4. Reflections on the outcomes of the research and validation of significant results through comparison with scientific literature can be found below.

4.2.1. Calcification SSD

Reflections on the Results

OA has varying impacts on different marine organisms. This variation is based on the physiological characteristics of the species groups. Each species has a different range of chemistry in which they optimally function. For instance, the carbonate chemistry in the habitats affect the rate of calcification ability of the organisms. The aragonite saturation state decreases with increasing acidity and as a consequence the calcification rate of the calcifying species declines. Additionally, when the bioavailability of carbonate ions decreases to a level outside this optimal range of operation, more energy needs to be spent to form shells and skeletons (Fallis, 2013). This implies that there is less energy left for other life processes such as growth and fertilization. The effect of reduced aragonite saturation state is therefore not limited to calcification ability (McOwen et al., 2019). Overall, the calcifying organisms are

expected to react more to OA based on the suggestions from scientific literature (Fabry et al., 2008; Azevedo et al., 2015; Kroeker et al., 2013).

The influence of the calcification ability of the marine species on the extent of negative responses to changing pH is tested through modelling separate SSDs for calcifying and slightly calcifying organisms. The SSD models for calcification category indicate that the calcifying species are more sensitive to OA compared to slightly calcifying species. The effect factor for the calcifying group (5.508×10^4 *(PAF)* m^3*/ mol)* is higher than the slightly calcifying group (3.165×10^4 *(PAF)* m^3*/ mol*). This implies that with each additional mol of hydrogen ions, more species will be potentially affected in the calcifying group. These effect factors can be utilized together with regionalized fate and exposure models in LCIA, especially for the biodiversity hotspots such as coral reefs and conservation areas. Furthermore, separate effect factors for calcifying and slightly calcifying species can be coupled with other relevant biodiversity indicators such as "warm water coral degradation" (Woods et al., 2016) to better understand the extent of impact of multiple stressors such as global warming and ocean acidification.

Reducing and mitigating the effects of OA for all marine species can be done by regulating and decreasing the GHG emissions released to the atmosphere. However, the results indicate that more urgent attention is required to conserve and recover calcifying marine species. This can be done by developing comprehensive conservation strategies for the marine ecosystems that are dense with calcifying organisms such as coral reefs. These ecosystems are facing other major threats along with global warming and OA, such as overharvest, pollution, and destructive fishing practices. Knowing that there is a higher extent of pressure exerted on calcifying species by OA, the focus on relief from other stressors and threating aspects should be amplified to conserve these endangered ecosystems.

Last but not least, it needs to be considered that there is high variability in responses and that genetic adaptation to these changing conditions remains a possibility in the long run (Fallis, 2013). Along with this, other environmental conditions such as nutrient availability, temperatures and light levels in the habitats also have an effect on the physiological conditions of the organism, as well as the ecosystem level impacts. Though it is demanding to set all of these as control variables in the experiments, future studies should incorporate these aspects as much as possible within the modelling processes to obtain more realistic estimations of the responses in near future.

Validation of Results

The results obtained from the calcification SSDs are compared to two scientific resources with the purpose of validation. The first comparison is with the study of Wittmann et al. (2013). In this study, the sensitivity results of 5 different taxa are calculated (see Appendix G). For the sake of comparison with the results of this thesis, the p_{CO2} values corresponding to the 50% PAFs were converted into pH values using Eq. 2.2.4 (see Appendix G). Crustaceans (pH_{50} = 7.416) were found to be less sensitive compared to cnidaria, echinoderms and molluscs (pH_{50}

= 7.789), while fish (pH_{50} = 7.869) show the highest vulnerability (Wittmann et al., 2013). This high vulnerability is explained by Wittmann et al. (2013) through the limited number of fish data included in the dataset. In this research, the dataset of this study was expanded and taxa vulnerabilities were recalculated (refer to Appendix G). While a slightly higher value for pH_{50} was obtained for Crustaceans (pH_{50} = 7.427), this taxonomic group remained to be the least sensitive to OA. Furthermore, the sensitivity of the fish data was reduced significantly to a pH_{50} = 7.23. Overall, when the taxonomic groups are classified as slightly calcifying versus calcifying species, the results of this research and Wittmann's study are aligned. Both results suggest that the calcifying species have a higher sensitivity to OA.

The second comparison is with the study done by Azevedo et al. (2015). 3 different SSDs are constructed by this paper that gives the relation between PAF and pH change in the marine environment. These SSDs are solely focused on calcifying species. Moreover, unlike this research, the categorization of the dataset was made on different life processes: growth (pH_{50} = 7.28), survival (pH_{50} = 7.35) and reproduction (pH_{50} = 7.11). There are some similarities in the trends of the results such as the lack of detrimental effects for the crustaceans and higher sensitivity for highly calcifying species (Azevedo et al., 2015). However, the pH_{50} results obtained by Azevedo et al. (2015) are different compared to the ones obtained from the SSD model for calcifying species in this research (pH_{50} = 7.74) (see Chapter 3.2 for the model).

Potential reasons for this difference could be listed as; the number of species data utilized to construct the SSDs, the scope of variable types included in the analysis and the differences in modelling methods. 40 out of the 82 species response data was considered detrimental in their SSDs whereas the number of calcifying species data was 96 in this research, which is a higher degree of representativeness of species. In terms of the variables, responses reflecting metabolic changes were excluded from the scope of their model. Such variables were included within the scope of this research. Metabolic changes might be less reflective of the disappeared fraction of species, thus, it could have created a bias in the results obtained from the SSDs. Last but not least, as discussed in Chapter 2.4, due to the data availability, the SSDs were calculated by using the negatively affected fraction of species for the calcifying category rather than obtaining individual pH_{50} values for each species before constructing the SSDs. This variation in approaches can be considered as the main reason for the differences in the results.

4.2.2. Climate SSDs

Reflections on the Results

Three different climate zones were assessed in this research in terms of the species sensitivity to OA. The results of the analysis revealed that there is no significant difference in the responses of the organisms in the polar, temperate and tropical regions. Therefore, no individual characterization factors were calculated for these regions. This might be due to the resilience and adaptation capabilities of the different species groups that live in these climate zones. The communities may adapt to the variations in pH over the long term and tolerate its effects. Moreover, the results could be biased as the temperatures in the experiments are not

always the same as the habitat temperatures of the species. The seasonal changes within these regions are also not taken into consideration as most of the experiments measured the responses in a fixed environment with a specific temperature**.** Overall, the results do not indicate a significant species sensitivity variance between the 3 climate zones.

4.2.3. Duration SSDs

Reflections on the Results

Both the species and ecosystem-based responses to OA in the long-term is largely unknown (Fabry et al., 2008). It is crucial to model and estimate these effects to determine the right course of action for mitigation. In this research, the SSDs based on experiment duration did not show any significant difference from each other. The chronic and acute responses to a chemical would be expected to differ in severity. However, the results indicate that the sensitivity of acute and chronic groups are the almost the same whereas the sub chronic SSD revealed a higher pH_{50} value compared to both acute and chronic responses. As there is no significant difference between the duration based SSDs, it is found that there is no requirement for prioritizing chronic or acute responses for the development of characterization models for OA.

The reasons for obtaining such results could be that the experiments are not considering the pH change in a gradual manner. One being the control group, there tend to be 2-3 different pH levels introduced in separate containers during the experiments. In reality, the species are exposed to pH change incrementally. In longer durations with gradual pH change, the species can adapt to the environment and make trade-offs in terms of energy with other life processes to ensure their survival (Doney et al., 2009). This could lead to lowered sensitivity in chronic experiments. Incorporation of this aspect to future studies might produce more realistic results in terms of the effects of experiment duration. The method of collecting and analysing the species response data could be another point of improvement for the future models. The variables and species types are very different from each other in the dataset that was utilized in this research. The durations are categorized regardless of these types in this study. In future studies, measuring one response type, such as growth rate, for the same species in different durations might reveal the impacts of exposure duration more accurately.

4.2.4. Characterization Model

Reflections on the Results

The model consists of 3 different characterization factors that represents the ecosystem damage indicators for OA. CO_2 is the substance with the highest endpoint characterization factor for OA ($4.833 \times 10^4 (\text{PDF})\text{m}^3/\text{kg}_{\text{GHG}}$). This is a logical result because it has the highest fate factor as there is no chemical conversion required in the atmosphere. This value is the lowest for CH_4 ($4.072 \times 10^4 (\text{PDF})\text{m}^3/\text{kg}_{\text{GHG}}$) as CH_4 partially reaches the atmosphere and needs to be converted to CO_2. CO on the other hand has a factor closer to CH_4. This indicates that the distribution factor has a considerable impact on the fate of these elementary flows.

Obtaining these characterization factors allows for the conversion of the inventory results of the 3 GHG in an LCA study into category indicator results for OA. This will provide insights regarding protection and conservation of marine ecosystems. Knowing the impacts of different GHG enables the practitioners to identify the hotspots and design targeted solutions to reduce the impact on oceans. These characterization factors provide a comprehensive indication of the implications of the impacts of emissions by incorporating the effects further along the cause-effect chain.

Validation of Results

Comparing these factors with reference literature is not currently possible. So far, the characterization factor for marine acidification is only calculated by Bulle et al. (2019). In their approach, the fate model utilizes GTP100 as a proxy for marine acidification and the effect model is based on the work of Azevedo et al. (2015), which solely focuses on calcifying species. GTP100 focuses on the temperature change potential in the atmosphere over 100 years only due to CO2 emissions. Beyond these differences, the characterization factors for marine acidification are provided in a different unit (PDF $m^2\times$ yr/kg_{CO2}), which eliminates the possibility of comparison. Through researching characterization factors for several indicators for the marine environment, it was found that there is a need for harmonization of the units while reflecting biodiversity. This would both make it easier to understand and enable comparison of different indicators in terms of impact.

4.4. Limitations of Research & Suggestions for Further Research

Fate and Exposure Models

The fate and exposure models used in this research can be developed further considering several aspects. First of all, not all acidifying substances are included in these models. Examples of such substances are nitrogen and sulphur oxides (NO_x, SO_x). These chemicals can be directly released into the ocean, especially creating a higher impact in the coastal ecosystems (Pierre et al., 2011), or can react with water in the atmosphere and form acid rain (Bach et al., 2016). Either way, both NO_x and SO_x alter the ocean chemistry towards reducing the pH. As a result, the pathways of these emissions need to be explored further to understand their contribution to OA and incorporated into the fate and exposure models for LCIA.

Another significant point is the absence of the time element in the fate and exposure models. The time from the initial pH change until the time the ocean might recover from this change is not represented in the current models. For most of the fate factors, such as GWP, the time aspect (in terms of year or day) is incorporated to consider the temporal scope of the impacts, which represents the duration of the GHGs emissions remaining in the atmosphere. This temporal scope has different implications for different sections of the cause-effect model for OA. The emissions that reach the atmosphere react into different chemical forms and then dissolve in the ocean. This is then followed by a series of reactions within the ocean that result in the alteration of the acidity by the release of H^+ ions. Then, various life processes of the marine species get affected by the gradual pH change. None of these processes occur instantaneously. This would be an of improvement for the models for OA in future research.

Geographical differentiation is yet another aspect that can be considered as an improvement for the fate model for OA. The characteristics of the ocean (such as temperature or salinity) at the point of dissolution might alter the extent of pH change in different regions (Doney et al., 2009). The types of species are also variable in different latitudes. According to literature, 25-30% of the total CO_2 is assumed to be dissolving, but higher accuracy in the dissolution rates can be obtained if regional values are obtained in the future for the fate model. From the 3 climate zones analysed in this research, the polar regions are expected to be more affected by OA compared to temperate and tropical regions (see Figure 16). There are several reasons for this. First of all, polar oceans have lower temperatures. This indicates higher solubility of the atmospheric CO_2, and therefore a higher magnitude of change in surface pH by any additional unit of dissolved CO_2. Lower temperatures also lead to lower aragonite saturation states as described in *Chapter 1.2*. With lower saturation states, a higher number of species are affected by OA due to lower calcification rates, and dissolving shells and skeletons of organisms (Fallis, 2013). Besides the high temperatures, the reduction of sea ice cover induced by global warming increases the ocean surface area that is in direct contact with the atmosphere. More CO_2 dissolves in the ocean with increasing air-water contact. When this is coupled with the fresh water originating from the melting sheets, the surface ocean pH in polar regions is expected to decrease even more in the near future (Fallis, 2013). Such conditions influence the extent of

impact of OA on species richness. Understanding and incorporating these impacts to the fate and exposure models is important to identify the zones and species that require the most immediate attention.

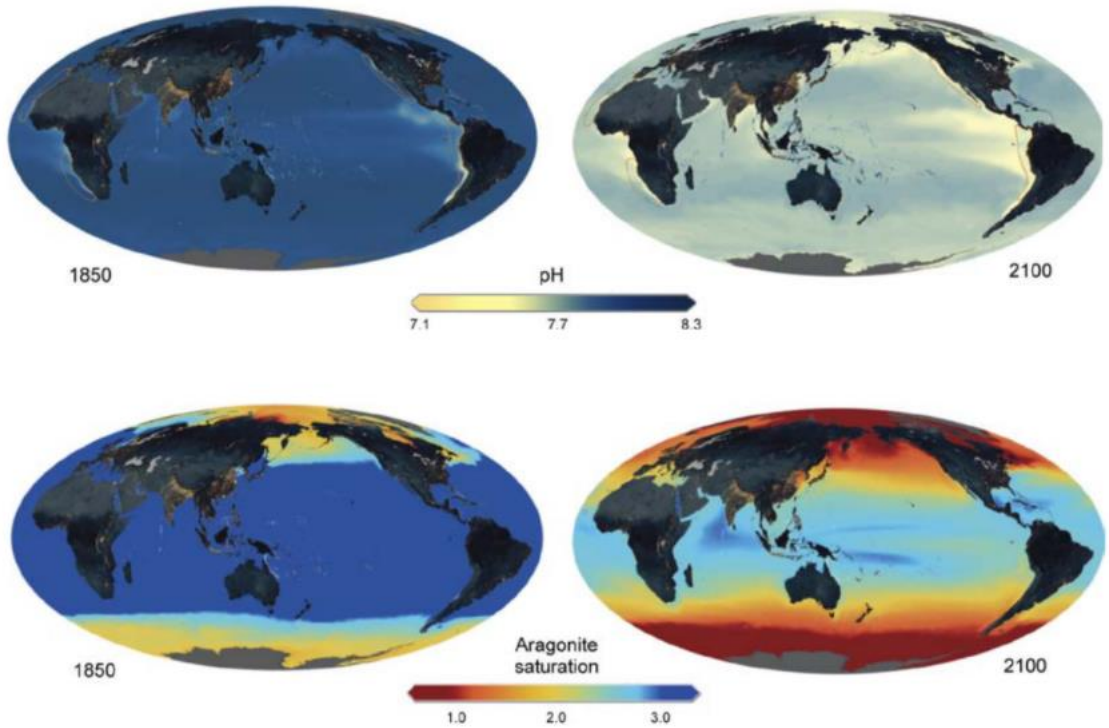


Figure 16 Model-derived maps of historical and projected global ocean pH levels (up) and aragonite saturation states (down), based on Fallis (2013)

Another level of detail for future fate and exposure models would be the incorporation of the vertical differentiation within the ocean (Doney et al., 2009). The CO_2 dissolves from the surface of the ocean, which has a different temperature compared to the bottom of the ocean, and there are different circulation pathways that affect the flow of water from one location to the other. Moreover, the species types and distributions differ in benthic and pelagic regions. With the differences in pH in between these regions, the exposure of different organisms to different pH levels should be considered to develop a more robust exposure factor.

Species Response Data

Discovery and synthesis of species response data in this thesis research has proven to be challenging. The research on the impact of OA on marine species gained acceleration within the last two decades. While there were only 18 published papers per year in 2004, this number increased to 365 studies in 2014 (Yang et al, 2016). Despite the recent developments, the research area is still relatively novel which imposes some challenges around data collection. Some of the experimental data are not even archived or not accessible and even if they are, there are several repositories which present the data in different formats. The representation of

the carbonate chemistry, the parameters used for reporting the outcomes of the experiments and their units vary significantly (Yang et al., 2016). This makes it hard to collect and compare the species response data, thus there is a need for harmonization in the reporting of the results in experiment-based OA research.

The taxonomic representativeness of the dataset is open for improvement. The species response data are modelled and evaluated to be reflective of the biological response on a global scale. The overarching challenge in achieving this is the vast number of marine species and ecosystems. The number of estimated species in marine life is around 1.4 - 1.6 million and only 226,000 of them have been identified so far (Bouchet, 2006). Considering only a small fraction of these identified species are utilized in OA experiments, it is not currently possible to find and include species response data with a full taxonomic coverage.

Within the scope of this thesis, 5 different taxa were included (echinodermata, mollusca, cnidaria, fish and crustacea). Photosynthetic organisms which include large taxonomic groups such as phytoplanktons were excluded from the scope. Moreover, geographical location of the species data is not evenly distributed. According to Yang et al. (2016), the majority of the reported responses belong to the species in the Northern Hemisphere. The extent of research for the species in the southern hemisphere and polar regions is still limited. Along with this, the reporting of the habitats of species is not consistent and not always clearly denoted. Some studies indicate the species habitats as the polar region, whereas, in other studies the same species habitat is denoted as temperate region. This can indeed be the case for some species, but it presented challenges in classifying (in terms of habitats) and collating different experiment results for some species.

Lastly, the fact that experimental data is utilized in this analysis creates a limitation as it represents responses in highly specific conditions rather than reflecting the reality. Most of the time the experiments report the responses of cultured organisms that are observed in an isolated environment. The laboratory conditions may impose changes in responses compared to the actual behaviour of the species in their natural habitats. The marine ecosystems are complex and dynamic and involve interactions of the organisms with each other and with the marine environment. This is inevitably excluded in a laboratory setting. The reduction in accuracy is especially the case for the experiments in which interaction-based variables, such as predatory behaviour, are utilized. Moreover, within the marine ecosystems, the chemical balances and temperature are not fixed qualities. However, these are static control variables in the experimental setups, and they are also different in most of the experiments. According to Fallis et al. (2013), mesocosm studies or incorporation of natural gradients could be addressing the complexity of the environment more realistically and thus might be considered as preferable setups for future research to resolve such issues.

Effect Modelling Approach

Initially, the method of the study from Azevedo et al. (2015) was initially selected to construct the models. The raw data was not provided by the authors; thus, the supplementary information of the article was utilized to trace back the steps of the method. The experimental data utilized in the calculation of one of the SSD models were acquired and the same approach was applied to test the applicability of the method. Some of the calculations did not lead to the same results as denoted in the publication, therefore, other meta-analyses were examined to obtain raw data. This led to a shift from the original choice of methods to construct the effect model.

The dataset of Wittmann et al. (2013) was used as the base dataset and expanded further to improve the species representativeness for polar regions and fish taxon. The format of the dataset that was constructed by the authors is therefore maintained. There are implications of this format on the choice of the SSD modelling approach. The method suggested by Rosenbaum (2008) and applied by Azevedo et al. (2015) starts with fitting the responses (in relation to the control responses) of a single species into a logistic regression to obtain EC_{50} values (effect concentration affecting 50% of the individuals). Then, these EC_{50} values are utilized in another regression which gives the HC_{50} value. It wasn't possible to apply this method to the dataset on hand. This is because the responses are recorded as negative, positive or none per each species along 6 p_{CO2} bins rather than the values of the actual responses. Therefore, once the negatively affected percentage of species were calculated for the given category, this data is directly fit into a logistic regression to obtain HC_{50}. This change in methodology can be considered as a limitation of this research and improvements can be made by applying the Rosenbaum (2008) approach to a similar data scope of species in future research. This way, the method would be fully aligned with the established ecotoxicology impact assessment approach for LCA. Observing the extent of the difference in the results would be interesting to assess the effectiveness of the approach used in this research.

According to Wittmann et al. (2013) crustaceans tend to build lighter skeletons and have a more efficient pH regulation mechanism compared to cnidaria, echinoderms and molluscs. On the other hand, even though fish mostly do not display calcifying structures, some fish species produce $CaCO_3$ based components such as the otoliths, as well as their skeletons (Grossel, 2019). Therefore, crustaceans and fish are categorized as the slightly calcifying category in this analysis. The choice of categorizing the taxonomic groups as such creates biases in the results. This is due to the gradual differences both between and within the groups. Not all species within these taxonomic groups have the same calcification ability. However, if more distinctions than 5 taxonomic groups were made in terms of categorization with the extent of data available, the statistical power of the models would decrease significantly.

The approach selected for assessing goodness-of-fit presents limitations regarding the statistical power of the models. Nagelkerke R^2 was selected as the statistic to evaluate the goodness-of-fit. However, these values are considerably high (see Chapter 3). considering the limited number of data points that are fitted into the regression to construct the SSDs When other R^2 values such as Efron R^2 were calculated for the regressions, the results differed from

the Nagelkerke R^2 values. As Nagelkerke R^2 is a commonly used statistic, these values were presented in the report. However, to ensure a greater statistical certainty and coherence with regards to the models, more data points should be incorporated into the models.

A categorization around life processes (growth, reproduction, survival) as done by Azevedo et al. (2015) was originally intended to be included as a part of the analysis. However, within the current data collection format, there is no distinction between experiment variables. Instead, the number and types of variables were collected and listed per species. Moreover, Azevedo et al. (2015) excluded variables associated with metabolic processes or behavioural aspects. The variety of experiment variables were higher within the dataset of Wittmann et al. (2013). These variables were grouped together rather than being recorded separately for each experiment, which made it harder to classify into distinct life processes. Consequently, life process categorization was not included in the scope of this thesis. The effect of swimming behaviour and the effect of fertilization success are different on the loss of biodiversity. Therefore, the variable types should be classified depending on their influence on PDF and explored accordingly in future studies.

5

Conclusion

Chapter 5. Conclusion

This research explores the relationship between the changing acidity of the oceans and marine biodiversity loss. This is done through developing an endpoint characterization model for OA to be utilized in LCIA. The model includes 3 different characterization factors based on the type of GHG (CO, CH_4 and CO_2). With 4.883×10^4 (PDF)m^3/kg_{GHG}, CO_2 emissions has the highest impact on marine biodiversity. From these factors CH_4 turned out to be the lowest (4.072×10^4 (PDF)m^3/kg_{GHG}. Along with the model development, influences of different climate zones (polar, temperate, tropical), calcification ability and duration of exposure (acute, sub chronic, chronic) on species responses were analysed. The results revealed that duration and climate zone are not significant in terms of species response to OA, whereas the calcifying species (mollusca, echinodermata, cnidaria) were found to be more sensitive to OA compared to slightly calcifying ones (crustacean, fish).

The model developed in this research differs from previous models in scientific literature due to incorporating slightly calcifying species in SSDs and assessing different influencing parameters on species response. Including this endpoint indicator for OA in LCA makes it possible to quantify the extent of impact that the service and product systems have on marine biodiversity loss. This allows for creating targeted solutions for both limiting the emissions from the production hotspots, as well as developing strategies to conserve threatened ecosystem such as coral reefs.

To sum up, OA has adverse effects on marine species richness. Most of these effects are currently not well-understood. More research is required to expand the collection of experimental data and to explore the unprecedented consequences of OA when coupled with other stressors such as global warming. The changes in ocean chemistry on a regional scale as well as the socio-economic and ecosystem level implications of OA need to be monitored closely. Incorporating the quantified impacts of OA in analytical tools such as LCA is of vital importance to have a grasp of the implications of our actions. With the addition of temporal and geographical aspects into the characterization model, future studies could contribute to developing a more robust category indicator for OA. Urgent attention is needed to further understand and mitigate the impacts OA, and to conserve the marine ecosystems.

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Appendices

Appendix A: Reference list for the species dataset expansion

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Appendix B: pCO_2 – pH conversion

Table 11. pCO2 ranges of the bins, average pCO2 per bin and the corresponding pH values

pCO2 range	***pCO2 average***	***pH***
500 - 650	550.0	7.922
651 - 850	750.5	7.804
851 - 1370	1110.5	7.655
1371 - 2900	2135.5	7.406
2901 - 10000	6450.5	6.986
10000	10000	6.820

Appendix C: Global normalization factors and number of extant species for each taxonomic group

Table 12 Global normalization factors and number of extant species per taxon, and their corresponding references

Taxon	*Global normalization factor*	*Number of extant species*	*Reference*
Echinodermata	0.053	7000	Ho & Rast, 2016
Mollusca	0.379	50000	Appeltans et al., 2012
Crustacea	0.303	40000	Hobbs, 2012
Fish (Actinopterygii)	0.197	26000	Dixon et al., 2016
Cnidaria	0.068	9000	Fautin et al., 2020

Appendix D: Fate Model Calculations

Distribution Factor

Both CO and CH_4 are converted into CO_2 in the atmosphere by reacting with oxygen (Wuebbles and Hayhoe, 2002). The troposphere is the layer of the atmosphere where this conversion occurs. In order to know the extent of these conversions, first, the distribution of these emissions within the atmosphere should be determined. The distribution factor indicates this percentage of the emissions entering the troposphere. All of the emitted CO_2 initially ends up in the troposphere. While this is the case for CO_2, only 87.1% of the CO reaches the troposphere. A similar but slightly higher percentage, 87.8%, is suggested by the literature for CH_4 (Kirscheke et al., 2013). The distribution factors for each elementary flow are therefore;

Distribution Factor$_{CO}$ = 0.871
Distribution Factor $_{CH4}$ = 0.878
Distribution Factor$_{CO2}$ = 1

Conversion Factor

The troposphere is a natural sink for methane. While CO directly transforms into CO_2 in the troposphere, CH_4 goes through a series of reactions. CH_4 first gets oxidized through reacting

with OH^- ions which eventually results in the formation of CH_2O and H_2O. This oxidation is influenced by the bioavailability of ozone and nitrogen oxides within the troposphere (Bach et al., 2016). Then, CH_2O further reacts into CO. The percentage of CH_4 converted to CO is estimated as 95% based on the suggestion Holloway and Wayne (2010). According to literature, 100% of the CO converts to CO2 through oxidation.

Overall, the total amount of CO_2 in the troposphere is a sum of direct (CO_2) and indirect emissions (CH_4 and CO). Conversion factor allows the calculation of the latter. This factor is considered as 1 for CO_2 as it is the required chemical formulation to dissolve in the ocean. The conversion factors of the elementary flows are:

Conversion Factor$_{CO}$ = 1 g_{CO2}/g_{CO}
Conversion Factor $_{CH4}$ = 0.95 g_{CO2}/g_{CH4}
Conversion Factor$_{CO2}$ = 1 g_{CO2}/g_{CO2}

Dissolution Factor

Following the conversion of all of the elementary flows into CO_2, the dissolution of CO_2 in the ocean is calculated. The dissolution factor is accounting for the fact that the selected environment is a water body for the fate model. There is a certain chemical equilibrium within the ocean regarding the fate of CO_2. This equilibrium explains how aquatic CO_2 is transformed or stored (IPCC, 2013). On one hand, the CO_2 is converted into different chemical forms to be utilized by the marine species to support their life processes and there is a continuous flow of CO_2 in between different layers of depth within the ocean. On the other hand, some of the dissolved CO_2 is stored on the floor of the ocean in sediment form rather than dynamically being converted and transported within the water. This static form of CO_2 within the ocean does not have an effect on OA and is 1% of the total amount of CO_2 dissolved in the ocean.

According to IPCC (2013), the percentage of CO_2 dissolving in the ocean is between 25 - 30%. The average of these two numbers, 27.5%, is assumed as the percentage of all atmospheric CO_2 ending up in the ocean. Thus, 1% of 27.5% of the dissolved CO_2 reflects the percentage of stored CO_2, which is equal to 0.225%. 0.225% is subtracted from the dissolved percentage, 27.5%, leading to 27.225% as the total amount of dissolved CO_2 contributing to OA.

Total amount of dissolved CO_2 = 27.225%

The dissolution factor gives the ratio of the total amount of dissolved CO_2 to the share of CO_2 able to be dissolved (see Eq. 2.3.3). To calculate the latter, the shares of each elementary flow that can dissolve in the ocean are calculated individually and added together using Eq. 2.3.4. These shares are determined by multiplying the distribution and conversion factors of each elementary flow.

Share of CO able to be dissolved = 0.871 x 1 = 0.871

Share of CH_4 able to be dissolved = 0.878 x 0.95 = 0.834
Share of CO_2 able to be dissolved = 1 x 1 = 1

The sum of these three values is equal to 2.705. The dissolution factor for all the elementary flows is therefore 0.27225/2.705 = 0.1008 (see Eq. 2.3.3).

Dissolution $Factor_{CO,CH4,CO2}$ = 0.1008

Fate Sensitivity Factor

Fate sensitivity factor translates the percentage of aquatic CO_2 into the dissolved H^+ ions as these ions cause the alteration of the acidity of the water body. As can be seen in Eq. 1.2, the initial release of H^+ ions is due to the conversion of CO_2 into HCO_3^-. Within this conversion, one H^+ ion is released per one CO_2 molecule. According to Doney et al. (2009), the probability of this reaction taking place is 90%. In other words, 90% of the CO_2 molecules will be converted into H^+ ions through the first conversion. The second part of the equilibrium reaction expresses the conversion from HCO_3^- to CO_3^{-2} and two H^+ ions. The value found in literature for the probability of this happening is 9%. To calculate the total number of released H^+ ions, the number of H^+ ions per equation is multiplied with the probability of that reaction and these two values are added together;

(1 H^+ ion) x 0.9 + (2 H^+ ions) x 0.09 = 1.08 H^+ ions released per one CO_2 molecule.

In order to find the category indicator, which is the "moles of released H^+ ions per gram of CO_2", the number of H^+ ions is divided by the molar mass of CO_2 (44 g/mol);

Fate sensitivity factor = 1.0844 g/mol= 2.45 x 10^{-2} mol H^+/gram CO_2.

Ocean Acidification Potential

So far, the journeys of each substance from emission to the ocean are explored in 3 distinct stages. The emissions get distributed within the atmosphere, get converted into CO_2 and a share of this atmospheric CO_2 dissolves within the ocean. By obtaining the product of these 3 factors, it is possible to calculate the fate factors of each elementary flow using Eq.2.3.2;

Fate $Factor_{CO}$ = 0.871 x 1 x 0.1008 = 0.0878 g_{CO2}/g_{CO}
Fate $Factor_{CH4}$ = 0.878 x 0.95 x 0.1008 = 0.0841 g_{CO2}/g_{CH4}
Fate $Factor_{CO2}$ = 1 x 1 x 0.1008 = 0.1008 g_{CO2}/g_{CO2}

As previously described, the OAP_i is the product of these individual fate factors and the fate sensitivity factor (see Eq. 2.3.1);

OAP_{CO} = 0.0878 x 2.45 x 10^{-2} = 2.15 x 10^{-3} mol H^+/g_{GHG}

$OAP_{CH4} = 0.0841 \times 2.45 \times 10^{-2} = 2.06 \times 10^{-3}$ mol H^+/g_{GHG}

$OAP_{CO2} = 0.1008 \times 2.45 \times 10^{-2} = 2.47 \times 10^{-3}$ mol H^+/g_{GHG}

Appendix F: Characterization factor calculations for calcifying and slightly calcifying species

Calcifying Species:

$$CF_{CH4} = \left(\frac{2.06\times 10^{-3}\ mol}{g_{GHG}}\right)\times\left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right)\times\left(\frac{5.508\ \times 10^{4}(PAF)m^{3}}{mol}\right)\times\frac{1\ (PDF)}{2\ (PAF)}$$
$$= 5.673\times 10^{4}(PDF)m^{3}/kg_{GHG}$$

$$CF_{CO} = \left(\frac{2.15\times 10^{-3}\ mol}{g_{GHG}}\right)\times\left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right)\times\left(\frac{5.508\ \times 10^{4}(PAF)m^{3}}{mol}\right)\times\frac{1\ (PDF)}{2\ (PAF)}$$
$$= 5.921\times 10^{4}(PDF)m^{3}/kg_{GHG}$$

$$CF_{CO2} = \left(\frac{2.47\times 10^{-3}\ mol}{g_{GHG}}\right)\times\left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right)\times\left(\frac{5.508\ \times 10^{4}(PAF)m^{3}}{mol}\right)\times\frac{1\ (PDF)}{2\ (PAF)}$$
$$= 6.802\ \times 10^{4}(PDF)m^{3}/kg_{CO2}$$

Slightly Calcifying Species:

$$CF_{CH4} = \left(\frac{2.06\times 10^{-3}\ mol}{g_{GHG}}\right)\times\left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right)\times\left(\frac{3.165\times 10^{4}(PAF)m^{3}}{mol}\right)\times\frac{1\ (PDF)}{2\ (PAF)}$$
$$= 3.260\times 10^{4}(PDF)m^{3}/kg_{GHG}$$

$$CF_{CO} = \left(\frac{2.15\ \times 10^{-3}\ mol}{g_{GHG}}\right)\times\left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right)\times\left(\frac{3.165\times 10^{4}(PAF)m^{3}}{mol}\right)\times\frac{1\ (PDF)}{2\ (PAF)}$$
$$= 3.402\times 10^{4}(PDF)m^{3}/kg_{GHG}$$

$$CF_{CO2} = \left(\frac{2.47\times 10^{-3}\ mol}{g_{GHG}}\right)\times\left(\frac{1000 g_{GHG}}{1 kg_{GHG}}\right)\times\left(\frac{3.165\times 10^{4}(PAF)m^{3}}{mol}\right)\times\frac{1\ (PDF)}{2\ (PAF)}$$
$$= 3.909\times 10^{4}(PDF)m^{3}/kg_{GHG}$$

Appendix G: Taxon based SSD results

Results calculated in this research:

Table 13 Taxon based model parameters, number of species and goodness of fit measure

Taxon	*pH50*	*Hillslope*	*Number of Species*	*Pseudo R²*
Echinodermata	7.745	-2.821	30	0.864
Mollusca	7.751	-2.392	44	0.982
Crustacea	7.427	-2.185	39	0.911
Fish	7.723	-2.971	41	0.843
Cnidaria	7.666	-2.565	22	0.951

Results of Wittmann et al. (2013):

Table 1 | Parameters, goodness of fit and resulting P_{50} values of the taxon sensitivity curves in Fig. 3.

	Taxon	A	B	R^2	P_{50} (µatm)
Fig. 3a,b reported	Corals	3.058	1.597	0.9157	1,143
	Echinoderms	3.021	1.627	0.7991	1,050
	Molluscs	2.924	1.448	0.7152	840
	Crustaceans	3.361	1.830	0.9731	2,298
Fig. 3c,d including estimates	Corals	3.001	1.973	0.9378	1,003
	Echinoderms	2.892	1.998	0.8582	870
	Molluscs	2.892	1.953	0.8638	781
	Crustaceans	3.319	2.097	0.9888	2,086
	Fishes	2.801	4.391	0.7653	632

Curve equation $Y = 100/(1+10^{(A-X)*B})$, $A = \log_{10} P_{50}$. P_{50}: p_{CO_2} at which 50% of the species were negatively affected.

Figure 17 Parameters, goodness of fit and resulting pH50 values of the taxon sensitivity curves from Witmann et al. (2013)

Table 14 P50 values obtained by Wittmann et al. (2013) that are converted to pH for the sake of comparison with the results of this research

Taxon	*pH50*	*pCO2*
Echinodermata	7.748	870
Mollusca	7.789	781
Crustacea	7.416	2086
Fish	7.869	632
Cnidaria	7.694	1003

Appendix H: The modelling method of Azevedo et al. (2015)

Experimental species response data for calcifying species were collected by the authors and further categorized into three main life processes: growth, survival and reproduction. The next steps in the approach of Azevedo et al. (2015) are:

1. Adjusting the species response data to empirical relative responses (eRR_i) per species, using the formula:

$$eRR_i = 1 - R_i/R_r \quad \text{(H.1)}$$

where R_i is the reported response at pH *i* and R_r is the reference response (i.e., highest reported pH level).

2. Fitting eRR_i and pH_i values into individual logistic regressions to obtain pH_{50} values (equivalent of EC_{50} for pH) using the formula:

$$cRR = \frac{1}{1+10^{(pH50-pH)/\beta}} \quad \text{(H.2)}$$

where cRR stands for calculated relative response and β is the slope of the logistic function. The logistic function has two parameters and 1 degree of freedom, therefore only the experiments with 3 or more eRR_i and pH values were utilized to create logistic regressions.

3. Classifying the regression results based on β and p values:
   - Detrimental if $\beta < 0$ and p value <= 0.05
   - Beneficial if $\beta > 0$ and p value <= 0.05
   - Uncertain if $\beta = 0$ or p value > 0.05

4. Calculating of means (μ) and standard deviations (σ) of the pH_{50} values obtained from regressions that were classified as detrimental in step 3.

5. Constructing SSDs per life process by fitting μ and σ values into a cumulative normal distribution indicated by the equation:

$$PAF_i = \frac{1}{\sqrt{2\pi\sigma}} e^{-(pH-\mu)^2/2\sigma^2} \quad \text{(H.3)}$$

where PAF denotes potentially affected fraction of species.

The intention was to expand the scope of the dataset of Azevedo et al. (2015) by including data for both slightly-calcifying and calcifying species, as well as species from the polar region to replicate the approach described above for a larger number of data. The purpose of this was to construct more comprehensive SSDs based on geographical classification rather than life processes. However, the raw data was not provided by the authors. The only available information from this study was the results of the logistic regressions from step (2) and the list of experiments included in the assessment. With the attempt to utilize this information and test the approach, the methodological steps from (1) to (5) were replicated for 5 of the experiments with the data found from the original papers referred by the authors. Some of the obtained results did not align with the results that were presented in the paper. Therefore, the approach was no longer utilized for the effect model.

Appendix I: Code in R

Code for modelling the Calcification Category SSDs:

```
library(readxl)
library(ggplot2)
library("rcompanion")

#code to model the SSD for calcifying species data with a taxonomic grouping
#step 1: weighted averages per bin per taxon; c(mollusca, echinodermata, cnidaria)
bin0 <- c(0,0,0) #control
bin1 <- c(50 , 62.5, 40) # response of the first pco2 bin - each number represent one taxa
bin2 <- c(64.7, 33.3, 38.5)
bin3 <- c(51.4, 67.9, 44.4)
bin4 <- c(90.3, 84.6, 85.7)
bin5 <- c(93.9, 100, 100)
bin6 <- c(100,100,100)

#step 2: calculating the weighted average of each bin using the global normalization factors per taxonomic group
w_gsr_c <- c(0.379, 0.053, 0.068)
w_avg_b0 <- weighted.mean(bin0, w_gsr_c)
w_avg_b1 <- weighted.mean(bin1, w_gsr_c)
w_avg_b2 <- weighted.mean(bin2, w_gsr_c)
w_avg_b3 <- weighted.mean(bin3,w_gsr_c)
w_avg_b4 <- weighted.mean(bin4, w_gsr_c)
w_avg_b5 <- weighted.mean(bin5, w_gsr_c)
w_avg_b6 <- weighted.mean(bin6, w_gsr_c)
y_c <- c(w_avg_b0, w_avg_b1, w_avg_b2, w_avg_b3, w_avg_b4, w_avg_b5, w_avg_b6)

#step 3: defining the pH values including the average control variable of the category
x_c <- c(8.0461, 7.922231, 7.804119, 7.655225, 7.406747, 6.986673, 6.820071)

#step 4: defining weights of the bins based on the total number of species data entry per given bin
```

```
bin_weights_c <- c(1, 0.358, 0.62963, 1, 0.8765, 0.83, 0.802)

#step 5: defining the logistic regression function with two parameters
cfunc <- function(x,a,b) {100 / (1 + 10 ^ ((a - x) * b))}

#step 6: defining the nonlinear least squares (nls) function for the regression
cal_fit <- nls(y_c ~ cfunc(x_c,a,b), start = list(a = 7.5, b = -2), weights = bin_weights_c)
summary(cal_fit)

#step 7: calculating the nagelkerke R2
nullfunct = function(x, m){m}
null.model = nls(y ~ nullfunct(x, m), start = list(m = 50), weights = bin_weights_c)
nagelkerke(cal_fit, null = null.model)

#------------------
#code to model the SSD for slightly calcifying species data with a taxonomic grouping
#step 1: weighted averages per bin per taxon; c(crustacea, fish)
bin0 <- c(0,0) #control
bin1 <- c(16.7, 30) # response of the first pco2 bin - each number represent one taxa
bin2 <- c(18.2, 52.9)
bin3 <- c(30, 57.1)
bin4 <- c(48, 91.3)
bin5 <- c(91.7, 74.2)
bin6 <- c(100,100)

#step 2: calculating the weighted average of each bin using the global normalization factors per taxonomic group
w_gsr_sc <- c(0.303, 0.197)
w_avg_b0 <- weighted.mean(bin0, w_gsr_sc)
w_avg_b1 <- weighted.mean(bin1, w_gsr_sc)
w_avg_b2 <- weighted.mean(bin2, w_gsr_sc)
w_avg_b3 <- weighted.mean(bin3, w_gsr_sc)
w_avg_b4 <- weighted.mean(bin4, w_gsr_sc)
w_avg_b5 <- weighted.mean(bin5, w_gsr_sc)
w_avg_b6 <- weighted.mean(bin6, w_gsr_sc)
y_sc <- c(w_avg_b0, w_avg_b1, w_avg_b2, w_avg_b3, w_avg_b4, w_avg_b5, w_avg_b6)

#step 3: defining the pH values including the average control variable of the category
x_sc <- c(7.9833, 7.922231, 7.804119, 7.655225, 7.406747, 6.986673, 6.820071)

#step 4: defining weights of the bins based on the total number of species data entry per given bin
bin_weights_sc <- c(1, 0.2909, 0.50909, 0.8727, 0.8727, 1, 0.982)

#step 5: defining the logistic regression function with two parameters
cfunc <- function(x,a,b) {100 / (1 + 10 ^ ((a - x) * b))}

#step 6: defining the nonlinear least squares (nls) function for the regression
scal_fit <- nls(y ~ cfunc(x,a,b), start = list(a = 7.5, b = -2), weights = bin_weights_sc)
summary(scal_fit)

#step 7: calculating the nagelkerke R2

nullfunct = function(x, m){m}
null.model = nls(y ~ nullfunct(x, m), start = list(m = 50), weights = bin_weights_sc)
nagelkerke(scal_fit, null = null.model)

#----------------------

#step 8:visualization of the SSD including the regression and the data points per bin per each taxon
#define dataframe for calcifying and slightly calcifying species
df_calcification <- read_excel("~/Desktop/dataset OA V4.xlsx", sheet = "calcification results")
x <- df_calcification$pH
y <- df_calcification$neg_affected
category <- df_calcification$`calcification`
#plot SSDs
g <- ggplot(df_calcification, aes(x,y, color = category, shape = category)) + xlim(5,10) + ylim(0,105)
g  + labs(x = "pH", y = "Potentially Affected Fraction of Species (PAF)") +
  stat_function(fun = cfunc, args = list(coef(cal_fit)["a"], coef(cal_fit)["b"]), color = "orangered1") +
```

```
  stat_function(fun = cfunc, args = list(coef(scal_fit)["a"], coef(scal_fit)["b"]), color = "cornflowerblue") + theme_classic()
+ geom_point()
#-------------------

#step 9: interaction term test
#define variables
w <- df_calcification[c(1:14), c(5)]$weight
ind <- df_calcification[c(1:14), c(4)]$ind  #identification variable for categories

#it --> interaction variable for testing
# fit the data to the function
it_test <- nls(y ~ 100 / (1 + 10 ^ ((a+a_it*ind - x) * (b+b_it*ind))), start = list(a = 7.5, b = -2, a_it = 0, b_it = 0), weights =
w)
summary(it_test)
```

Code for modelling the Climate Category SSDs:

```
library(readxl)
library(ggplot2)
library("rcompanion")

#code to model the SSD for polar data with a taxonomic grouping
#step 1: weighted averages per bin per taxon; c(mollusca, crustacea, echinodermata, fish)
bin0 <- c(0,0,0,0) #control
bin1 <- c(100, 50, 100, 0) # response of the first pco2 bin - each number represent one taxa
bin2 <- c(75, 66.7, 50, 0)
bin3 <- c(60, 60, 50, 100)
bin4 <- c(100, 80, 66.7, 100)
bin5 <- c(100, 100, 100, 50)
bin6 <- c(100,100,100, 100)

#step 2: calculating the weighted average of each bin using the global normalization factors per taxonomic group
w_gsr_p <- c(0.379, 0.053, 0.303, 0.197) #mollusca, echinodermata, crustacea, fish
w_avg_b0 <- weighted.mean(bin0, w_gsr_p)
w_avg_b1 <- weighted.mean(bin1, w_gsr_p)
w_avg_b2 <- weighted.mean(bin2, w_gsr_p)
w_avg_b3 <- weighted.mean(bin3,w_gsr_p)
w_avg_b4 <- weighted.mean(bin4, w_gsr_p)
w_avg_b5 <- weighted.mean(bin5, w_gsr_p)
w_avg_b6 <- weighted.mean(bin6, w_gsr_p)
y_p <- c(w_avg_b0, w_avg_b1, w_avg_b2, w_avg_b3, w_avg_b4, w_avg_b5, w_avg_b6)

#step 3: defining the pH values including the average pH value of the experiments within the category

x_p <- c(8.0548, 7.922231, 7.804119, 7.655225, 7.406747, 6.986673, 6.820071) #average pH values of each bin

#step 4: defining weights of the bins based on the total number of species data entry per given bin
bin_weights_p <- c(1, 0.3125, 0.75, 1, 0.8125, 0.81, 0.75)

#step 5: defining the logistic regression function with two parameters
cfunc <- function(x,a,b) {100 / (1 + 10 ^ ((a - x) * b))}

#step 6: defining the nonlinear least squares (nls) function for the regression
polar_fit <- nls(y_p ~ cfunc(x_p,a,b), start = list(a = 7.5, b = -2), weights = bin_weights_p)
summary(polar_fit)

#step 7: calculating the nagelkerke R2

nullfunct = function(x, m){m}
null.model = nls(y ~ nullfunct(x, m), start = list(m = 50), weights = bin_weights_p)
nagelkerke(polar_fit, null = null.model)


#------------
#code to model the SSD for temperate data with a taxonomic grouping
#step 1: weighted averages per bin per taxon; c(mollusca, crustacea, echinodermata, fish, cnidaria)
bin0 <- c(0,0,0,0,0) #control
```

```
bin1 <- c(45.5, 0, 66.7, 0,0) # response of the first pco2 bin - each number represent one taxa
bin2 <- c(75, 0, 37.5, 25, 25)
bin3 <- c(64.7, 20, 71.4, 22.2, 25)
bin4 <- c(94.1, 40, 84.6, 100, 100)
bin5 <- c(88.9, 90, 100, 87.5, 100)
bin6 <- c(100,100,100, 100,100)

#step 2: calculating the weighted average of each bin using the global normalization factors per taxonomic group
w_gsr_te <- c(0.379, 0.053, 0.303, 0.197, 0.068) #mollusca, echinodermata, crustacea, fish, cnidaria
w_avg_b0 <- weighted.mean(bin0, w_gsr_te)
w_avg_b1 <- weighted.mean(bin1, w_gsr_te)
w_avg_b2 <- weighted.mean(bin2, w_gsr_te)
w_avg_b3 <- weighted.mean(bin3,w_gsr_te)
w_avg_b4 <- weighted.mean(bin4, w_gsr_te)
w_avg_b5 <- weighted.mean(bin5, w_gsr_te)
w_avg_b6 <- weighted.mean(bin6, w_gsr_te)
y_te <- c(w_avg_b0, w_avg_b1, w_avg_b2, w_avg_b3, w_avg_b4, w_avg_b5, w_avg_b6)

#step 3: defining the pH values including the average pH value of the experiments within the category

x_te <- c(7.9860, 7.922231, 7.804119, 7.655225, 7.406747, 6.986673, 6.820071) #average pH values of each bin

#step 4: defining weights of the bins based on the total number of species data entry per given bin
bin_weights_te <- c(1, 0.3519, 0.5, 1, 0.889, 0.91, 0.852)

#step 5 is the same function definition for all regressions

#step 6: defining the nonlinear least squares (nls) function for the regression
temperate_fit <- nls(y_te ~ cfunc(x_te,a,b), start = list(a = 7.5, b = -2), weights = bin_weights_te)
summary(temperate_fit)

#step 7: calculating the nagelkerke R2

nullfunct = function(x, m){m}
null.model = nls(y ~ nullfunct(x, m), start = list(m = 50), weights = bin_weights_te)
nagelkerke(temperate_fit, null = null.model)

#-----------------------------------------------------
#code to model the SSD for tropical data with a taxonomic grouping
#step 1: weighted averages per bin per taxon; c(mollusca, crustacea, echinodermata, fish, cnidaria)
bin0 <- c(0,0,0,0,0) #control
bin1 <- c(50, 0, 50, 37.5, 50) # response of the first pco2 bin - each number represent one taxa
bin2 <- c(40, 0, 22.2, 66.7, 44.4)
bin3 <- c(30.8, 20, 70, 70.6, 50)
bin4 <- c(81.8, 40, 90, 86.7, 83.3)
bin5 <- c(100, 90, 100, 73.7, 100)
bin6 <- c(100,100,100, 100,100)


#step 2: calculating the weighted average of each bin using the global normalization factors per taxonomic group
w_gsr_tr <- c(0.379, 0.053, 0.303, 0.197, 0.068) #mollusca, echinodermata, crustacea, fish, cnidaria
w_avg_b0 <- weighted.mean(bin0, w_gsr_tr)
w_avg_b1 <- weighted.mean(bin1, w_gsr_tr)
w_avg_b2 <- weighted.mean(bin2, w_gsr_tr)
w_avg_b3 <- weighted.mean(bin3,w_gsr_tr)
w_avg_b4 <- weighted.mean(bin4, w_gsr_tr)
w_avg_b5 <- weighted.mean(bin5, w_gsr_tr)
w_avg_b6 <- weighted.mean(bin6, w_gsr_tr)
y_tr <- c(w_avg_b0, w_avg_b1, w_avg_b2, w_avg_b3, w_avg_b4, w_avg_b5, w_avg_b6)


#step 3: defining the pH values including the average pH value of the experiments within the category

x_tr <- c(8.0432, 7.922231, 7.804119, 7.655225, 7.406747, 6.986673, 6.820071) #average pH values of each bin

#step 4: defining weights of the bins based on the total number of species data entry per given bin
bin_weights_tr <- c(1, 0.35, 0.6667, 0.9833, 0.9667, 1, 1)
```

```
#step 5 is the same function definition for all regressions

#step 6: defining the nonlinear least squares (nls) function for the regression
tropical_fit <- nls(y_tr ~ cfunc(x_tr,a,b), start = list(a = 7.5, b = -2), weights = bin_weights_tr)
summary(tropical_fit)

#step 7: calculating the nagelkerke R2

nullfunct = function(x, m){m}
null.model = nls(y ~ nullfunct(x, m), start = list(m = 50), weights = bin_weights_tr)
nagelkerke(tropical_fit, null = null.model)


#----------------------
##step 8:visualization of the SSD including the regression and the data points per bin per each taxon
df_climate <- read_excel("~/Desktop/dataset OA V4.xlsx", sheet = "climate zones results")

x <- df_climate$pH
y <- df_climate$neg_affected
category <- df_climate$`climate zone`

g <- ggplot(df_climate, aes(x,y, color = category, shape = category)) + xlim(5,10) + ylim(0,105)
g   + labs(x = "pH", y = "Potentially Affected Fraction of Species (PAF)") +
  stat_function(fun = cfunc, args = list(coef(polar_fit)["a"], coef(polar_fit)["b"]), color = "orangered1") +
  stat_function(fun = cfunc, args = list(coef(temperate_fit)["a"], coef(temperate_fit)["b"]), color = "limegreen") +
  stat_function(fun = cfunc, args = list(coef(tropical_fit)["a"], coef(tropical_fit)["b"]), color = "cornflowerblue") +
theme_classic() + geom_point()
#-------------------
#step 9: interaction term test

#polar vs temperate
#define variables
x <- df_climate[c(1:14), c(2, 3)]$pH
y <- df_climate[c(1:14), c(2, 3)]$neg_affected
w <- df_climate[c(1:14), c(4)]$weight
ind <- c(1,1,1,1,1,1,1,0,0,0,0,0,0,0)  #identification variable for categories
#ind <- c(0,0,0,0,0,0,0,0,1,1,1,1,1,1,1)

#it --> interaction variable for testing
# fit the data to the function
it_test_temp_polar <- nls(y ~ 100 / (1 + 10 ^ ((a+a_it*ind - x) * (b+b_it*ind))), start = list(a = 7.5, b = -2, a_it = 0, b_it =
0), weights = w)
summary(it_test_temp_polar)

#polar vs tropical
#define variables
x <- df_climate[c(1:14), c(2, 3)]$pH
y <- df_climate[c(1:7,15:21), c(2, 3)]$neg_affected
w <- df_climate[c(1:7,15:21), c(4)]$weight
ind <- c(1,1,1,1,1,1,1,0,0,0,0,0,0,0)  #identification variable for categories
#it --> interaction variable for testing
# fit the data to the function
it_test_trop_polar <- nls(y ~ 100 / (1 + 10 ^ ((a+a_it*ind - x) * (b+b_it*ind))), start = list(a = 7.5, b = -2, a_it = 0, b_it =
0), weights = w)
summary(it_test_trop_polar)


#temperate vs tropical
#define variables
x <- df_climate[c(8:21), c(2, 3)]$pH
y <- df_climate[c(8:21), c(2, 3)]$neg_affected
w <- df_climate[c(8:21), c(4)]$weight
#ind <- c(0,0,0,0,0,0,0,1,1,1,1,1,1,1)  #identification variable for categories
ind <- c(1,1,1,1,1,1,1,0,0,0,0,0,0,0)
#it --> interaction variable for testing
# fit the data to the function
```

```
it_test_trop_temp <- nls(y ~ 100 / (1 + 10 ^ ((a+a_it*ind - x) * (b+b_it*ind))), start = list(a = 7.5, b = -2, a_it = 0, b_it = 0), weights = w)
summary(it_test_trop_temp)
```

Code for modelling the Duration Category SSDs:

```
library(readxl)
library(ggplot2)
library("rcompanion")

#code to model the SSD for acute data with a taxonomic grouping
#step 1: weighted averages per bin per taxon; c(mollusca, crustacea, echinodermata, fish, cnidaria)
bin0 <- c(0,0,0,0,0) #control
bin1 <- c(0, 100, 50, 50, 0) # response of the first pco2 bin - each number represent one taxa
bin2 <- c(33, 100, 12.5, 77.8, 50)
bin3 <- c(30, 50, 70, 73.3, 16.7)
bin4 <- c(85.7, 100, 80, 100, 33.3)
bin5 <- c(100, 100, 100, 66.7, 100)
bin6 <- c(100,100,100, 100,100)

#step 2: calculating the weighted average of each bin using the global normalization factors per taxonomic group
w_gsr_a <- c(0.379, 0.053, 0.303, 0.197, 0.068) #mollusca, echinodermata, crustacea, fish, cnidaria
w_avg_b0 <- weighted.mean(bin0, w_gsr_a)
w_avg_b1 <- weighted.mean(bin1, w_gsr_a)
w_avg_b2 <- weighted.mean(bin2, w_gsr_a)
w_avg_b3 <- weighted.mean(bin3,w_gsr_a)
w_avg_b4 <- weighted.mean(bin4, w_gsr_a)
w_avg_b5 <- weighted.mean(bin5, w_gsr_a)
w_avg_b6 <- weighted.mean(bin6, w_gsr_a)
y_a <- c(w_avg_b0, w_avg_b1, w_avg_b2, w_avg_b3, w_avg_b4, w_avg_b5, w_avg_b6)

#step 3: defining the pH values including the average pH value of the experiments within the category
x_a <- c(8.0329, 7.922231, 7.804119, 7.655225, 7.406747, 6.986673, 6.820071) #average pH values of each bin

#step 4: defining weights of the bins based on the total number of species data entry per given bin
bin_weights_a <- c(1, 0.1818, 0.52273, 0.9773, 0.7727, 0.98, 1)

#step 5: defining the logistic regression function with two parameters
cfunc <- function(x,a,b) {100 / (1 + 10 ^ ((a - x) * b))}

#step 6: defining the nonlinear least squares (nls) function for the regression
acute_fit <- nls(y_a ~ cfunc(x_a,a,b), start = list(a = 7.5, b = -2), weights = bin_weights_a)
summary(acute_fit)

#step 7: calculating the nagelkerke R2

nullfunct = function(x, m){m}
null.model = nls(y ~ nullfunct(x, m), start = list(m = 50), weights = bin_weights_a)
nagelkerke(acute_fit, null = null.model)


#------------
#code to model the SSD for sub-chronic data with a taxonomic grouping
#step 1: weighted averages per bin per taxon; c(mollusca, crustacea, echinodermata, fish, cnidaria)
bin0 <- c(0,0,0,0,0) #control
bin1 <- c(50,0, 100, 25,0)
bin2 <- c(100, 0, 50, 28.6, 0)
bin3 <- c(100, 16.7, 85.7, 40, 0)
```

```
bin4 <- c(100, 44.4, 85.7, 71.4, 100)
bin5 <- c(100, 88.9, 100, 100, 100)
bin6 <- c(100,100,100, 100,100)

#step 2: calculating the weighted average of each bin using the global normalization factors per taxonomic group
w_gsr_sc <- c(0.379, 0.053, 0.303, 0.197, 0.068) #mollusca, echinodermata, crustacea, fish, cnidaria
w_avg_b0 <- weighted.mean(bin0, w_gsr_sc)
w_avg_b1 <- weighted.mean(bin1, w_gsr_sc)
w_avg_b2 <- weighted.mean(bin2, w_gsr_sc)
w_avg_b3 <- weighted.mean(bin3,w_gsr_sc)
w_avg_b4 <- weighted.mean(bin4, w_gsr_sc)
w_avg_b5 <- weighted.mean(bin5, w_gsr_sc)
w_avg_b6 <- weighted.mean(bin6, w_gsr_sc)
y_sc <- c(w_avg_b0, w_avg_b1, w_avg_b2, w_avg_b3, w_avg_b4, w_avg_b5, w_avg_b6)

#step 3: defining the pH values including the average pH value of the experiments within the category

x_sc <- c(8.0229, 7.922231, 7.804119, 7.655225, 7.406747, 6.986673, 6.820071) #average pH values of each bin

#step 4: defining weights of the bins based on the total number of species data entry per given bin
bin_weights_sc <- c(1, 0.2857, 0.67857, 0.9643, 1, 0.93, 0.929)

#step 5: defining the logistic regression function with two parameters
cfunc <- function(x,a,b) {100 / (1 + 10 ^ ((a - x) * b))}

#step 6: defining the nonlinear least squares (nls) function for the regression
sc_fit <- nls(y_sc ~ cfunc(x_sc,a,b), start = list(a = 7.5, b = -2), weights = bin_weights_sc)
summary(sc_fit)

#step 7: calculating the nagelkerke R2

nullfunct = function(x, m){m}
null.model = nls(y ~ nullfunct(x, m), start = list(m = 50), weights = bin_weights_sc)
nagelkerke(sc_fit, null = null.model)


#------------------
#code to model the SSD for chronic data with a taxonomic grouping
#step 1: weighted averages per bin per taxon; c(mollusca, crustacea, echinodermata, fish, cnidaria)
bin0 <- c(0,0,0,0,0) #control
bin1 <- c(53.8, 0, 60, 0, 40) # response of the first pco2 bin - each number represent one taxa
bin2 <- c(66.7, 20, 44.4, 0, 40)
bin3 <- c(52.4, 33.3, 54.5, 33.3, 58.3)
bin4 <- c(90, 50 , 88.9, 100, 100)
bin5 <- c(90.5, 90, 100, 75, 100)
bin6 <- c(100,100,100, 100,100)

#step 2: calculating the weighted average of each bin using the global normalization factors per taxonomic group
w_gsr_ch <- c(0.379, 0.053, 0.303, 0.197, 0.068) #mollusca, echinodermata, crustacea, fish, cnidaria
w_avg_b0 <- weighted.mean(bin0, w_gsr_ch)
w_avg_b1 <- weighted.mean(bin1, w_gsr_ch)
w_avg_b2 <- weighted.mean(bin2, w_gsr_ch)
w_avg_b3 <- weighted.mean(bin3,w_gsr_ch)
w_avg_b4 <- weighted.mean(bin4, w_gsr_ch)
w_avg_b5 <- weighted.mean(bin5, w_gsr_ch)
w_avg_b6 <- weighted.mean(bin6, w_gsr_ch)
y_ch <- c(w_avg_b0, w_avg_b1, w_avg_b2, w_avg_b3, w_avg_b4, w_avg_b5, w_avg_b6)
```

```
#step 3: defining the pH values including the average pH value of the experiments within the category

x_ch <- c(8.0096, 7.922231, 7.804119, 7.655225, 7.406747, 6.986673, 6.820071) #average pH values of each bin

#step 4: defining weights of the bins based on the total number of species data entry per given bin
bin_weights_ch <- c(1,0.4915, 0.62712, 1, 0.9492, 0.9, 0.831)

#step 5: defining the logistic regression function with two parameters
cfunc <- function(x,a,b) {100 / (1 + 10 ^ ((a - x) * b))}

#step 6: defining the nonlinear least squares (nls) function for the regression
ch_fit <- nls(y_ch ~ cfunc(x_sc,a,b), start = list(a = 7.5, b = -2), weights = bin_weights_ch)
summary(ch_fit)

#step 7: calculating the nagelkerke R2

nullfunct = function(x, m){m}
null.model = nls(y ~ nullfunct(x, m), start = list(m = 50), weights = bin_weights_ch)
nagelkerke(ch_fit, null = null.model)

#----------------
##step 8:visualization of the SSD including the regression and the data points per bin per each taxon
df_duration <- read_excel("~/Desktop/dataset OA V4.xlsx", sheet = "duration results")

x <- df_duration$pH
y <- df_duration$neg_affected
category <- df_duration$`effect`

g <- ggplot(df_duration, aes(x,y, color = category, shape = category)) + xlim(5,10) + ylim(0,105)
g + labs(x = "pH", y = "Potentially Affected Fraction of Species (PAF)") +
  stat_function(fun = cfunc, args = list(coef(acute_fit)["a"], coef(acute_fit)["b"]), color = "orangered1") +
  stat_function(fun = cfunc, args = list(coef(ch_fit)["a"], coef(ch_fit)["b"]), color = "limegreen") +
  stat_function(fun = cfunc, args = list(coef(sc_fit)["a"], coef(sc_fit)["b"]), color = "cornflowerblue") + theme_classic() +
geom_point()
#-------------------

#interaction term

#Acute vs subchronic
#define variables
x <- df_duration[c(1:14), c(2, 3)]$pH
y <- df_duration[c(1:14), c(2, 3)]$neg_affected
w <- df_duration[c(1:14), c(4)]$weight
ind <- c(1,1,1,1,1,1,1,0,0,0,0,0,0,0)  #identification variable for categories
#it --> interaction variable for testing
# fit the data to the function
it_test_a_sc <- nls(y ~ 100 / (1 + 10 ^ ((a+a_it*ind - x) * (b+b_it*ind))), start = list(a = 7.5, b = -2, a_it = 0, b_it = 0),
weights = w)
summary(it_test_a_sc)

#acute vs chronic
#define variables
x <- df_duration[c(1:7,15:21), c(2, 3)]$pH
y <- df_duration[c(1:7,15:21), c(2, 3)]$neg_affected
w <- df_duration[c(1:7,15:21), c(4)]$weight
ind <- c(1,1,1,1,1,1,1,0,0,0,0,0,0,0)  #identification variable for categories
#it --> interaction variable for testing
# fit the data to the function
```

```
it_test_a_ch <- nls(y ~ 100 / (1 + 10 ^ ((a+a_it*ind - x) * (b+b_it*ind))), start = list(a = 7.5, b = -2, a_it = 0, b_it = 0), weights = w)
summary(it_test_a_ch)

#temperate vs tropical
#define variables
x <- df_duration[c(8:21), c(2, 3)]$pH
y <- df_duration[c(8:21), c(2, 3)]$neg_affected
w <- df_duration[c(8:21), c(4)]$weight
ind <- c(0,0,0,0,0,0,0,1,1,1,1,1,1,1)  #identification variable for categories
#it --> interaction variable for testing
# fit the data to the function
it_test_sc_c <- nls(y ~ 100 / (1 + 10 ^ ((a+a_it*ind - x) * (b+b_it*ind))), start = list(a = 7.5, b = -2, a_it = 0, b_it = 0), weights = w)
summary(it_test_sc_c)
```