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(article starts on next page)

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Prospective environmental risk screening of seven advanced materials based on production volumes and aquatic ecotoxicity

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ABSTRACT

The number and volume of advanced materials being manufactured is increasing. In order to mitigate future impacts from such materials, assessment methods that can provide early indications of potential environmental risk are required. This paper presents a further development and testing of an environmental risk screening method based on two proxy measures: aquatic ecotoxicity and global annual production volumes. In addition to considering current production volumes, this further developed method considers potential future production volumes, thereby enabling prospective environmental risk screening. The proxy measures are applied to seven advanced materials: graphene, graphene oxide, nanocellulose, nanodiamond, quantum dots, nano-sized molybdenum disulfide, and MXenes. Only MXenes show high aquatic ecotoxicity, though the number of test results is still very limited. While current production volumes are relatively modest for most materials, several of the materials (graphene, graphene oxide, nanocellulose, nano-sized molybdenum disulfide, and MXenes) have the potential to become high-volume materials in the future. For MXenes, with both high aquatic ecotoxicity and high potential future production volumes, more detailed environmental risk assessments should be considered. For the other materials with high potential future production volumes, the recommendation is to continuously monitor their aquatic ecotoxicity data. Based on the application of the proxy measures combined with future scenarios for production volumes, we recommend this environmental risk screening method be used in the early development of advanced materials to prioritize which advanced materials should be subject to more detailed environmental assessments.

1. Introduction

An increasing number of new materials being explored and innovated are so-called advanced materials, which are "engineered to exhibit novel or enhanced properties that confer superior performance relative to conventional materials" (Kennedy et al., 2019). Alternatively, such materials may be referred to as sophisticated materials, which "exhibit novel, dynamic and multifaceted functionality" (Maynard et al., 2011). Engineered nanomaterials (ENMs), often defined as materials with at least one dimension in the 1–100 nm size range and with novel properties due to this size (Boholm and Arvidsson, 2016), are examples of such materials. While the ENMs currently developed and used in society are mainly metal and metal oxide nanoparticles, such as silica and titanium dioxide nanoparticles (Furberg et al., 2016), there is a strong research and innovation focus on more complex multi-component ENMs and advanced nanostructures, including two-dimensional materials such as the graphene family and the transition metal carbides or nitrides called MXenes (Khan et al., 2020; Wick et al., 2014). In the 2000s, a transition from early ENMs (e.g., metal nanoparticles) into next-generation ENMs with more elaborate functions was predicted (Roco, 2004; Tour, 2007). A bibliometric analysis identified such a shift towards more active nanostructures in the scientific literature starting already in 2006 (Subramanian et al., 2010). There is even development of highly elaborate ENMs such as medical nanorobots, consisting of, e.g., small nano-sized metal rods or folded DNA molecules, which are able to move and deliver drugs inside organisms (Arvidsson and Hansen, 2020). It thus seems like the transition to a more widespread use of advanced ENMs is beginning to be realized.

Considering this emergence of advanced materials, there is an increasing need to assess their potential environmental implications in the early stages of material development and commercialization, i.e. when the materials still have low technology readiness levels (TRLs)

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(ISO, 2019) and manufacturing readiness levels (MRLs) (United States Department of Defense, 2015). For ENMs, several environmental risk screening methods exist, such as LICARA nanoSCAN (van Harmelen et al., 2016), NanoRiskCat (Hansen et al., 2014) and the Precautionary Matrix (Höck et al., 2008). However, these methods may not be directly applicable to advanced materials. For example, the Precautionary Matrix requires input data that presupposes certain configurations of the material assessed, such as nanoparticles and nanorods. Future advanced materials may not comply with such configurations, two-dimensional materials being a case in point. For LICARA nanoSCAN and NanoRiskCat, the assessment objects are products containing ENMs. However, for very novel materials being researched, such products may not exist yet. There is thus a need for a flexible environmental risk screening method with a material focus that can be applied even at early stages of material development and commercialization, when risk-related data will be scarce.

To address this need, Arvidsson et al. (2018) proposed the use of two so-called proxy measures of environmental risk: global annual production volumes (unit: metric t/year) and aquatic ecotoxicity (unit: L/mg). The idea was that together, these two measures could screen materials for their potential risk to freshwater organisms at a minimum data requirement level. Using this approach, Arvidsson et al. (2018) assessed six metal and metal oxide nanoparticles, along with carbon nanotubes and graphene. Only silver nanoparticles were shown to have high aquatic ecotoxicity, while several nanomaterials had high production volumes (e.g., silica and titanium dioxide). None of the assessed nanomaterials had both high aquatic ecotoxicity and high production volumes.

In the present study, the proxy measure risk screening method is applied to a novel set of advanced materials. In addition, the proxy measure production volume is further developed by considering also future production scenarios according to three different approaches. This was suggested, but not implemented, in the previous study (Arvidsson et al., 2018). Besides the obvious aim of performing early environmental risk screening for potentially important future materials, the study also aims to test the feasibility of this approach for materials at even earlier stages than the previously assessed ENMs. For comparison, graphene is included in this study too, along with six other advanced materials: graphene oxide (GO), nanocellulose, nanodiamonds, quantum dots, nano-sized molybdenum disulfide (nano-MoS_2), and MXenes.

2. Materials and methods

2.1. Selected advanced materials

Graphene consists of a single layer of carbon atoms and offers many outstanding properties, including high strength and conductivity (Geim, 2009). For this reason, it has several promising applications, such as in composites, electronics, flame retardants, supercapacitors, and photonics (Arvidsson and Sandén, 2017; Ferrari et al., 2015; Janković and Plata, 2019; Novoselov et al., 2012).

GO is oxidized graphene and is another member of the graphene-based materials family (Wick et al., 2014). While GO also has several promising future applications, most of its envisioned applications require reduced GO, which is similar to graphene given a high enough reduction (Dideikin and Vul", 2019; Ray, 2015). GO thus shares most applications with graphene by being a precursor material for graphene produced via oxidation of graphite and subsequent reduction of GO, which is the most common large-scale preparation method of graphene (Poh et al., 2012). In fact, a significant share of products labeled as graphene on the market might rather be GO or reduced GO (Kauling et al., 2018).

Nanocellulose consists of nano-sized cellulose fibers and comes in three main types: nanofibrillated cellulose, nanocrystalline cellulose and bacterial cellulose (Klemm et al., 2011). Its main promising applications include composites, packaging, paper coatings/fillers, and textiles (Dufresne, 2013; Janković and Plata, 2019; Shatkin et al., 2014).

The term nanodiamond is used for a range of nano-sized diamond materials, including diamond films produced by chemical vapor deposition and small diamondoid molecules (Shenderova and McGuire, 2006). However, the currently most industrially produced nanodiamond type is detonation nanodiamonds produced from explosives, typically roughly spherical with 5 nm diameter (Mochalin et al., 2012; Shenderova and Nunn, 2017). Detonation nanodiamonds have envisioned applications in metal plating, composites, polishing, lubricants, as well as in biomedical applications, such as drug delivery and imaging (Dolmatov, 2006; Mochalin et al., 2012).

Quantum dots are a wide range of nano-sized (often $<$10 nm) particles with discrete size-dependent band gaps that make them tunable semiconductors, examples being lead sulfide and cadmium selenide (Bera et al., 2010; Reshma and Mohanan, 2019). They can be doped, alloyed, or coated with other materials (Bera et al., 2010; Reshma and Mohanan, 2019). The properties of quantum dots can be utilized in applications such as light emitting diodes, solar cells, and biomedical applications such as imaging (Bera et al., 2010; Cotta, 2020; Reshma and Mohanan, 2019).

Nano-MoS_2 is a nano-sized layered material of MoS_2 with early envisioned applications in contaminant adsorption, membrane filtration, gas sensing, photocatalysis, batteries, electronics, and medical applications, such as biosensing, disinfection, and cancer therapy (Akbari et al., 2018; Lembke et al., 2015; Lu et al., 2020; Radisavljevic et al., 2011; Shi et al., 2016; Wang and Mi, 2017; Xie et al., 2015). Furthermore, micro-sized MoS_2 ("bulk MoS_2") is commercially used as solid lubricant (Vazirisereshk et al., 2019). Recently, there are also attempts to use nano-sized MoS_2 in liquid lubricants (Xu et al., 2018).

MXenes are two-dimensional, layered materials with the general formula $M_{n+1}X_nT_x$, where M is a transition metal (e.g., titanium), X is carbon or nitrogen, and T is a surface terminator (e.g., oxygen or fluorine) (Gogotsi and Anasori, 2019). Examples include $Ti_3C_2T_x$, Ti_2CT_x and Mo_2NT_x (Papadopoulou et al., 2020). Envisioned uses for MXenes include catalysis, electronics, sensors, battery electrodes, as well as water purification and bioimaging (Gogotsi and Anasori, 2019; Papadopoulou et al., 2020; Ronchi et al., 2019).

Together, these seven advanced materials span different applications as well as fiber-shaped (nanocellulose), sheet-shaped (graphene, GO, nano-MoS_2, and MXenes), and particle-shaped (nanodiamonds and quantum dots) materials. It should be noted that most of the seven advanced materials contain subgroups. For example, nanodiamonds can have different functionalizations and quantum dots have different chemical compositions (e.g., CdSe and CdTe). Still, they are assessed on group bases here, since that is how materials are often considered and evaluated in environmental regulation and governance (Hansen and Lennquist, 2020).

2.2. Aquatic ecotoxicity data

Aquatic ecotoxicity data in the form of XC50 values (i.e., either of LC50, EC50, and IC50) are gathered from aquatic ecotoxicity tests, in line with the method of the previous publication (Arvidsson et al., 2018), because such XC50 values are the most reliable ecotoxicological parameters and are often accessible even for materials at early stages. Aquatic XC50 values from laboratory test systems can also be used as conservative proxies for the actual XC50 values in the natural environment, where natural organic matter influences ecotoxicity (Arvidsson et al., 2020). Median XC50 values are calculated, when possible, in order to obtain most likely estimates for benchmarking the advanced materials. This reduces the risk of a single value influencing the assessment considerably, as might be the case if, e.g., the lowest XC50 value is used for benchmarking.

For graphene, four XC50 values from Pretti et al. (2014), Lu et al. (2015), and Sanchís et al. (2016) are used to calculate median, 25th percentile, and 75th percentile values. For GO, Markovic et al. (2018)

report five XC50 values (LC50 and EC50), which are used to calculate median, 25th percentile, and 75th percentile values. For nanocellulose, 20 aquatic EC50 and LC50 values are reported by Ong et al. (2017, 1 value) and Kovacs et al. (2010, 19 values), from which median, 25th percentile, and 75th percentile values are calculated. For nanodiamond, only a single published LC50 value exists (Brand et al., 2020) and four additional unpublished values (three EC50 values and one LC50 value) from the EU-funded NANOSOLUTIONS project (FP7–309329) are kindly provided by researchers at the Water Research Group at North-West University in South Africa (Botha and Wepener, 2021). Median, 25th percentile, and 75th percentile values are calculated based on these five values. For quantum dots, 33 XC50 values (mainly for CdSe as well as some CdTe, CdS, and carbon quantum dots) are obtained from various sources but mostly from the extensive review by Rocha et al. (2017), enabling the calculation of median, 25th percentile, and 75th percentile values. For nano-MoS_2, two XC50 values are reported by Arefi-Oskoui et al. (2020) and their average value is used as most likely estimate. For MXenes, only one single LC50 value is reported, specifically for $Ti_3C_2T_x$ (Nasrallah et al., 2018). This value is therefore used as most likely estimate, considering that $Ti_3C_2T_x$ is the by far most researched MXene to date (Gogotsi and Anasori, 2019). All aquatic ecotoxicity data can be found in Table S1 in the Supplementary Material (SM). The 1 mg/L (or, reciprocally, 1 L/mg) threshold for aquatic acute toxicity in the Classification, Labeling and Packaging (CLP) regulation (European Parliament and the Council of the European Union, 2008) is applied as benchmark threshold.

2.3. Current global production volume data

When estimating global production volumes, the most recent estimate from each individual source is considered, and data older than 10 years (i.e., from before 2011) are not considered. One global production estimate for graphene is obtained by summing the production data from major graphene producers listed in Ren and Cheng (2014), which are from varying years between 2012 and (estimates for) 2019, resulting in approximately 1000 t/year. Janković and Plata (2019) report a range of 20–525 t/year, giving an average value of about 270 t/year. Lin et al. (2019) provide estimates of graphene nanoflake production in China, Europe, and the United States in 2017, amounting to about 2000 t/year in total. Finally, a market report by Future Markets (2014) provide production volumes from various producers, mainly for the years 2013–2015, which add up to approximately 2500 t/year. The median value (1500 t/year), as well as 25th and 75th percentiles, are calculated from these four estimates.

Data on GO production are still scarce, but it was reportedly 100 t/year in 2013 according to Ren and Cheng (2014), although this number only includes one company. Furthermore, Lin et al. (2019) report graphene oxide production in China, Europe, and the United States in 2017, adding up to about 780 t/year in total. The average value of these two estimates (440 t/year) is taken as most likely estimate for the year 2021.

Both Trache et al. (2020) and Rebouillat and Pla (2013) provide production data from known nanocellulose producers, which add up to similar results (601 and 609 t/year, respectively). Stoudmann et al. (2019) provide three estimates based on different market reports: one at about 21,000 t/year in 2017, one at about 600 t/year in 2015, and one at about 6100 t/year in 2014. Janković and Plata (2019) provide an estimate at 1140–7560 t/year in 2021, with an average of about 4400 t/year. The median value of these six estimates (2500 t/year), as well as 25th and 75th percentiles, are calculated.

Little production data are available for nanodiamonds, but Shenderova and Nunn (2017) report that detonation nanodiamonds, which are the currently cheapest and most produced nanodiamonds, are produced at "ton quantities annually". Furthermore, Petrov and Shenderova (2006) report that the company Altai produced more than 5 t/year already in 1993. The market report values cited in Janković and Plata (2019) say 28–42 t/year in 2021, from which an average of 35 t/year is calculated. This value is used as most likely estimate.

For quantum dots, global median, 25th percentile, and 75th percentile production volumes are reported in Piccinno et al. (2012) at 0.6, 0.6 and 5.5 t/year, respectively. The market report values provided in Janković and Plata (2019) say >5 t/year in 2020, which is in line with the 75th percentile in Piccinno et al. (2012). Based on these values, a most likely estimate of 5 t/year is assumed for 2021.

Unfortunately, no current production data for nano-MoS_2 is available. Data on ENM production from consultancy reports generally include many ENMs, but often not nano-MoS_2 (see, e.g., Janković and Plata (2019)), which is probably due to limited current production. It is also clear that the research interest into nano-MoS_2 has followed that of graphene (Akbari et al., 2018; Lembke et al., 2015), which makes it probable that the production of nano-MoS_2 is lower than that of graphene. Since most envisioned applications for nano-MoS_2 are at the experimental level, its production volumes are probably much lower than those of graphene. For example, Song et al. (2015) write that "large-scale synthesis of single layers [of MoS_2] with single crystalline domain is still not achieved."

No current production data for MXenes are available either, but similarly to nano-MoS_2, production volumes are expected to be low compared to, e.g., graphene. Recent review papers state that MXenes, while showing great promises, are still at an early stage of technological development (Gogotsi and Anasori, 2019), for example referring to "potential" and "possible" (rather than existing) applications (Papadopoulou et al., 2020).

All production volume data can be found in Table S2 in the SM. The high production volume threshold of 1000 t/year, as applied by the Organisation for Economic Co-Operation and Development (OECD, 2004), is used as benchmark. In addition, the production volume results are also benchmarked against those of two high-volume chemicals (ascorbic acid and acetone) in order to put the results into perspective.

2.4. Future annual global production scenarios

There is no generally acknowledged method for estimating future production volumes of advanced materials (Cowie et al., 2014), but two types of approaches can be distinguished. The first involves estimating the future market share (x_i) of an advanced material in an application i (e.g., a device or conventional material), as well as the future market volume of that application (m_i), and the concentration of the advanced material in that application (c_i):

$$m = \sum_i x_i c_i m_i \tag{1}$$

Sometimes, future scenarios of m_i are considered in this approach, preferably temporally aligned with x_i. We refer to this approach as "the market share approach"; see Boxall et al. (2007) for an example of its use in environmental risk assessment of ENMs.

In the second approach, the production volume of the material is scaled up by extrapolation to the time t based on some temporal trend, such as an exponential relationship with a growth rate a and a current production volume m_0:

$$m(t) = m_0 a^t \tag{2}$$

The parameter a is related to the annual exponential growth rate r, sometimes referred to as compound annual growth rate (CAGR), as $r = a - 1$. We refer to this approach as "the extrapolation approach"; see Robichaud et al. (2009) for an example of its use on titanium dioxide nanomaterials. In addition to the exponential relationship, alternative relationships are possible, such as the logistic relationship, which recognizes the possibility of reaching market saturation:

$$m(t) = \frac{L}{1 + e^{-k(t-t_0)}} \tag{3}$$

where L is the maximum value of the annual production rate of the advanced material, k is the growth rate, and t_0 is the value of t at the curve's midpoint. Much used in human and ecological population dynamics, the logistic function has also found applications in economics for modelling, e.g., long-term GDP growth (Modis, 2013), the diffusion of management systems (To and Lee, 2014), and sales growth for innovative products (Rietmann et al., 2020).

Relating to the scenario framework by Börjesson et al. (2006), the market share approach is often used for "what-if scenarios" of *possible* futures, while the extrapolation approach is often used for deriving future scenarios perceived as *likely*. Both approaches involve parameters which are challenging to estimate, such as x_i in the market share approach and a or k in the extrapolation approach. While the exponential extrapolation approach requires knowledge about the current production rate of the advanced material (m_0), the market share approach is independent of this. On the other hand, the extrapolation approach provides an explicit relationship between m and t, whereas the market shares can apply for some unspecified future point in time in the market share approach. The market share approach becomes more challenging to apply if there are many envisioned applications, i.e., for higher values of i, since it then requires investigations into many markets.

For graphene, applications such as in composites (Geim and Novoselov, 2007) and transparent electrodes (Berger, 2008) are pointed out as the most imminent ones. However, when looking further into the future, graphene clearly has many other potential applications (Section 2.1). This makes it challenging to apply the market share approach for graphene. Hence, the exponential extrapolation approach is applied with m_0 as in Table S2 (assumed for 2021), $r = 26\%$ as a low estimate and $r = 43\%$ as a high estimate (Janković and Plata, 2019). Other authors report a similar annual growth rate of 40% for graphene (Reiss et al., 2019). The data is extrapolated to year 2030 using Eq. 2.

As discussed in Section 2.1, GO is strongly linked to graphene. Although no growth rates published in scientific journals are available, online market reports typically provide rates similar to those for graphene, i.e., 30–40%. Considering the strong link to graphene, we apply the same growth rates as for graphene (26% as low estimate and 43% as high estimate) in an exponential extrapolation from an m_0 value as in Table S2 in 2021 until 2030 using Eq. 2. However, it should be noted that if other production processes for graphene than oxidation of graphite become increasingly popular in the future, e.g., liquid exfoliation of graphite by ultrasound (Bonaccorso et al., 2012), this link may become broken.

Future production volumes of nanocellulose are estimated using the market share approach in two consecutive papers (Cowie et al., 2014; Shatkin et al., 2014). In the first paper, 33 future applications of nanocellulose are identified. In the second, global production volumes of nanocellulose are estimated, resulting in "optimistic", "reasonable", and "pessimistic" scenarios. Different market shares x_i are assumed depending on the application. The estimations are stated to assume "favorable performance, technological readiness and economics", which may lead to an overestimation of the production volume. On the other hand, no growth of the application markets (m_i) is assumed, which may lead to an underestimation of future production volumes. Although these estimates are conducted some years ago and without specifying a time horizon, they constitute the most comprehensive market-share estimates available for nanocellulose and are therefore used in the present study. In addition, we also include a high and low estimate scenario using the exponential extrapolation approach for comparison, starting with an m_0 value as in Table S2 in 2021 with growth rates of 21 and 31% until 2030 in a low and high estimate, respectively (Janković and Plata, 2019). The lower growth rate is similar to the 19% reported by Stoudmann et al. (2019).

Similar to graphene, nanodiamonds have a wide range of potential applications (Section 2.1), which makes the market share approach challenging to apply. Instead, the exponential extrapolation approach is applied until 2030 with m_0 as in Table S2 in 2020, as well as with $r = 12\%$ in a low estimate and $r = 15\%$ in a high estimate (Janković and Plata, 2019).

Quantum dots also have several envisioned applications (Section 2.1). Several of these, such as light emitting diodes and photovoltaics, might be of significant magnitude, while, e.g., biomedical applications might be more limited. Again, we therefore used the exponential extrapolation approach with m_0 as in Table S2 in 2021 and using $r = 58\%$ in an extrapolation to 2030 (Janković and Plata, 2019).

Since neither current production m_0 nor any growth rates are available for nano-MoS_2, the extrapolation approach cannot be used. Nano-MoS_2 also has numerous potential application (Section 2.1), making the market approach challenging. There is, however, one application of nano-MoS_2 which is reported to be particularly promising, near-term plausible, and potentially involving large material volumes: liquid lubricants. A limited market share scenario with this application only is therefore performed using Eq. 1. Based on a mini review of experimental studies applying nano-MoS_2 in various liquid lubricants, thereby lowering friction significantly, a range of 0.1–1% cover most concentrations ($c_{\text{lubricant}}$) applied (Table S3 in the SM). Regarding the future market share $x_{\text{lubricant}}$, we apply the values 1%, representing limited use of nano-MoS_2 in particular niches only, and 50%, representing wide use of nano-MoS_2 in a considerable share of lubricants. The set of lower numbers is referred to as a "pessimistic scenario" and the set of higher numbers as an "optimistic scenario", as in the previous market share estimation for nanocellulose (Cowie et al., 2014). Regarding the lubricant market $m_{\text{lubricant}}$, it has been estimated at 35.6 million t/year in 2015 (Mang and Gosalia, 2017).

For MXenes, no growth rates have been found. Like most of the advanced materials, MXenes have several envisioned applications (Section 2.3). However, using MXenes for energy storage, specifically as electrode material in lithium-ion batteries, is among the first explored applications and constitutes a large proportion of MXene activities (Gogotsi and Anasori, 2019). A limited market share scenario comprising the electrode application only is therefore conducted, where $c_{\text{electrode}}$ is based on a mini review of 17 experimental studies (Table S4 in the SM), mainly obtained from a previous review (Greaves et al., 2020). Table S4 shows that 80% is a common MXene concentration in electrodes, which is applied in the present study. Consistent with our treatment of nano-MoS_2, a "pessimistic scenario" with 1% market penetration and an "optimistic scenario" with 50% market penetration are assumed. The market for lithium-ion battery anode materials has been estimated at 0.19 million t in 2017 and 1.75 million metric t in 2028 (Lasley, 2020), which are used in the "pessimistic" and "optimistic" scenarios, respectively.

For curve-fitting the logistic extrapolation model, it is preferable to have a long historical dataset. For this reason, we rely on the supporting information in Janković and Plata (2019), which reproduces data from a market report (Future Markets Inc, 2016), since that offers the most extensive and internally consistent set of time series for graphene, nanocellulose, and nanodiamonds. Time series for GO, quantum dots, nano-MoS_2, and MXenes are not available and thus no extrapolation based on the logistic relationship is performed for these materials. The results from the exponential and logistic extrapolations are also compared in terms of improvements in correlation coefficients based on the dataset from Janković and Plata (2019).

3. Results and discussion

This section first reports and discusses aquatic ecotoxicity results (horizontal axis in Fig. 1), then current and future potential production volume results (vertical axis in Fig. 1). Finally, combined risk screening results from Fig. 1 are discussed. Limitations and potential methodological improvements are discussed in each subsection.

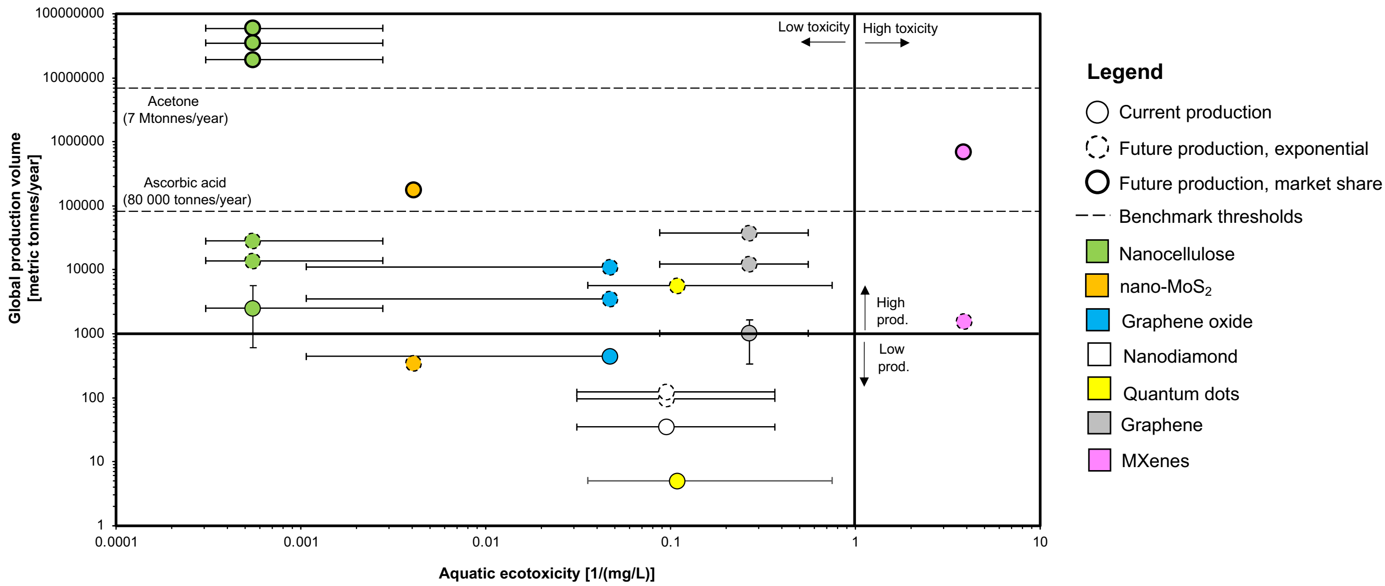

Fig. 1. Results from using two proxy measures (global annual production volume and aquatic ecotoxicity) on seven advanced nanomaterials. Error bars show 25th and 75th percentiles. The 1 L/mg threshold is a European CLP regulation criterion for acute aquatic toxicity. The 1000 t/year threshold marks high-volume chemicals according to the OECD (2004). Number of aquatic ecotoxicity data points: 20 for nanocellulose, 2 for nano-MoS_2, 5 for graphene oxide, 5 for nanodiamond, 33 for quantum dots, 4 for graphene, and 1 for MXenes.

3.1. Aquatic ecotoxicity

Only one of the seven advanced materials, the $Ti_3C_2T_x$ MXene, has an estimated aquatic ecotoxicity value above 1 L/mg. Most of the advanced materials do not raise considerable aquatic ecotoxicity concerns. In particular, nanocellulose and nano-MoS_2, as well as the 25th percentile for GO, show very low aquatic ecotoxicities. However, the results for MXenes and nano-MoS_2 are based on very few XC50 values (one and two, respectively). The aquatic ecotoxicity results for these two materials are therefore highly uncertain and the risk screening would benefit greatly from additional XC50 values. Reporting the number of XC50 values underpinning the assessment in connection to the result, as done in the caption of Fig. 1, is recommended in order to communicate uncertainty from limited data availability. Furthermore, as has been shown for first generation nanomaterials, technical issues related to generating XC50 values arise when testing novel materials with existing test methods (Skjolding et al., 2016). This raises questions related to the relevance and reliability of such aquatic ecotoxicity data for decision making (Hartmann et al., 2017), including decisions based on the proxy risk screening approach. However, the reliability of the outcome of the risk screening approach may improve when larger datasets become available by introducing a weighing of XC50 values based on their quality (Sørensen et al., 2020). If the proxy measures are considered for use in stricter governance contexts, such as regulatory frameworks, it is also possible to impose requirements on the number of XC50 values for each advanced material. For example, three XC50 values representing species at different trophic levels are required in the hazard assessment procedure of the European Chemicals Agency (ECHA, 2008) and in the USEtox method for deriving ecotoxicity characterization factors in life cycle assessment (Rosenbaum et al., 2008). Given such a requirement, more data gathering of XC50 values would have been required for nano-MoS_2 and MXenes in the present study.

3.2. Global production volumes

Our analysis shows that the seven materials fall in three groups according to their current production volumes: one group with high production volumes at about 1000 t/year (graphene, GO, and nanocellulose), one with lower production volumes (nanodiamond and quantum dots), and one with unknown but probably also low production volumes (nano-MoS_2 and MXenes) (Fig. 1). However, future production volumes are estimated to increase considerably for most of the materials, to the extent where they might approach or even surpass, e.g., those of high-volume chemicals like ascorbic acid.

A particularly notable future production scenario is the market share estimation for nanocellulose, which resulted in very high estimates, even surpassing the current production of acetone (Fig. 1). Clearly, the estimation by Cowie et al. (2014) is, as they put it, "favorable" for nanocellulose. In fact, based on the extrapolation approach used in parallel, it would take until between 2055 (given 31% growth rate) and 2068 (given 21% growth rate) before even the pessimistic market share scenario of ca 19,000 Mt/year is reached. The logistic modelling of data from Janković and Plata (2019) likewise suggests that such values for nanocellulose should not be expected until the second half of the century at the earliest (Table 1). In general, the market share estimations, applied for nanocellulose, nano-MoS_2, and MXenes in this study, resulted in relatively high production values compare to those derived using the extrapolation approaches, especially in the "optimistic" estimates. Such market share-based estimates should therefore not necessarily be expected to become realized in the near future, but more be seen as cornerstone scenarios of high production volumes.

Results from using the logistic relationship for extrapolation can be found in Table 1 for graphene, nanocellulose, and nanodiamond. For graphene, the coefficient of determination generated by fitting data to a logistic curve is slightly higher than for an exponential curve. For nanocellulose and nanodiamond, the difference in coefficient of determination between logistic and exponential curves is insignificant. For the silicon dioxide, included as an example of a more mature material, the improvement in the coefficient of determination between logistic and exponential relationships is highest.

The estimated future production volumes of graphene in 2030 differ considerably between the logistic and exponential relationships. The key reason for this is the different starting points. For the exponential extrapolation, the initial value was 1500 t/year in 2021, whereas the longer historical and estimated dataset in Janković and Plata (2019) used in the logistic curve fitting has values for 2021 based on estimates made in 2016. The minimum and maximum values for 2021 from Janković and Plata (2019) are relatively low: 20 and 525 t/year of

Table 1
Results from the logistic modelling for graphene, nanocellulose, and nanodiamond as well as for silicon dioxide nanomaterials, which represents a relatively mature market benchmark included for comparison. Primary estimates based on exponential extrapolation and/or the market share approach are also provided for comparison.

Nanomaterial	Estimate type label	Coefficient of determination (R^2)	Improvement over exponential correlation (%)	Curve midpoint year (t_0)	Maximum value (L) [t/year]	Value year 2030 [t/year]	Primary estimate from market share or extrapolation modelling	Primary estimate type
Graphene	Min	0.9963	0.832	2024	170	170	12,000	Extrapolation
	Max	0.9991	1.597	2022	1400	1400	38,000	Extrapolation
Nanocellulose	Min	0.9974	0.004	2059	5,200,000	8300	14,000	Extrapolation
	Max	0.9987	0.011	2045	8,800,000	100,000	28,000	Extrapolation
	Pessimistic	–	–	–	–	–	19,000,000	Market share
	Reasonable	–	–	–	–	–	35,000,000	Market share
	Optimistic	–	–	–	–	–	60,000,000	Market share
Nanodiamond	Min	0.9993	0.000	2124	7,100,000	83	97	Extrapolation
	Max	0.9984	0.010	2106	11,000,000	160	120	Extrapolation
Silicon dioxide	Min	0.9945	3.353	2018	680,000	630,000	n/a	n/a
	Max	0.9984	2.488	2019	5,800,000	5,200,000	n/a	n/a

graphene, respectively. The estimates for nanodiamonds in Janković and Plata (2019) are much closer to the median value in this study, which is why results for 2030 are more similar. In the case of nanocellulose, the logistic estimates for 2030 differ by a factor of three or less from the exponential estimates, helped by the fact that our starting point (2500 t/year) is close to the range (1100–7600 t/year) of the minimum and maximum estimates in Janković and Plata (2019) for 2021. Interestingly, the undated market share estimates from Cowie et al. (2014) are only an order of magnitude different from the maximum values suggested by logistic modelling of data from Janković and Plata (2019). On the other hand, in the cases of nanodiamond and nanocellulose, the benefits of logistic modelling over exponential modelling of the data in Janković and Plata (2019) are barely apparent given the minimal differences between the correlation coefficients. In these two cases and based on these underlying datasets, the main value may be to demonstrate that the estimated logistic curve midpoints are probably far (>2050) into the future.

The situation that several advanced materials have *many* envisioned applications means that the market share approach is challenging to apply unless one undertakes large, dedicated studies, like that of Cowie et al. (2014) for nanocellulose. For multi-purpose advanced materials, the extrapolation approach might therefore be the most feasible of the two approaches outlined in Section 2.4. Furthermore, it is noteworthy that several of the materials are envisioned for *the same* applications, e.g., composites (graphene, nanocellulose, and nanodiamonds), biomedical applications (nanodiamonds and quantum dots), and membrane filtration (GO and nano-MoS_2). This might result in interactions between different advanced materials in these applications, such that the production volumes of the materials will be influenced by each other. The most obvious interaction would be competition for market shares, but there might also be symbiotic interactions (Sandén and Hillman, 2011), e.g., due to transferable knowledge on how to produce composites. Such interdependencies among advanced materials are challenging for estimating future production volumes regardless of the approach.

3.3. Risk screening

None of the materials assessed currently have both high (>1 L/mg) aquatic ecotoxicity and high (>1000 t/year) production volumes. However, when considering future production volumes, MXenes could potentially become such materials. Five of the advanced materials (graphene, GO, nanocellulose, nano-MoS_2, and quantum dots) are characterized by low aquatic ecotoxicity but potentially high production volumes in the future. Finally, nanodiamonds have both low aquatic ecotoxicity as well as low current and future production volumes, and are thus less likely to pose an environmental risk to freshwater organisms than the other advanced materials in the near future (<2030).

Fig. 2 shows how the environmental risk screening results can be translated into action, elaborating on the previous recommendations by Arvidsson et al. (2018). No materials in the present study have both high aquatic ecotoxicity and high current production volumes. However, MXenes has high aquatic ecotoxicity and high potential future production volumes. Therefore, more detailed environmental risk assessments are recommended to investigate whether such future production volumes might lead to environmental risk. Baumann and Cowell (1999) refers to this as a consecutive relationship between environmental

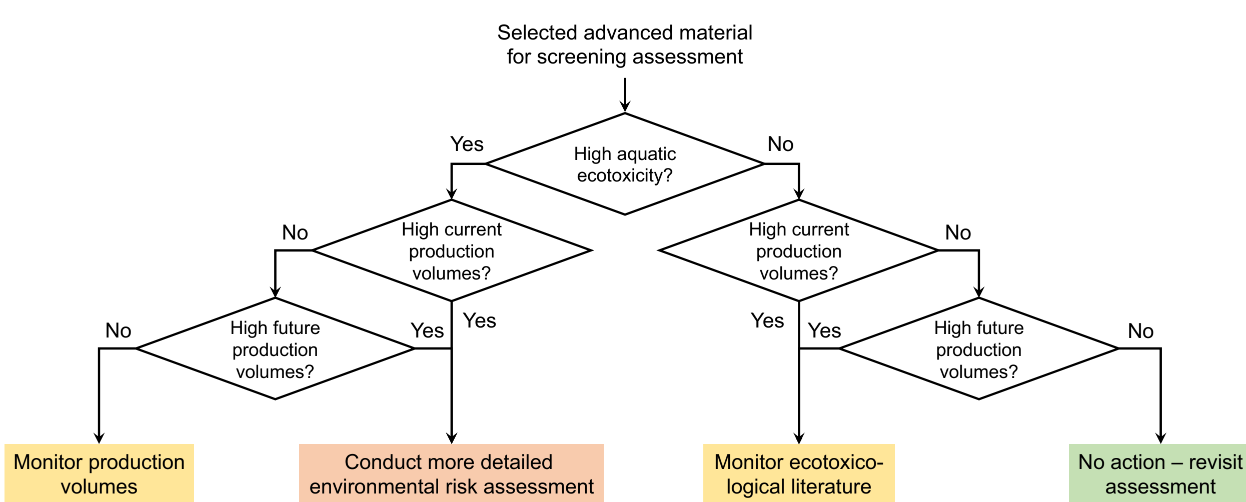

Fig. 2. Recommended actions depending on the outcome of the proxy measure risk screening approach.

assessment approaches. For graphene, graphene oxide, nanocellulose, quantum dots, and nano-MoS_2, which have low aquatic ecotoxicity but high future potential (and, for nanocellulose, also current) production volumes, careful monitoring of the ecotoxicological literature is recommended in order to ensure that the aquatic ecotoxicity does not come to exceed the threshold. In addition, for such current or future high-production materials, it is possible to initiate exposure assessments and material flow analyses as previously done for, e.g., carbon nanotubes and silicon dioxide nanomaterials (Gottschalk et al., 2009; Wang and Nowack, 2018) as well as for nanocellulose (Stoudmann et al., 2019). This will be of high importance for more detailed environmental risk assessments. For nanodiamonds, which have low aquatic ecotoxicity, low current production volumes, and also low future potential production volumes, no action is currently recommended, but the proxy measure screening might be revisited in the future.

Clearly, aquatic ecotoxicity and global production volumes alone cannot determine whether an advanced material will constitute an environmental risk in specific contexts. That would depend on a number of additional parameters, including emission profiles, environmental fate, exposure, and non-aquatic ecotoxicities. Since the proxy measure approach only considers aquatic ecotoxicity and production volumes, it cannot be considered a final determination of environmental risk, but instead provides early indications of potential environmental risk to freshwater organisms and prioritize advanced materials for more detailed environmental risk assessments. In addition, the proxy measure approach can suggest advanced materials that might not require more detailed environmental risk assessments. While there are other potential proxy measures for advanced materials, they often suffer from either low data availability and/or a weak link to environmental risk (Arvidsson et al., 2018). Low data availability is particularly challenging at early stages of technological development. For example, the release of MXenes from battery electrodes will probably depend on the end-of-life handling of lithium-ion batteries, which is currently difficult to predict since several different development pathways are being explored (Harper et al., 2019). However, more detailed environmental risk assessments need to also consider emissions, environmental fate, exposure, and non-aquatic ecotoxicities of advanced materials.

4. Conclusions

The results indicate that MXenes have the potential to become an aquatic ecotoxic high-volume material and should therefore be considered further in terms of more detailed environmental risk assessments. On the contrary, nanodiamonds are shown to have neither high aquatic ecotoxicity nor high future production volumes, and are therefore not priority for more detailed environmental risk assessments. However, the availability of aquatic ecotoxicity data varied considerably between the materials, from one XC50 value for MXenes to 33 for quantum dots. Further data acquisition is thus recommended, in particular regarding the aquatic ecotoxicity of MXenes and nano-MoS_2. Still, due to the low data demand and the consideration of future scenarios for production volumes, it is possible to apply this method to provide early indications of potential environmental risk to freshwater organisms even at early development stages of advanced materials. We therefore recommend this early-stage environmental risk screening method be included among the other tools aimed at achieving advanced materials that are safe and sustainable by design, such as risk assessment and life cycle assessment (Gottardo et al., 2021). Potential users of the method include technology developers themselves as well as researchers and consultants involved in technology development projects with an expertise in sustainability and/or environmental risk assessment.

CRediT authorship contribution statement

Rickard Arvidsson: Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Visualization, Writing – original draft, Writing – review & editing. **Gregory Peters:** Conceptualization, Formal analysis, Investigation, Methodology, Writing – original draft, Writing – review & editing. **Steffen Foss Hansen:** Conceptualization, Funding acquisition, Methodology, Project administration, Writing – review & editing. **Anders Baun:** Conceptualization, Methodology, Writing – review & editing.

Declaration of Competing Interest

The are no conflicts of interest to declare.

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Appendix A. Supplementary data

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