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Characterization model to assess ocean acidification within life cycle assessment

Vanessa Bach^{1*}, Franziska Möller¹, Natalia Finogenova¹, Yasmine Emará¹, Matthias Finkbeiner¹

Abstract

Purpose Ocean acidification due to the absorption of increasing amounts of atmospheric carbon dioxide has become a severe problem in the recent years as more and more marine species are influenced by the decreasing pH value as well as by the reduced carbonate ion concentration. So far, no characterization model exists for ocean acidification. This paper aims to establish such a characterization model to allow for the necessary future inclusion of ocean acidification in life cycle assessment (LCA) case studies.

Methods Based on a cause-effect chain for ocean acidification, the substances carbon monoxide, carbon dioxide, and methane were identified as relevant for this impact category. In a next step, the fate factor representing the substances' share absorbed by the ocean due to conversion, distribution, and dissolution is determined. Then, the fate sensitivity factor is established reflecting the changes in the marine environment due to the amount of released hydrogen ions per gram of substance (category indicator). Finally, fate and fate sensitivity factors of each substance are multiplied and set in relation to the reference substance, carbon dioxide, thereby delivering the respective characterization factors (in kg CO₂ eq) at mid-point level.

Results and discussion Characterization factors are provided for carbon monoxide (0.87 kg CO₂ eq), carbon dioxide (1 kg CO₂ eq), and methane (0.84 kg CO₂ eq), which allow conversion of inventory results of these substances into category indicator results for ocean acidification. Inventory data of these substances is available in common LCA databases and software. Hence, the developed method is directly applicable. In a subsequent contribution analysis, the relative contribution of the three selected substances, along with other known acidifying substances, to the ocean acidification potential of 100 different materials was studied. The contribution analysis confirmed carbon dioxide as the predominant substance responsible for more than 97 % of the total ocean acidification potential. However, the influence of other acidifying substances, e.g., sulfur dioxide, should not be neglected.

Conclusions Evaluation of substances contributing to ocean acidification is of growing importance since the acidity of oceans has been increasing steadily over the last decades. The introduced approach can be applied to evaluate product system related impacts of ocean acidification and include those into current LCA practice.

Keywords Acidifying substances · CO₂ · Life cycle assessment · Life cycle impact assessment · Marine environment · Ocean acidification

1 Introduction

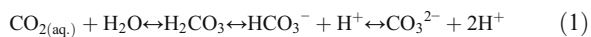
On April 2014, the Intergovernmental Panel on Climate Change (IPCC) released its latest assessment report which has evoked new discussions about climate change and its impacts on the environment and society (IPCC 2014). Since then, the topic of ocean acidification continued to grow in importance as research results indicate that more and more

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marine ecosystems will be significantly influenced (Widdicombe and Spicer 2008; Carew 2010; Harrould-Kolieb and Herr 2012). Since 1750, around 155 pentagram carbon dioxide (CO₂) emissions - the main cause for ocean acidification - have been absorbed by the oceans, resulting in an increase of the prevailing hydrogen ion (H⁺) concentration by approximately 30 % (Hall-Spencer et al. 2008; Rhein et al. 2013). The change in ocean chemistry has led to lowering of the oceans' mean pH value from 8.2 to 8.1. This is an enormous effect considering that the pH scale is logarithmic and that the volumes of water affected are huge (Royal Society Great Britain 2005; Carew 2010). Furthermore, the carbonate ion concentration has decreased by 16 % compared to pre-industrial conditions (Royal Society Great Britain 2005; Carew 2010). As all forecasts regarding future carbon dioxide emissions imply further increase (Carew 2010; IPCC 2013), ocean acidification and its impacts on the marine environment are expected to become even more severe over time. In a business-as-usual scenario, ocean acidity is expected to become 150 % higher than its pre-industrial levels by the end of the century, thereby reaching unprecedented pH values, which have not been observed in more than 20 million years (IPCC 2014). In light of this steadily growing threat to the environment, the need to include ocean acidification in life cycle assessment (LCA) can no longer be overlooked. This paper presents a characterization model, which will allow converting inventory results of acidifying substances into category indicator results on midpoint level, quantifying the impact of product systems on ocean acidification.

When CO₂ dissolves in the ocean, it reacts with water and forms carbonic acid (H₂CO₃) (see Eq. 1). This acid dissociates in the first step to bicarbonate ions (HCO₃⁻) and hydrogen ions (H⁺) and in the second step to carbonate ions (CO₃²⁻) and H⁺. This reaction is called the chemical equilibrium of carbon dioxide in seawater (Dickson 2010; Eisler 2011).



In Fig. 1, the cause-effect chain for ocean acidification is shown, illustrating relevant environmental mechanisms as well as suggesting elementary flows (left) and possible midpoint (middle) and endpoint (right) indicators. Considered elementary flows contributing to ocean acidification are CO₂ as well as its precursors: carbon monoxide (CO) and methane (CH₄). Whereas CO₂ can be dissolved in the ocean immediately, CO and CH₄ have to be transformed to CO₂ before dissolution can occur (Seinfeld and Pandis 2006; IPCC 2013). Not all of the emitted or generated, i.e., derived from precursors, CO₂ dissolves in the ocean; a part of it also stays in the atmosphere contributing to global warming. Due to the dissolution of CO₂ in the ocean, the H⁺ concentration increases which leads to a lower pH value. Furthermore, already existing CO₃²⁻ are bound by the newly generated H⁺. Given

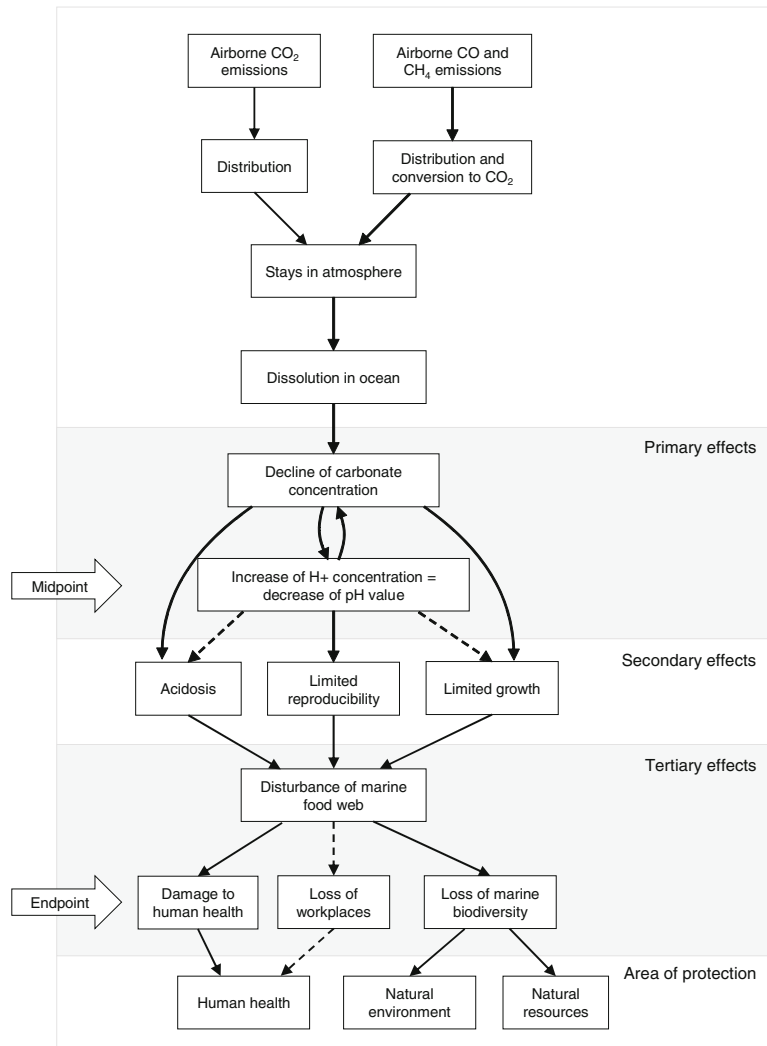
that 90 % of the carbonic acid formed by the dissolution of CO₂ in seawater quickly dissociates into bicarbonate and H⁺ whereas only 9 % breaks down further to CO₃²⁻ and another H⁺, the released H⁺ ions outnumber the increase in carbonate ions (Royal Society Great Britain 2005; Doney et al. 2009; Feely et al. 2009). Consequently, the effect of binding already existing carbonate ions by H⁺ dominates, resulting in a decrease of the total number of available carbonate ions. Hence, the more CO₂ is absorbed by the oceans, the more acidic the water is and the less carbonate ions are available (Zeebe and Wolf-Gladrow 2001; Eisler 2011). These impacts are called primary effects (see Fig. 1). Secondary effects of increasing CO₂ absorption into ocean waters and related ocean acidification include the following:

1. Acidosis (carbon dioxide diffuses into the blood of marine species and increases its acidity) (Fabry et al. 2008; Eisler 2011)
2. Limited survival of fish larvae (rising CO₂ levels act as a stressor) (Hurst et al. 2013)
3. Depleted levels of carbonate ions (primary effect) create many parts of the ocean which are undersaturated with calcium carbonate minerals. As a result, calcifying marine organisms lack the building blocks for their skeletons and shells (Gazeau et al. 2007; Widdicombe and Spicer 2008; Eisler 2011; Schroeder 2013).

The above listed secondary effects are likely to disturb the marine food web (tertiary effect) and modify the overall structure of marine ecosystems (Fabry et al. 2008; Schroeder 2013). As predator-prey relationships change, marine biota is bound to change in composition, leading to the depletion of certain populations and, essentially, to a loss of biodiversity (endpoint impact) (Lindeijer et al. 2002; Carew 2010). The decrease in biotic resources may affect human health as fish is the nutritional basis for many people. Lack of fish can also influence workplaces in the fishery and tourism sector. How far ocean acidification impacts will cascade throughout the marine food chain and ultimately result in tertiary effects is still unknown. However, there is general consensus that all three areas of protection - natural environment, natural resources, and human health - will be influenced by the increasing ocean acidification (Zeebe and Wolf-Gladrow 2001; Kroeker et al. 2010).

Despite the pertinence of the problem, so far, ocean acidification has not been considered within LCA, as no characterization model exists to determine the consequences of CO₂ (and its precursors) absorbed by oceans (Jolliet et al. 2014). Therefore, the authors developed an approach to quantify the potential impact of acidifying emissions on ocean acidification

Fig. 1 Cause-effect chain for ocean acidification based on Fabry et al. (2008), Widdicombe and Spicer (2008), Carew (2010), and Harrould-Kolieb and Herr (2012)



(midpoint modeling), thereby enabling a more comprehensive assessment of a product’s environmental profile.

2 Model for ocean acidification

As the first step, flows contributing to ocean acidification are identified on the basis of a cause-effect chain (classification). For midpoint methods, it is recommended to use primary effects for the category indicator, because these are easier to measure than secondary and tertiary effects and can be easily related to the main causes of the environmental problem (Klöpffer and Grahl 2009). To define the midpoint characterization factors (CFs) for the three identified elementary flows, fate and fate sensitivity factors must first be established. The fate factor represents the share of the substances that is absorbed by the environment (e.g., the ocean) due to

conversion, distribution, and dissolution (Lindeijer et al. 2002; Margni et al. 2008). It is calculated by multiplying the conversion, distribution, and dissolution factors of each elementary flow i (see Eq. 2).

$$\text{Fate factor}_i = \text{conversion factor}_i \times \text{distribution factor}_i \times \text{dissolution factor}_i \quad (2)$$

The conversion factor specifies how much of a substance is transformed into another substance. Before and/or after transformation, the considered substances can be distributed (distribution factor), e.g., between the layers of the atmosphere. Additionally, for models considering the environmental compartment water, the dissolution factor, i.e., the dissolved share of a substance into water bodies, has to be identified.

The fate sensitivity factor reflects the changes in the considered environmental compartment when the substance

enters it (Margni et al. 2008). In this case, the fate sensitivity factor indicates the potential increase in the H^+ ion concentration and thus a decrease in the pH value of the ocean water, when CO_2 is absorbed. Fate and fate sensitivity factors of each substance i are multiplied (see Eq. 3) to determine the ocean acidification potential factor (OAP_i).

$$OAP_i = \text{fate factor}_i \times \text{fate sensitivity factor}_i \quad (3)$$

To calculate the final characterization factors (in kg CO_2 eq), the OAPs of each substance are set in relation to the OAP of the reference substance, CO_2 (see Eq. 4). CO_2 was chosen as the reference substance as it is the main contributor to ocean acidification (Carew 2010).

$$CF_i = \frac{OAP_i \text{ kg } CO_2 \text{ eq.}}{OAP_{CO_2} \text{ kg emission}} \quad (4)$$

After the general approach for developing the characterization model for ocean acidification has been introduced, the specifics of the characterization model will now be determined. Fate factors for the three selected elementary flows - CO_2 , CH_4 , and CO - are first established. For CO_2 , no conversion factor is needed as it is dissolved in the ocean without further transformation. For CO and CH_4 , conversion factors have to be calculated as both substances only contribute to ocean acidification after they have been transformed into CO_2 (Doney et al. 2009). Since this transformation only occurs via hydroxide radicals (OH^-) in the troposphere, the amount of CO and CH_4 emissions entering the troposphere has to be identified (Wuebbles and Hayhoe 2000). According to Wuebbles and Hayhoe (2000), IPCC (2007), and Kirschke et al. (2013), 87.1 % of emitted CO and 87.8 % of emitted CH_4 enter the troposphere (see Fig. 2). These distribution shares present the basis for determining the distribution factors for CH_4 and CO .

In Fig. 2, the distribution, conversion, and dissolution shares of CO , CO_2 , and CH_4 used to calculate the distribution, conversion, and dissolution factors are shown.

The oxidation of CH_4 by OH^- leads to the formation of formaldehyde (CH_2O) and water vapor and, depending on the

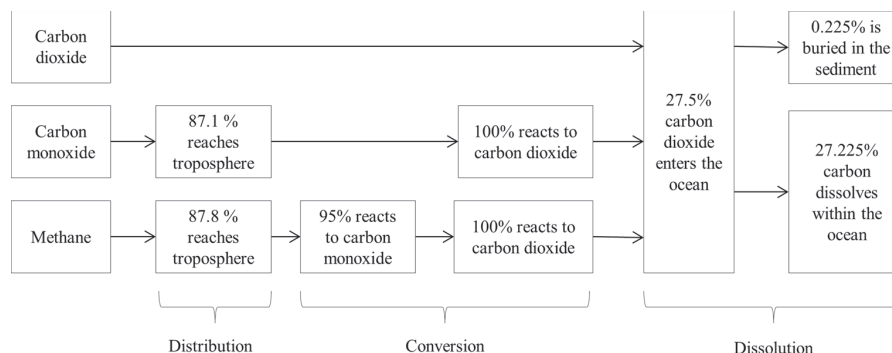
amount of nitrogen oxides, ozone (O_3). CH_2O reacts further to CO which is then converted to CO_2 (Wuebbles and Hayhoe 2002). Information on the exact shares of CH_4 and CO actually oxidized to CO_2 is not available in the literature. However, several sources indicate that most of the CH_2O will actually react to CO_2 (Wuebbles and Hayhoe 2000, 2002; Schlesinger 2005; Isaksen 2012). Thus, the share of CO produced by CH_4 is assumed to be 95 %. Produced CO will further react completely to CO_2 in the troposphere (Holloway and Wayne 2010; Isaksen 2012). The conversion factor for CH_4 into CO_2 is thus set to 0.95. Correspondingly, the conversion factor for CO entering the troposphere is set to 1, as the same assumption is applied: CO reacts to 100 % to CO_2 .

Not all of the overall CO_2 emissions will dissolve in the ocean as a certain amount stays in the atmosphere. According to Brewer and Barry (2008), Eakin et al. (2008), Hood et al. (2011), and the IPCC (2013), approximately 25–30 % of all (directly) released and (from precursors) generated CO_2 emissions are dissolved in the ocean. When CO_2 enters the ocean, it is participating in the ocean's equilibrium of storing and transforming CO_2 , which includes uptake of carbon by marine biota; dissolution in the ocean water; transport between surface, intermediate, and deep sea ocean; as well as sedimentation on the ocean floor (IPCC 2013). Only 1 % of the CO_2 entering the ocean is leaving this equilibrium by being buried in the sediment (CO_2 sinks due to sedimentation on the ocean floor) (Ducklow et al. 2001). Thus, out of the 27.5 % dissolving in the ocean, 1 % will not directly affect ocean acidification, leading to a final share of dissolved CO_2 of 27.225 % (see Eq. 5).

$$\begin{aligned} \text{Share of } CO_2 \text{ dissolving in the ocean} &= \text{Share of } CO_2 \text{ dissolving in the ocean} \\ &- \text{Share of } CO_2 \text{ captured in sediment} = 27.5\% - \frac{1\%}{27.5} \\ &= 27.5\% - 0.225\% = 27.225\% \end{aligned} \quad (5)$$

The dissolution share of 27.225 % relates to total CO_2 emissions (i.e., those directly emitted as CO_2 and those generated from precursors (CO and CH_4)) and thus represents the

Fig. 2 Distribution, conversion, and dissolution shares of CO , CO_2 , and CH_4



overall amount of dissolved CO₂, which in this case is equal to a *total fate factor* for all the three substances. The *total fate factor* represents the sum of the individual fate factors of CO, CO₂, and CH₄. However, it cannot be equally distributed to all three substances as their final dissolved share, or more precisely, their individual fate factors vary according to substance specific characteristics (e.g., CO and CH₄ have to be distributed and transformed into CO₂ first before being able to be dissolved in the ocean). Hence, the individual fate factors must be determined for each substance separately. This includes the determination of the dissolution factor, which is the same for CO, CO₂, and CH₄ as CH₄ and CO have already been distributed and converted to CO₂ at the point of dissolution into the ocean water (see Fig. 2). Therefore, the dissolution factor expresses a common characteristic of all CO₂ emissions regardless whether they have been emitted directly or generated from precursors. The individual or substance specific characteristics are expressed by the already established distribution and conversion factors and hence are considered in the individual fate factors of each substance. To determine the dissolution factor, the overall amount of dissolved CO₂ (27.225 %) is set in relation to the overall share of CO₂ able to be dissolved (see Eq. 7). The overall share able to be dissolved can be calculated by summing up the individual shares able to dissolve (see Eq. 6).

Overall share able to be dissolved

$$\begin{aligned}
 &= \text{Share of CO able to dissolve} \\
 &+ \text{Share of CO}_2 \text{ able to dissolve} \\
 &+ \text{Share of CH}_4 \text{ able to dissolve} \\
 &= 0.871 + 1 + 0.834 = 2.705 \quad (6)
 \end{aligned}$$

As CO₂ does not have to be converted and distributed prior to its dissolution, it is able to be dissolved in the ocean instantly (share of CO₂ able to be dissolved=1). To determine the share of CO able to be dissolved, the already identified distribution and conversion shares are used. Given that 100 % of the CO reaching the troposphere is assumed to be converted to CO₂, the share of CO distributed in the troposphere, i.e., the abovementioned distribution factor of 87.1 %, is equal to the individual share of CO able to be dissolved. The situation for CH₄ is in so far different, as only 95 % of CH₄ is assumed to be converted into CO, which is eventually converted into CO₂. Hence, of the 87.8 % of CH₄ reaching the troposphere (distribution share of CH₄), only 95 % will - after conversion to CO and CO₂ - be able to be dissolved. The individual share of CH₄ able to be dissolved is therefore 83.4 % (see Fig. 2).

The dissolution factor can be then calculated according to Eq. 7

$$\begin{aligned}
 &\text{Dissolution factor}_i \\
 &= \frac{\text{Overall amount of dissolved CO}_2}{\text{Overall share of CO}_2 \text{ able to be dissolved}} \quad (7)
 \end{aligned}$$

Based on Eqs. 6 and 7, the dissolution factor for CO, CO₂, and CH₄ is determined (see Eq. 8).

$$\text{Dissolution factor}_{\text{CO,CO}_2,\text{CH}_4} = \frac{0.27225}{2.705} = 0.1008 \quad (8)$$

Now that the conversion, distribution, and dissolution factors have been determined for each selected elementary flow, the fate factor for CO, CO₂, and CH₄ according to Eq. 2 is calculated (see Eqs. 9, 10, and 11) as follows:

$$\text{Fate factor}_{\text{CO}} = 1 \times 0.871 \times 0.1008 = 0.0878 \quad (9)$$

$$\text{Fate factor}_{\text{CO}_2} = 1 \times 1 \times 0.1008 = 0.1008 \quad (10)$$

$$\text{Fate factor}_{\text{CH}_4} = 0.95 \times 0.878 \times 0.1008 = 0.0841 \quad (11)$$

The fate factor represents the probability of substances entering the environment and thus is dimensionless. Next, the fate sensitivity factor is determined. Based on the approach of Heijungs et al. (1992) for calculation of the acidification potential of substances for terrestrial and freshwater acidification, the amount of released H⁺ per gram of substance is identified, which acts as the category indicator. As shown in Eq. 1, an equilibrium is established when CO₂ dissociates within the ocean. Based on Royal Society Great Britain (2005), Doney et al. (2009), and Feely et al. (2009), around 90 % of the CO₂ dissociates into HCO₃⁻ and one H⁺ and 9 % dissociates further into CO₃²⁻ and another H⁺ (see Table 1). Based on the calculations in Table 1, the fate sensitivity factor of ocean acidification sums up to $2.25 \times 10^{-2} \frac{\text{mol}_i}{\text{g}_{\text{CO}_2}}$ for CO₂, including indirect emissions and CO₂ derived from CO and CH₄.

With the fate and fate sensitivity factor identified, the OAP_i for CO, CO₂, and CH₄ can now be calculated according to Eq. 3 (see Eqs. 12, 13, and 14)

$$\begin{aligned}
 \text{OAP}_{\text{CO}} &= 0.0878 \times 2.45 \times 10^{-2} \frac{\text{mol}_i}{\text{g}_{\text{CO}_2}} \\
 &= 2.15 \times 10^{-3} \frac{\text{mol}_i}{\text{g}_{\text{CO}_2}} \quad (12)
 \end{aligned}$$

$$\begin{aligned}
 \text{OAP}_{\text{CO}_2} &= 0.1008 \times 2.45 \times 10^{-2} \frac{\text{mol}_i}{\text{g}_{\text{CO}_2}} \\
 &= 2.47 \times 10^{-3} \frac{\text{mol}_i}{\text{g}_{\text{CO}_2}} \quad (13)
 \end{aligned}$$

Table 1 Calculation of the fate sensitivity factor for ocean acidification including reaction equations, number of released H⁺ ions, molar mass, released H⁺ mole per gram CO₂, and probability of reaction taking place

Substance	Reaction equation	Number of released H ⁺ ions	Molar mass (g/mol)	Released H ⁺ ions mol per g CO ₂	Probability of reaction taking place
CO ₂	CO ₂ +H ₂ O↔H ₂ CO ₃ ↔HCO ₃ ⁻ +H ⁺	1	44	1/44	0.9
CO ₂	CO ₂ +H ₂ O↔H ₂ CO ₃ ↔CO ₃ ²⁻ +2H ⁺	2	44	2/44	0.09
CO ₂	(CO ₂ +H ₂ O↔H ₂ CO ₃ ↔)HCO ₃ ⁻ +H ⁺ ↔CO ₃ ²⁻ +2H ⁺	0.9 × 1H ⁺ + 0.09 × 2H ⁺ = 1.08H ⁺	44	1.08/44 = 2.45 × 10 ⁻²	0.99

$$\begin{aligned} \text{OAP}_{\text{CH}_4} &= 0.0841 \times 2.45 \times 10^{-2} \frac{\text{mol}_i}{\text{g}_{\text{CO}_2}} \\ &= 2.06 \times 10^{-3} \frac{\text{mol}_i}{\text{g}_{\text{CO}_2}} \end{aligned} \quad (14)$$

In the last step, the final characterization factors are determined (see Eqs. 15, 16, and 17) by setting the OAP_i of CO, CO₂, and CH₄ in relation to the OAP of the reference substance, CO₂, according to Eq. 4.

$$\text{CF}_{\text{CO}} = \frac{2.15 \times 10^{-3}}{2.47 \times 10^{-3}} = 0.87 \frac{\text{kg CO}_2 \text{ Eq.}}{\text{kg emission}} \quad (15)$$

$$\text{CF}_{\text{CO}_2} = \frac{2.47 \times 10^{-3}}{2.47 \times 10^{-3}} = 1 \frac{\text{kg CO}_2 \text{ Eq.}}{\text{kg emission}} \quad (16)$$

$$\text{CF}_{\text{CH}_4} = \frac{2.06 \times 10^{-3}}{2.47 \times 10^{-3}} = 0.84 \frac{\text{kg CO}_2 \text{ Eq.}}{\text{kg emission}} \quad (17)$$

To determine the ocean acidification potential of a product system, the characterization factor is multiplied with the mass of the elementary flow (ISO 14044 2006). In Table 2, the characteristics of the impact category ocean acidification are summarized.

3 Discussion

Fate factor The fate factor is determined by multiplying the distribution, conversion, and dissolution factors of each

substance. Thus, uncertainties of these factors are passed along to the fate factor. The determination of the distribution factors is based on several sources (i.e., Wuebbles and Hayhoe (2000); IPCC (2007); Kirschke et al. (2013)), which basically match in their statements. Thus, uncertainties can be considered low. The data of the conversion factors for CO and CH₄, on the other hand, are rather uncertain as no source clearly states how high the share of the transformed CO and CH₄ actually is, even though all sources (e.g., Wuebbles and Hayhoe 2002; Doney et al. 2009; Isaksen 2012) indicate that most of the CH₄ will be converted into CO and almost 100 % of emitted CO will be transformed into CO₂ after the intermediate reactions occurred. The data for the overall dissolution factor can be considered good, as several sources (e.g., Brewer and Barry 2008; Hood et al. 2011) agree on a range of 25–30 % of directly emitted and generated CO₂ emissions dissolving in the ocean.

Fate sensitivity factor For the fate sensitivity factor, specifications regarding the probability that the partial reactions occur, (based on which the potential amount of H⁺ ions released per gram CO₂ is calculated) originate from several sources (Royal Society Great Britain 2005; Doney et al. 2009; Feely et al. 2009). Consequently, the uncertainty in this factor can be considered low. As the OAPs as well as the CFs are composed of the fate and fate sensitivity, uncertainties of these factors are passed along.

Table 2 Characteristics of the impact category ocean acidification based on ISO 14044 (2006)

Impact category	Ocean acidification
LCI result	Amount of CO, CO ₂ , and CH ₄ per functional unit in kilogram
Characterization model	Introduced model by TUB SEE
Category indicator	Amount of H ⁺ ions released in mol/g CO ₂
Characterization factor	Ocean acidification potential (OAP) in kilograms CO ₂ equivalents per kilogram substance
Category indicator result	Kilograms of CO ₂ equivalents per functional unit
Category endpoint	Marine ecosystem, marine resources

Contribution of other acidifying substances Given that CO₂ is the main contributor to ocean acidification, the impacts of other acidifying substances (e.g., nitrogen oxides (NO_x) and sulfur dioxide (SO₂)) have so far not been considered. However, SO₂ and NO_x emission can rise high into the atmosphere, where they react with water, oxygen, and other chemicals to form acidic pollutants known as acid rain. The dissolution of these pollutants into ocean waters lowers the pH value by releasing H⁺ ions into the ocean. Impacts of such acidifying substances other than CO₂ (and its precursors) on marine ecosystems are not fully understood yet and may not necessarily trigger the exact same cause-effect chain as shown for CO₂ in Fig. 1. Consequently, they do not necessarily lead to the same secondary and tertiary effects. For instance at the current state of knowledge, it is not possible to predict if the released H⁺ ions (by the dissolution of these pollutants) impact the equilibrium of HCO₃⁻ and CO₃²⁻ in the ocean and therefore influence the calcification of organisms and their ability to build shells. Nonetheless, the reduced pH value is known, for instance, to cause disruption of the acid-base state of extracellular body fluid (e.g., blood), which leads to depressed metabolism, growth, and fitness in organisms unable to adapt to the changes in their environment (Pörtner et al. 2004; Michaelidis et al. 2005; Kroeker et al. 2010).

The developed approach for CO₂ (and its precursors) can serve as an example for expanding the characterization model to include other substances which affect the oceans' pH value. These substances, emitted into air, mostly reach the ocean via dry and wet deposition. Occasionally, acidifying substances, such as hydrogen chloride, are emitted into the ocean directly. Substances emitted into soil and freshwater will most likely not reach the ocean or will be too diluted to cause strong impacts (Goedkoop et al. 2009; Dunford et al. 2012; European Union 2014).

To give an example of how the proposed characterization model can be expanded to other substances, a first estimation of impacts of airborne NO_x and SO₂ emissions was made. According to Doney et al. (2007), about 33 % of all airborne NO_x and SO₂ emissions (or more precisely, of their corresponding acids: nitric acid (HNO₃) and sulfuric acid (H₂SO₄)) are dissolved into the ocean, resulting in a *total fate factor* of

0.33. As presented in Eq. 2, the individual fate factor is determined by multiplying the conversion factor (here, the total share of SO₂ and NO_x that is converted into the corresponding acids: H₂SO₄ and HNO₃) with the distribution factor (the total share of SO₂ and NO_x transported over the sea) and the dissolution factor (the total share of SO₂ and NO_x dissolving in the ocean). Similar to the *total fate factor* for CO₂, CO and CH₄ (27.255 %), the total fate factor of 33 % expresses the probability of both substances together, to be converted into acids, deposited over the ocean, and finally dissolved into the ocean (see Eq. 18).

$$\begin{aligned} \text{Fate factor}_{\text{NO}_x+\text{SO}_2} &= \text{conversion factor}_{\text{NO}_x+\text{SO}_2} \times \text{distribution factor}_{\text{NO}_x+\text{SO}_2} \\ &\times \text{dissolution factor}_{\text{NO}_x+\text{SO}_2} = 0.33 \end{aligned} \quad (18)$$

However, unlike the case of CO, CO₂, and CH₄, where data was available on the substance specific distribution and conversion factors and thus the breakdown of 27.225 % into individual fate factors was possible, no data is available on the individual distribution, conversion, and dissolution factors of NO_x and SO₂. Consequently, a simplified approach was applied in this context and the individual fate factors were determined by dividing the factor 0.33 equally on both substances. The study thus assumes that the individual probability of each substance to be distributed, converted, and finally dissolved in the ocean is the same, resulting in a fate factor of 0.165 for SO₂ as well as for NO_x. The fate sensitivity factor is determined as before (see Table 1) by accounting for the amount of hydrogen ions released for every gram of substance entering the ocean (see Table 3).

As shown in Eqs. 3 and 4, the characterization factor (in kg CO₂ eq) for substance *i* is determined by multiplying the fate and the fate sensitivity factor of each substance and dividing it by the OAP of the reference substance, CO₂ (see Eqs. 19 and 20).

$$CF_{\text{NO}_x} = \frac{0.165 \times 1.59 \times 10^{-2}}{2.47 \times 10^{-3}} = 1.06 \frac{\text{kg CO}_2 \text{ Eq.}}{\text{kg emission}} \quad (19)$$

$$\begin{aligned} CF_{\text{SO}_2} &= \frac{0.165 \times 2.04 \times 10^{-2}}{2.47 \times 10^{-3}} \\ &= 1.36 \frac{\text{kg CO}_2 \text{ Eq.}}{\text{kg emission}} \end{aligned} \quad (20)$$

Table 3 Calculation of the fate sensitivity factor for ocean acidification for HNO₃ and H₂SO₄

Substance	Reaction equation	Number of released H+ ions	Molar mass (g/mol)	Released H+ ions mol per g substance
HNO ₃	HNO ₃ →H ⁺ +NO ₃ ⁻	1	63	1/63
H ₂ SO ₄	H ₂ SO ₄ →2H ⁺ +SO ₄ ²⁻	2	98	1/49

Contribution analysis Following the approach of Berger and Finkbeiner (2011), a contribution analysis was performed to determine the relative contribution of each selected elementary flow (CO₂, CO, CH₄, NO_x, SO₂) to the overall ocean acidification resulting from production processes of 100 different materials. To guarantee that the results are not distorted by the choice of materials, they were selected from five distinct material groups: ores, metals, and alloys; monomers and polymers; organic and inorganic intermediates; and fuels (for detailed information on the materials considered, please see the [Electronic Supplementary Material](#)). Furthermore, in each group, 20 materials were considered, using 10 datasets from the GaBi database (Thinkstep 2016) and 10 from the Ecoinvent database (Ecoinvent 2016). The aims of the contribution analysis are (1) to identify which elementary flow contributes to the overall result and to what extent and (2) to determine whether other acidifying substances beside CO₂ (and its precursors) contribute to ocean acidification. As the first step, the total impact assessment result in the category ocean acidification for each material group is determined by summing up the individual impact category results of the 20 materials each group entails. The total result is set to 100 %, and the contribution share of each elementary flow to the

group's total impact is determined (for inventory results of the total mass contribution of each elementary flow across all 20 materials in every group, please see the [Electronic Supplementary Material](#)). In Table 4, the results of the contribution analysis are shown. They confirm carbon dioxide as the predominant substance causing ocean acidification, as its smallest contribution share is observed in the group fuels and lies at 97.72 %, whereas in the group monomers and polymers, it exceeds 99 %. Nevertheless, other substances like NO_x, SO₂, CO, and CH₄ contribute to ocean acidification as well, showing that their consideration is required to establish a comprehensive characterization method for this impact category.

Endpoint indicator As shown in Fig. 1, ocean acidification is likely to result in many (still widely unknown) damages at the endpoint level, such as loss of biodiversity and biotic resource depletion. Both endpoints are interlinked with each other as a loss of biodiversity can also lead to a reduction of biotic resources and vice versa. The here proposed midpoint characterization model will allow to quantify the expected increase in H⁺ ions and thus the potential degree (or gravity) of

Table 4 Contribution (in percentage) of elementary flows to the impact category ocean acidification for the five material groups

Groups	Elementary flows into the air	Contribution to impact category ocean acidification (%)
Ores, metals, and alloys	Carbon dioxide	98.56
	Carbon monoxide	0.56
	Nitrogen oxides	0.34
	Sulfur dioxide	0.38
	Methane	0.16
Monomers and polymers	Carbon dioxide	99.26
	Carbon monoxide	0.06
	Nitrogen oxides	0.20
	Sulfur dioxide	0.24
	Methane	0.34
Organic intermediates	Carbon dioxide	98.97
	Carbon monoxide	0.06
	Nitrogen oxides	0.19
	Sulfur dioxide	0.52
	Methane	0.26
Inorganic intermediates	Carbon dioxide	99.18
	Carbon monoxide	0.05
	Nitrogen oxides	0.18
	Sulfur dioxide	0.46
	Methane	0.12
Fuels	Carbon dioxide	97.72
	Carbon monoxide	0.51
	Nitrogen oxides	0.36
	Sulfur dioxide	0.71
	Methane	0.70

ocean acidification, when a given amount of acidifying substances is released during a product's life cycle. It does, however, not indicate in which way the marine species and the ecosystem as a whole will be affected exactly. In order to include secondary and tertiary effects of ocean acidification in a product's environmental assessment as well as to deliver more tangible interpretations of impact assessment results (yet at the expense of higher uncertainty), endpoint indicators for the category ocean acidification have to be developed. One way to establish such an endpoint indicator is to determine the potential disappeared fraction - a common measure for the loss of biodiversity - of marine species in response to ocean acidification based on the approach of Goedkoop et al. (2009). To this end, data of the research field oceanography is needed to find out the dose-response relationship between the potential disappeared fraction and the change in H^+ ion concentration. However, at the current state of knowledge, only few publications on this topic are available (e.g., Azevedo et al. 2015). It is, therefore, of vital importance to strengthen the science basis of the cause-effect chain for ocean acidification in order to introduce endpoint characterization models in the future.

4 Conclusions

Over the last decades, ocean acidification has been increasing at an accelerating and alarming rate, attracting much attention from scientists and policymakers alike. Despite the growing threat, it has until now not been considered in LCA due to the lack of a suitable characterization model. In this paper, a midpoint characterization model was introduced, which provides characterization factors for three selected acidifying substances (CO , CO_2 , and CH_4), thereby allowing for the first time to incorporate the category ocean acidification in future LCA case studies. The model can be expanded to include other acidifying substances, as was shown through estimates for the ocean acidification potential of NO_x and SO_2 . The identified substances contributing to ocean acidification are integrated in most existing LCA databases, as they also contribute to other important impact categories. Thus, less to no additional effort is necessary to collect data for the elementary flows contributing to ocean acidification. However, during interpretation of the impact assessment results, the uncertainties in the determined CFs have to be considered.

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