



Water quality footprint of agricultural emissions of nitrogen, phosphorus and glyphosate associated with German bioeconomy

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Fertiliser and pesticide application can cause extensive environmental damage. We use the water quality footprint to express nitrogen, phosphorus and glyphosate emissions from agriculture in volumes of water needed to virtually dilute pollution and apply the approach to agricultural imports for the German bioeconomy in 1995 and 2020. In total, the virtual German water quality footprint corresponds to 90 times the volume of Lake Constance. If water pollution had to be eliminated by dilution in export countries supplying Germany, volumes would be by a median of 300 times higher than the associated irrigation volumes there and could exceed natural water availability. Important and growing hotspots of clean water scarcity are China, Spain and India. The impact of German agricultural supply chains needs to be monitored with regard to the sustainability of national consumption and to the effectiveness of increasing fertiliser and pesticide use, especially in African, Asian and Pacific countries.

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In the sense of more sustainable production, the establishment of a bioeconomy has been regarded as a possible strategy in many countries. According to common definitions, the bioeconomy is not a separate economic sector, but rather an interdisciplinary concept that describes the use of biological resources to produce food, energy, chemicals and other products, and the integration of bio-based approaches into different sectors of the economy. The overarching goal is to build a sustainable and resource-efficient economy that meets the environmental challenges of the 21st century. Bioeconomy has been defined as “[...] production of renewable biological resources and the conversion of these resources and waste streams into value added products, such as food, feed, bio-based products and bioenergy [...]” by the European Commission¹. As a cross-sectoral area it permeates “[...] the sectors of agriculture, forestry, fisheries, food and pulp and paper production, as well as parts of chemical, biotechnological and energy industries”¹. In many countries, efforts are now being made to base a larger part of material demand on renewable raw materials, strengthen farmers and make use of biotechnologies². However, it has already been shown that bioeconomy is not inherently sustainable because of the use of renewable raw materials. Instead, the bioeconomy must also be oriented towards the planetary boundaries and its performance must be questioned with regard to sustainability criteria. Systematic monitoring can identify undesirable side effects of the bioeconomy on the environment and observe their development over time. Already observed impacts are for example land use changes, increased water use through irrigation or increased GHG emissions^{3–8}. These and others can very well be assessed by the footprint approach, as the climate footprint and the set of fossil energy, material, land and water footprint together cover 84% of the variance of environmental impacts, respectively⁹. In the context of bioeconomy, footprints for agricultural raw materials, primary timber, agricultural land, irrigation water withdrawals and greenhouse gas emissions have been determined considering global and life cycle-wide requirements of fully or partly biomass-based products that are annually produced or consumed in Germany⁸. Hereby, footprint-based monitoring framework for the German bioeconomy has been established.

In the course of this study, an indicator that assesses water pollution is added to this bundle. The aspect of water pollution is important because it has also a contribution to the scarcity of clean freshwater^{10,11}, as polluted water can no longer be used by users with higher quality demands. If their demand cannot be met from other water sources, scarcity may result. Comparable approaches to assess water pollution are more commonly known as grey water footprint^{12–17}.

Here, the concept of virtual dilution volume (VDV), recently presented as qualitative water scarcity footprint¹⁸, is used to express agricultural water pollution in virtual volumes of water that would be needed to dilute the pollution below a certain threshold. Advantages of the volumetric approach are that qualitative water use can be directly compared with quantitative use and that water stress indicators, which are also based on volumetric considerations, can be used to assess qualitative use in terms of regional scarcity of clean water. Here, the concept of the qualitative water scarcity footprint is adapted to agricultural use and referred to as water quality footprint from here on. Important differences to other grey water footprint approaches are resulting from a different definition: the water scarcity footprint¹⁸ is intended to assess the risk of natural freshwater scarcity for humans and nature caused by water use along human supply chains in a spatially explicit way, where natural freshwater refers to basin-specific water in its naturally occurring water quality. Moreover, water bodies within a basin are not considered separately from each other, but as a unit. It follows that (1)

dilution is calculated with demineralised water up to the naturally existing background concentration, instead of dilution with regionally pre-loaded water up to a threshold value, and that (2) threshold values from the WHO drinking water standard are applied for all types of water bodies equally. More detail and discussions on this is provided in the Methods and the publication¹⁸. Here, only the adaptations for the application of the qualitative water footprint for agricultural pollution are examined in more detail. For the German bioeconomy, we concentrate on the agricultural sector for the production of biobased products for the German bioeconomy (including animal feed, food, biofuels and others), i.e. the indicator is used to measure the share of agricultural production for the German bioeconomy in global water pollution and its contribution to clean water scarcity and thus complement the indicator set of the monitoring framework established for the German bioeconomy⁸. The scope of the study is to identify Germany’s global water quality footprint related to agricultural imports and to identify greatest hotspots.

Results

The water quality footprint of the German bioeconomy is calculated in the following steps: (1) The concept of VDV from the water scarcity footprint framework¹⁸ is extended to express agricultural water pollution per country in volumes of water that are required to virtually dilute the pollution below substance specific thresholds. Country level resolution is chosen in line with the scope of the study to identify hotspots of Germany’s global water quality footprint related to agricultural imports, and as best aggregation level of agreement of the different input data. Starting from a certain share of substances applied to the fields which is released into the soil, a VDV is calculated for the agricultural input of nitrogen (N), phosphorus (P) and glyphosate (G) by dividing the emission to water by the geogenic background concentration (naturally occurring substances N and P) or target concentration (G), respectively. Input data are taken from the global model IMAGE-GNM for N and P¹⁹ and from the global gridded map PEST-CHEMGRIDS²⁰ as well as the life cycle impact assessment model USEtox[®] model^{21,22} for G. Local to regional framework conditions that determine the amount of emission to water are taken into account, even if the results are presented at country level. For every country, the largest VDV represents the water quality footprint of agriculture under consideration of country water stress levels as withdrawal-to-availability ratios, including environmental flow requirements. (2) The raw material input into the German bioeconomy (RMI, including German domestic consumption and export) is determined from the multi-regional input-output table (MR-IOT) EXIOBASE for the years 1995 and 2020⁸. This study supplements the monitoring framework presented there with an indicator for water quality and is therefore calculated with an identical data basis, even though MRIOs with higher resolution are now available. To provide country level resolution for EXIOBASE rest-of-world regions, we use FAOSTAT data on production volume and agricultural area. For every country of origin, the total agricultural water quality footprint is multiplied by the share of agricultural raw material produced for export to Germany. (3) Resulting German water quality footprints are presented in m³ per German inhabitant for the years 1995 and 2020 together with country water stress levels according to an own calculation of the withdrawal-to-availability ratio (WTA)²³ based on AQUASTAT data²⁴. For G, results are only presented for 2020 due to data shortages. At this stage, this pilot study aims to test the suitability of a potential water quality footprint indicator, supplementing the monitoring of the German bioeconomy, and to identify first

hotspots. In the continuation of the monitoring, these initial results are planned to be observed and successively refined.

Water quality footprint of the German bioeconomy. In 2020, the total water volume needed to dilute the water pollution associated with agricultural production for the German bioeconomy is 4000 Giga cubic metres, which equals 90 times the volume of the Lake Constance (according to IGKB, International Water Protection Commission for Lake Constance). Domestic German production accounts for 22 % of this, which is 20 times the volume of Lake Constance. Compared to 1995, the total volume has increased by one third, while the share of domestic German production on the total water quality footprint has decreased by 16%.

Looking at the countries of origin, Germany is associated with high water quality footprints in 49 countries (Fig. 1). The largest one is caused by agricultural production in Germany itself. With approximately 14,000 m³ per German inhabitant, it is 300 times the German direct drinking water withdrawal per German inhabitant (GDW) of 46 m³ a⁻¹ (including households and small businesses²⁵). This is followed by Brazil and China, where the German water quality footprint is still about half and one third of the largest value. In the majority of the 49 countries (Netherlands to Germany), the footprint is more than twice the GDW. While most countries belong to Europe, countries from all continents are represented, showing the global relevance of water pollution linked to German activities.

Although most countries of origin have a low water stress level, some of the countries with footprints of 1000 m³ per German inhabitant and greater (Greece to Germany, at the basis of Fig. 1) show a medium water stress level (China, Spain, India). These are major hotspots of the German bioeconomy, because here the strong water pollution from agriculture further burdens the already stressed water resources (referred to as hotspots of clean water scarcity). Among the countries with lower footprints, there is a medium to high water stress level in Iran, Turkey, Bulgaria, Mexico, South Africa, Pakistan, Belgium and Kazakhstan. Overall, however, the German bioeconomy sources very little from countries with high water stress.

Virtual dilution volumes are arithmetically determined theoretical amounts of water use and are not actually consumed. Nevertheless, these volumes measure the use of water taking up pollution, and thus indicate the scarcity of clean water, an issue of growing global concern. They represent an own category of the water footprint and are not directly comparable with real volumes consumed, but it is nevertheless revealing to classify and evaluate the quantities in comparison: water quality footprints can be several orders of magnitude higher than volumes of actual water withdrawal. This is a well-known effect of the dilution concept, which uses calculated virtual volumes to express water pollution in volumes of water¹⁸ (see also uncertainty analysis). In comparison to related agricultural irrigation water withdrawals (AQUASTAT²⁴) this also applies for water quality footprints of the German bioeconomy: only in six countries (Fig. 2), namely Bahrain, Barbados, Cape Verde, Dominica, Brunei and Belize, does irrigation water exceed the dilution volume. However, none of these currently play a major role in the German bioeconomy. For about a quarter of countries, dilution volume can be up to 100 times the irrigation water withdrawals. Among the 24 countries of this category are many countries from the African continent as well as important European suppliers. For the majority of countries, the dilution volume exceeds for more than a hundred times the irrigation volume and for more than half of them, the ratio is even greater than a thousand. The list is headed by Mexico, Mongolia, Malaysia, India and Mali.

At this point, we would like to draw attention to the fact that the size of country level water quality footprints can be influenced by different factors that are not easily recognisable at first glance: absolute agricultural production of a country, absolute N, P or G application and Germany's share of agricultural production. We did not analyse absolute agricultural production and an evaluation of the influence of the other factors is not in the focus of our analysis, but we will point to correlations we consider relevant. Mexico, Malaysia and India as mentioned above for example are among the countries with the highest water quality footprints associated with the German bioeconomy (Fig. 1) which is predominantly due to high fertilizer application.

Hotspots of German water quality footprint. A principle of dilution volume is that the largest substance-specific volume dilutes all other substances with smaller volumes for which the same activity is responsible. For the substances investigated, it is shown that P is in almost all of the 198 investigated countries and island states responsible for the largest volume and can be regarded a substance-related hotspot in general. This is due to a combination of different influences: the natural background concentration of N, by which the applied amount is divided to calculate the dilution volume, is on average about 50 times higher than that of P, leading to smaller values for the dilution volume in comparison. For G, there is no natural background concentration, here the target concentration of drinking water quality is used for calculation. It is only a fraction of the geogenic background concentration of P (on average only about 1%), but here it is crucial that the quantities of G applied are smaller (see also uncertainty analysis). Belarus is the only country where N causes the highest dilution volume in 1995 and 2020. G is never responsible for the highest dilution volume in 2020.

Spatial hotspots of the German water quality footprint are countries with high water stress levels, high dilution volumes or a combination of both resulting in a varying degree of severity: weak (colours 1, 2 and 4 in Fig. 3), medium (colours 3, 5 and 7) and severe (colours 6, 8 and 9). Accordingly, severe hotspots are Iran, Spain, Turkey, India and China followed by Tunisia, Egypt, Sudan, Lebanon, Uzbekistan and Pakistan. High water quality footprints can result from high absolute values of agricultural production in large countries, even if the share of the German bioeconomy in agricultural production is small (<1%, Supplementary Fig. 3). For this reason, dilution volumes per German inhabitant are high in the USA and Canada, whereas Germany has in fact high shares in Brazilian and Australian production at 4% and 2%.

German water quality footprint over time. The German water quality footprint 2020 is compared to 1995 which is determined analogously. The most striking difference between both years are the lower absolute values of dilution volumes in 1995 (Supplementary Fig. 4, 6) compared to an even higher German value and consequently a lower number of countries exceeding the GDW: in 1995, Germany was only associated with a high water quality footprint in 33 countries compared to 49 in 2020. This is due to a general trend of increase in both the amount of fertilisers and pesticides applied between 1995 and 2020 and Germany's share of the respective agricultural production, especially in non-European countries. This trend is particularly evident in India, where the total dilution volume in the country has increased by almost 20% and Germany's share by about 0.3%. The associated dilution volume has increased sevenfold. However, there are also exceptions: first is Germany itself, where both the total dilution volume and the share of own consumption in domestic production have fallen, the latter by 4%. In the case of the Netherlands,

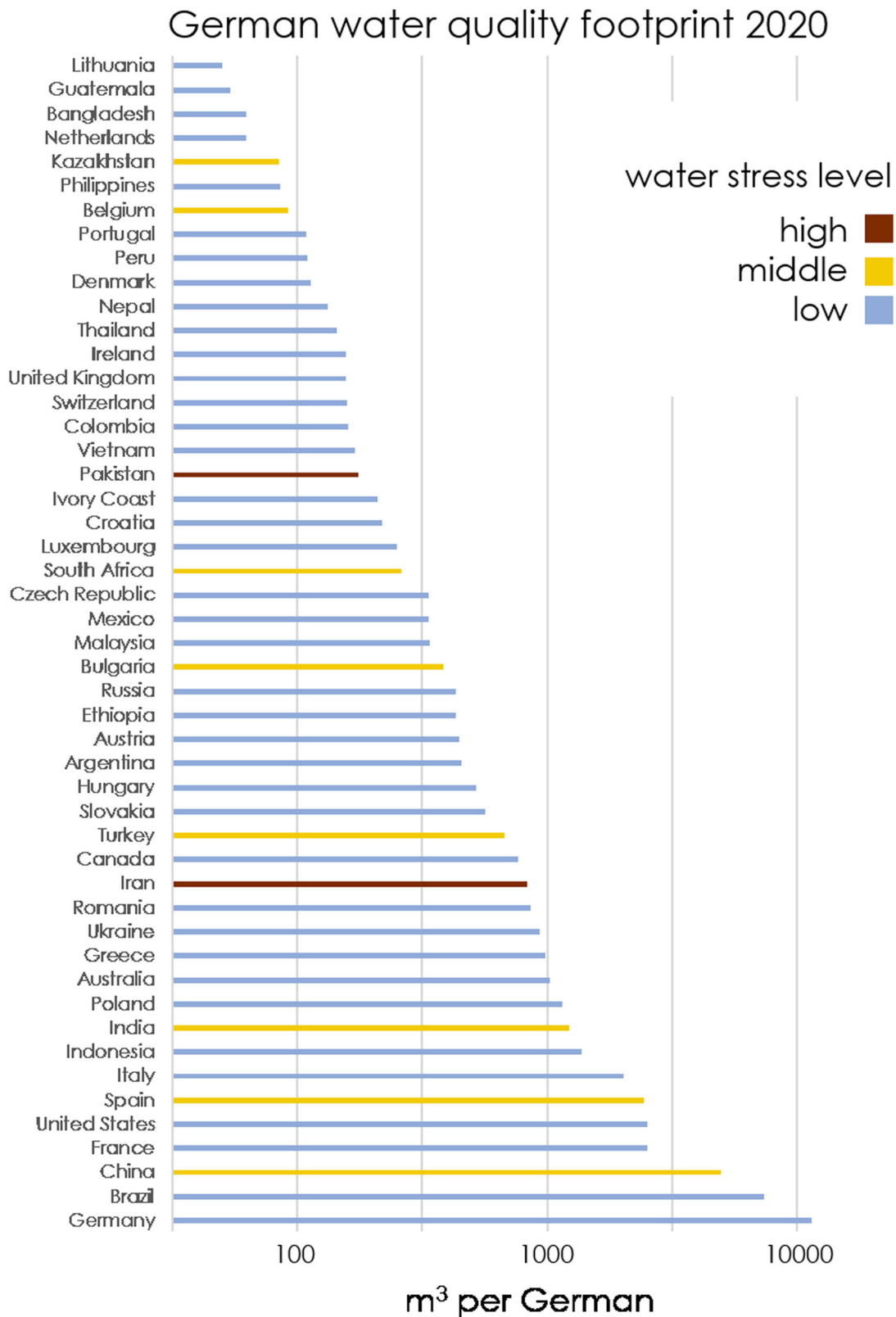


Fig. 1 German water quality footprint from agricultural imports 2020. Per country, it is the largest of the volumes required to dilute nitrogen, phosphorus or glyphosate related to agricultural production of the German bioeconomy, the so-called critical volume. Only countries where the German water quality footprint is larger than the German domestic direct water withdrawal are shown here. For a complete list, see Supplementary Fig. 1 and Supplementary Data 1. Water stress is expressed by an own calculation of the withdrawal-to-availability ratio (WTA)²³ based on AQUASTAT data²⁴ classified according to $WTA < 0.2$ (low), $0.2 \leq WTA < 0.4$ (middle) and $0.4 \leq WTA$ (high, see Supplementary Fig. 2).

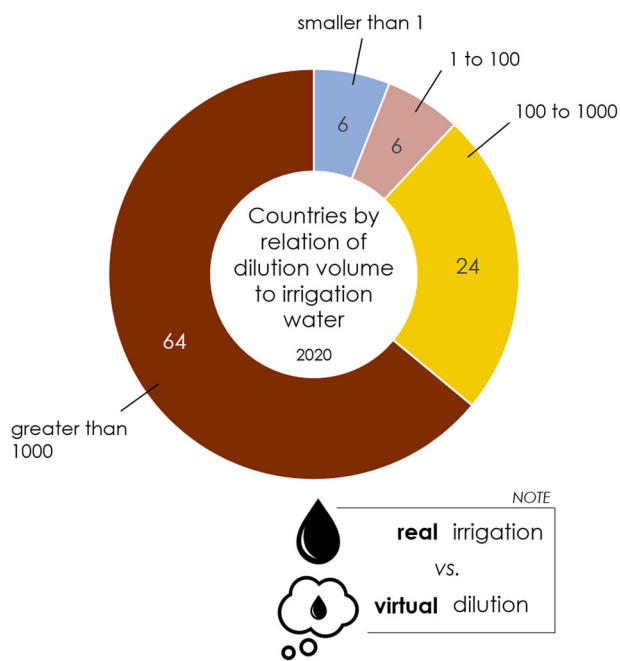


Fig. 2 Number of countries by relation of virtual dilution volume associated with agricultural production for Germany to actual irrigation volume 2020. Note that irrigation volumes are amounts of water used in reality, whereas virtual dilution is a purely calculated and not actually consumed amount of water. The comparison of “apples and oranges” here is made deliberately and serves to classify the order of magnitude. The four categories refer to a dilution volume that is smaller than irrigation water (blue), that is 1 to 100 times the irrigation water (rose), 100 to 1000 times the irrigation water (yellow) or more than 1000 times the irrigation water (red). Irrigation water withdrawals 2020 are available for 107 countries from AQUASTAT²⁴ and are related to agricultural production of the German bioeconomy. For values, see Supplementary Data 2.

Germany’s share of production has declined sharply from 35% in 1995 to 10% in 2020. The total dilution volume in the country has also decreased over the same period, indicating that the effect is not due to a strong increase in production. Another example is the Mexican agricultural production, where Germany had a share of 1% in 1995, while today it is 0.3%. Changed import structures are also reflected in the fact that countries from the African continent, Southeast Asia and the Pacific region are increasingly represented in 2020. The importance of single exporting countries for the German bioeconomy, measured by the size of the water quality footprint, has changed slightly in comparing Fig. 1 and Supplementary Figs. 4, 6. However, the ten countries with the largest water quality footprints have remained almost identical: compared to 1995, only Mexico and Canada have been replaced by India and Poland. A comparison of the spatial analyses (Fig. 2 and Supplementary Fig. 7) reveals that both changes in water stress levels and changes in dilution volumes can be important for the water quality footprint.

Comparing the agricultural virtual dilution volume per country in the period 1995 to 2020 with the natural water availability in calculating a virtual dilution-to-availability ratio (VTA) reveals that in a number of countries virtual dilution for agricultural pollution alone can exceed water availability (Fig. 4, Supplementary Data 3). In 1995, this mainly concentrates to European countries, while in 2020 it spreads over Northern Africa, the Middle East as well as India and China. The share of the VDV associated with the Germany bioeconomy in the total water availability of a country amounts to a maximum of values in the

range of 10^{-7} and to a median value in the range of 10^{-11} , i. e. reveals very small numbers.

Comparing the development of the total calculated critical dilution volume per country in the period 1995 to 2020 with the development of total agricultural yield according to FAOSTAT in the same period shows that there is no clear trend (Fig. 5). However, only a few countries have recorded strong increases in harvests with almost unchanged dilution volumes for fertiliser and pesticide use (Fig. 5, circle b). On the other hand, there are also many countries that have recorded constant or only small increases in harvests with remarkably higher dilution volumes (Fig. 5, circle a). Since the natural background or target concentration was not changed for the calculations over the period under consideration, 1995 to 2020, changes can originate from varying application, meaning that considerably more fertilisers and pesticides were applied without having a proportional effect on yields. Among the countries, where this applies, there is not a single European country; the majority are countries in Africa and the Asian and Pacific regions. Based on the data used, these could be places where increasing fertiliser and pesticide use disproportionately may do more harm than good – with German participation. In a number of countries, the dilution volume has increased only slightly compared to the harvests, indicating a more efficient use of fertilizers and pesticides. Among them is India, a number of European countries and Germany itself.

However, other effects could also play a role, e.g. a change in the crops cultivated between 1995 and 2020 which influences yields and nutrient demand, or climatic changes which can influence runoff and hence water stress levels. We do not necessarily expect a correlation here, but in countries where there is a large gap between harvest and fertiliser and pesticide application, water resources could be unnecessarily burdened by agriculture. In the case of P, for efficient application, it should be taken into account that the soil is also a P reservoir. In the case of N (Supplementary Fig. 8), it should be noted that N-use efficiency decreases with increasing fertiliser application and leaching and run-off then increase.

Uncertainty analysis. For the data from the global model IMAGE-GNM and the MR-IOT EXIOBASE, it is inherently difficult to specify concrete errors or error ranges. However, uncertainties of modelled data can be large and have a corresponding effect on the uncertainty of the dilution volume calculated from them. A sensitivity analysis is carried out to identify those variables that have the greatest influence on the result by changing one-factor-at-a-time: for the example of P, the variables load, geogenic background concentration and share of the German bioeconomy are varied by 1% one after the other, while the other two remain unchanged. For G, the variables application, mass fraction, target concentration and share of the German bioeconomy are varied accordingly. The change in the value for the calculated German water quality footprint is measured in each case.

As the dilution volume is calculated through simple mathematical operations, it is clear that it is directly proportional to the input variables load respectively application, mass fraction and share of the German bioeconomy, which are only linked by multiplication: a change in one of these inputs by a certain percentage results in a change of the result by the same percentage. (Supplementary Fig. 9, 10). More interesting is the sensitivity to the geogenic background and target concentration. The associated function is an inverse hyperbolic function which goes towards infinity for negative changes approaching 100%. There is a higher sensitivity to negative changes. If the geogenic

German water quality footprint 2020

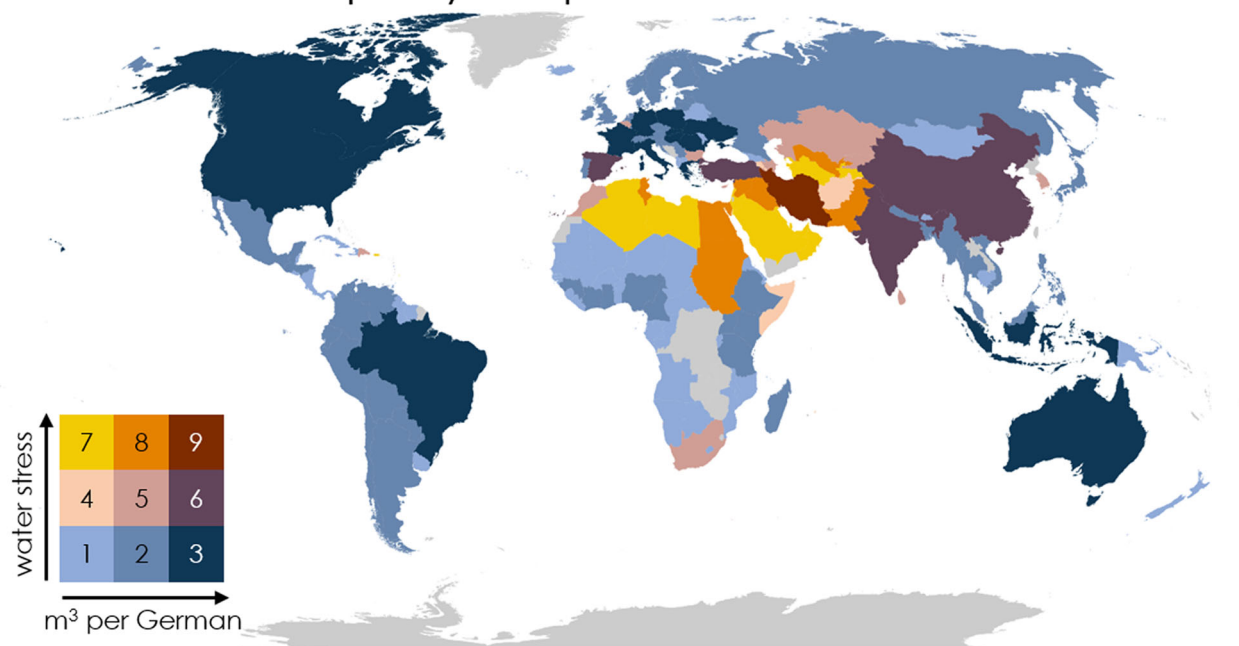


Fig. 3 German water quality footprint from agricultural imports 2020. Per country, it is the largest of the volumes required to dilute nitrogen, phosphorus or glyphosate related to agricultural production of the German bioeconomy, the so-called critical volume. Water stress is expressed by an own recalculation of the withdrawal-to-availability ratio²³. Columns of the colour matrix refer to low, medium and high dilution volumes (from left to right), while rows refer to low, medium and high water stress (from bottom to top). For values, the reader is referred to the methodology section. Colours 1, 2 and 4 refer to weak, 3, 5 and 7 to medium and 6, 8 and 9 to severe hotspots. Grey: no data. For values, see Supplementary Data 1.

background or target concentration is reduced by 20%, the dilution volume increases by 25%, and a reduction of 50% already increases the dilution volume by 100%. Conversely, for positive changes, there is a substantially lower sensitivity of only about 17% decrease in dilution volume for a 20% increase in the geogenic background and target concentration. For the data taken from IMAGE-GNM, EXIOBASE and PEST-CHEMGRIDS the uncertainties are largely unknown. For the geogenic background and target concentration, for which we take mostly country values from literature to derive median regional and global values, uncertainties are well known and can easily go up to 100%. If the geogenic background is overestimated, the resulting dilution volume can be extremely underestimated. An underestimation of geogenic background also influences the dilution volume, but much less strongly. In addition, it should be kept in mind that the possibilities for determining the geogenic background concentration are in themselves only an approximation to the actual values, which are largely unknown. Against the background of this high level of uncertainty, the results of this study should be seen as approximations that can help to identify hotspots.

Discussion

The monitoring concept for the German bioeconomy⁸ is used to record the global environmental impacts of the German bioeconomy by means of suitable indicators and to observe their development over time. This study has identified a number of arguments how the water quality footprint can contribute to expand this set to draw attention to the often neglected issue of water pollution and its contribution to the scarcity of clean freshwater.

First, it has become clear that German water quality footprints abroad are generally high. If water pollution had to be eliminated by dilution, dilution volumes could exceed the German direct

water use dramatically meaning that they play an important role in the water related impacts of the German bioeconomy. Also, it has been shown that they could exceed irrigation water withdrawals of exporting countries, which applies to the majority of countries examined here. As the volumetric concept allows a comparison with direct water use, agricultural water quality footprints that exceed irrigation withdrawals mean that water pollution makes a much greater contribution to the scarcity of clean freshwater than the direct abstraction of water. In those cases, the impact of water pollution on the availability of clean water resources is higher than of irrigation. While withdrawals for irrigation water are already subject to numerous assessment procedures and are often critically monitored, as is other direct water use, the relevance of water pollution has received too little attention in footprinting, so far. This should be taken as an opportunity to systematically record and evaluate water quality footprints as well.

Second, the analysis of water quality footprints, which explicitly include the consideration of regional water stress, allows to identify existing hotspots of clean water stress. This currently includes India, Spain and China with both high footprints and high water stress levels as well as Iran and Pakistan with lower footprints, but very high scarcity of clean freshwater. The observation of the development since 1995 reveals an increase in water stress levels for a few countries (e.g. Turkey and China), however, we do not see a general trend for the water quality footprint here, although a continuous and future expansion of water stress areas is observed²⁶. The country aggregation of water stress levels possibly masks such developments, for example in the southern USA, southern Europe and parts of Australia which were already considered water stress areas in 1995²³. Germany's contribution should be further monitored and evaluated here. Potential future hotspots, where the virtual dilution volume is already high and water stress levels are low to middle, must be

Agricultural virtual dilution-to-availability ratio

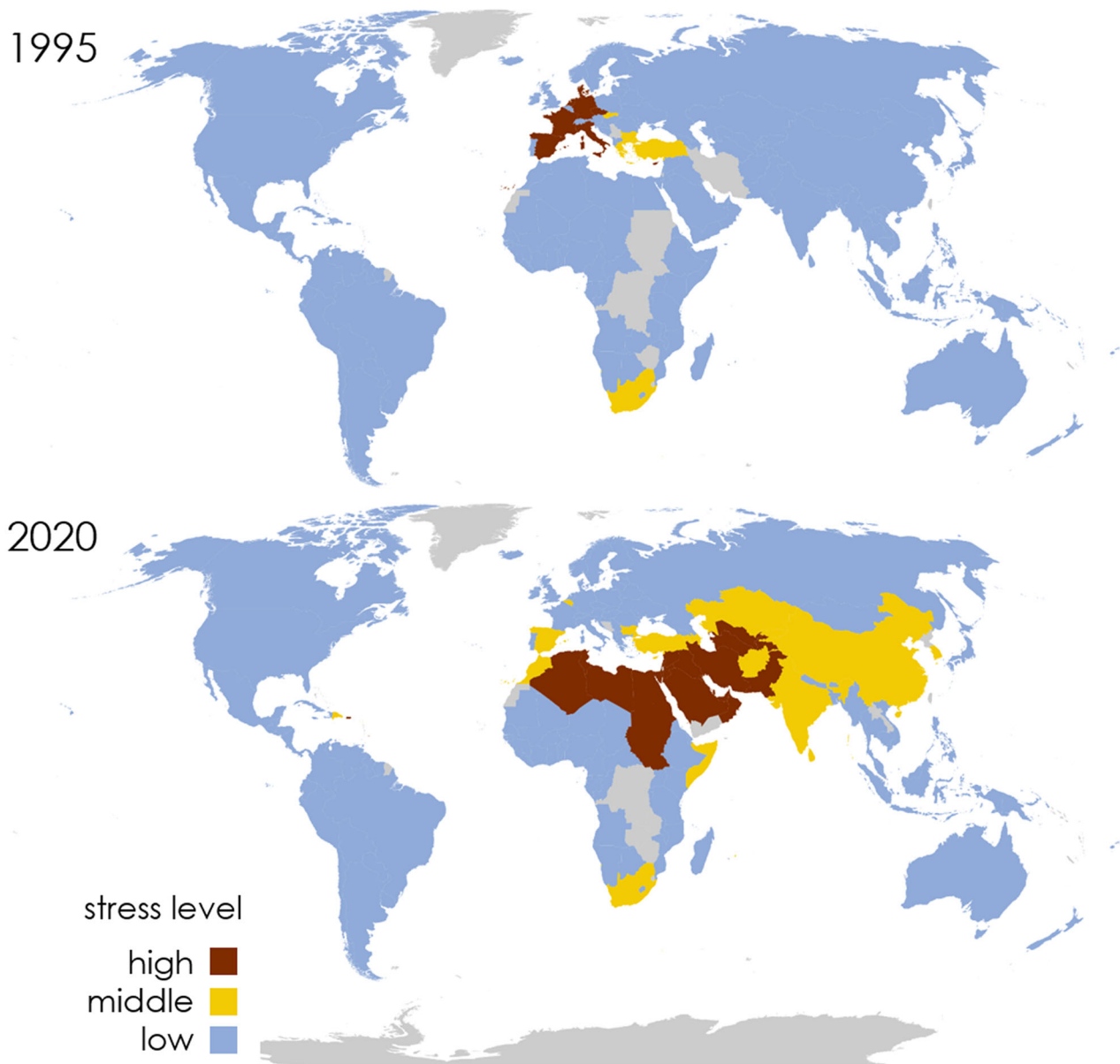


Fig. 4 Agricultural virtual dilution-to-availability ratio 1995 and 2020. Virtual dilution refers to agricultural emissions of nitrogen, phosphorus and glyphosate. Water availability is taken from AQUASTAT²⁴. The ratio is calculated following the concept of the withdrawal-to-availability ratio (WTA)²³ and the stress level is classified just as with WTA, where $WTA < 0.2$ is a low, $0.2 \leq WTA < 0.4$ a middle and $0.4 \leq WTA$ a high stress level.

kept in mind, as changes in water stress levels can easily lead to aggravation. Examples for such potential hotspots are the USA, Spain, the South of Europe, Ukraine, Turkey, China, India and Australia. The water quality footprint can be used to avoid potential future hotspots and defuse existing hotspots. In order to derive explicit policy recommendations for the concrete handling of hotspots, the present analysis should be further refined, which is the subject of future work. Third, the observation of water quality footprints over time allows for the identification of general trends, changes in single countries and evaluation of other trends: between 1995 and 2020, German water quality footprints have increased considerably worldwide, so that Germany is associated with a high water quality footprint exceeding GDW in 49 countries. This trend is most evident in Germany's water quality footprint in India. A shift in sources of supply also seems to play a

role here, as Mexico and the Netherlands have recorded sharp declines in the water quality footprint due to Germany's lower share of their agricultural production. A comparison with the development of crop yields, which we present here as possible application of the virtual dilution volume, has revealed that in a number of countries in Africa and the Asian and Pacific regions, fertilizer and pesticide use have strongly increased while the yields have not or only insufficiently grown. Based on the data used, this may indicate that serious environmental problems are emerging there with German involvement, which is seen as an important result of this study. However, since no positive correlation between dilution volume and harvest could be observed for European countries either, the issue may well be of a general nature and should be revealed, recorded and evaluated over time with the help of the water quality footprint and under

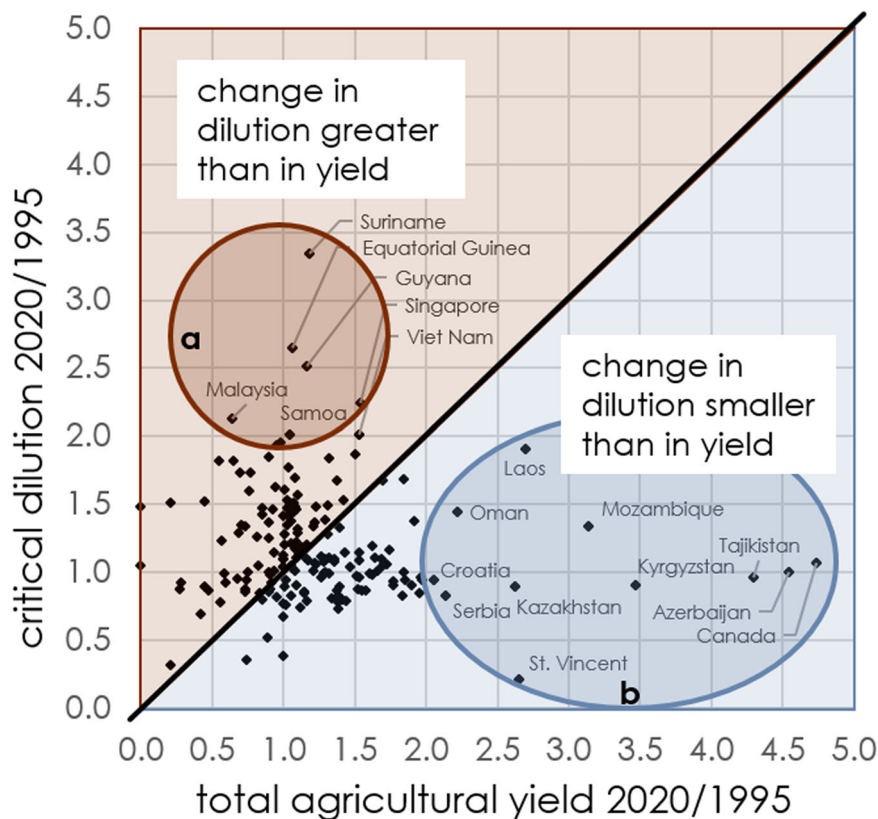


Fig. 5 Comparison of temporal development of the critical dilution volume and yield for all countries. The critical dilution volume is the highest substance-specific dilution volume, which in this study is most often due to phosphorus dilution. Black points represent single countries, the black line is $x = y$, i. e. for every country with a data point on the line the change in dilution volume equals the change in yield in the period 1995 to 2020. Countries where the dilution volume has changed more than the yield plot on the upper left side of the black line (reddish raster), while countries where the yield has changed more than the dilution volume plot on the lower right side (blueish raster). The circles a and b identify some countries with considerable differences between the development of the dilution volume compared to the yield. For values and countries, see Supplementary Data 4.

consideration of other possible influencing parameters. The development of suitable benchmarks is also conceivable in this context.

The spatial resolution of the present analysis is country level with respect to (1) the scope of the study, (2) the recommendations for the applied methodology and (3) the best aggregation level of agreement: (1) To quantify Germany's global water quality footprint within a national monitoring framework, we regard country-level resolution as reasonable to create a "knowledge base for hotspot identification"¹⁴. From the point of view of political levels of action where the results of the hotspot analysis are supposed to be considered, countries, which are politically and administratively relevant, are the most appropriate spatial setting according to current standards.

(2) This is also in line with the guidelines for the applied methodology, which is a combination of a modified LCA water scarcity footprint approach and a macroeconomic analysis: both LCA analyses in general and water footprint determinations in LCA do not require a specific spatial resolution, but it is dependent on the scope of the analysis, respectively^{27,28}. The spatial resolution of water footprint determinations outside the field of LCA also can vary with the research question from small catchment (where great catchment areas such as the Nile basin are subdivided) to national to global region level¹⁴ and there are numerous different examples of each, e.g. Ma et al.¹¹, Mekonnen & Hoekstra¹⁶ (both small catchment), Hoekstra & Mekonnen¹⁴ (national), Bringezu et al.⁸ (national and global regions).

(3) The representation of Germany's water quality footprint from agricultural imports under consideration of national water

stress levels requires the combination of different data sets with different resolution: nutrient emissions to water are available on grid cell level (0.5 by 0.5 degree), whereas substance-specific geogenic background and target concentrations as well as import quantities are partly only available at the level of global regions. Water stress assessment is performed with the help of a country-level aggregated index, although it has become common practice in hydrological modelling to determine water stress at catchment level. This is among other things related to the fact that from a hydrological point of view drainage directions which are needed to model the water resources situation are strongly connected to basins²³ and because the scarcity of clean freshwater is a regional issue^{11,29}. In fact, however, even high-resolution hydrological models, especially in the area of water use by humans, draw on national data and statistics that are disaggregated with the help of assumptions and generalisations. So far, the common spatial reference of these different data sets, the best aggregation level of agreement, is country level. At country level, the core statements of the analysis are valid with a certain degree of uncertainty resulting from assumptions made in the process of aggregation and disaggregation. For further downscaling, further assumptions have to be made at the cost of successively increasing uncertainties. In order to keep the balance between higher spatial resolution at higher uncertainties and greater validity of the results – and consequently better robustness within a national monitoring framework –, we decide to stay at country level. Further work is intended to increase the resolution of the analysis, which is primarily needed for a closer examination of identified hotspots with the aim of developing strategies to reduce impacts

on the local scale¹⁴. This is especially indicated for the water stress analysis as country level water stress factors are tending to disguise regional water stress (e.g. South of USA, South of Europe, Australia).

The temporal resolution of this work is also limited. 1995 and 2020 were compared for the beginning. More comprehensive time trends with narrower time steps, for example 5 years, can provide a clearer picture of the development of the water quality footprint in individual countries and, above all, help to identify the circumstances that influence this development in each case.

Our results suggest, that P is almost always responsible for the critical dilution volume comprising both of the other substance-specific volumes studied. However, we have only looked at G on the pesticide side. While this is one of the most commonly used pesticides, other pesticides are more commonly used, both regionally and crop-specifically, which may have higher leaching rates or lower target concentrations. A combination of these factors can lead to higher dilution volumes for these pesticides. Consequently, our water quality footprint may be considered a minimum.

A valid data basis is the basic prerequisite for calculating reliable water quality footprints. For the selection of input data, we have therefore relied on sophisticated state-of-the-art models and maps so that we are able to take into account the high spatial dependence of fertiliser and pesticide use and the resulting emissions to water bodies, even if final results are presented at country level. Nevertheless, we are aware that major uncertainties remain, especially because this is a global analysis: (1) In the case of G in particular, there is still a need for development in order to be able to quantify the actual emissions from soil into water bodies more precisely. This is also the reason why we present G water quality footprints only for 2020: for 1995, there are no reliable data on application quantities and emission factors available. Our work should help to assess the relevance of G for water quality in comparison to N and P based on the existing data. (2) With regard to the influence of geogenic background concentrations, dilution volumes can easily be underestimated and could possibly be substantially larger in reality.

In order to present a suitable methodology and data basis for the water quality footprint as a monitoring indicator, we accept these and other uncertainties and limitations. Our results must be seen as a first approximation that can be used to identify potential hotspots. This knowledge can be used to derive further research needs and raise awareness among decision makers about hotspots of water pollution in the German agricultural supply chain.

Conclusion

We present the water quality footprint of agricultural emissions of nitrogen, phosphorus and glyphosate associated with agricultural emissions from the German bioeconomy.

We use a modified grey water footprint approach to calculate the virtual dilution volume that would be required to dilute the pollution below natural background concentration or drinking water thresholds¹⁸. A strong literature base on the grey water footprint in the back, we have opted for a concept that focuses on the natural state of water before pollution. A core element of this concept is that blue and green water are not distinguished, although it is due to the special impact pathway of fertiliser and pesticide emissions from agriculture that these primarily end up in groundwater and surface waters, i. e. classic blue water compartments. It follows, that comparable works would probably refer to the water quality footprint calculated here as blue water quality footprint.

The water quality footprint based on the substance-specific virtual dilution volumes is intended to complement the indicator

set for the German bioeconomy⁸ which so far has only identified irrigation water footprints of agricultural production. To ensure comparability and complementarity, the same data basis, EXIOBASE, is used, even if it has a limited spatial resolution. Resolution is refined with the help of FAOSTAT data. In the ongoing continuation of the monitoring of the German bioeconomy the use of a better database is already initiated. In this course, not only spatial resolution, but also for example food product differentiation will be enhanced.

The uncertainties of our global and economy-wide analysis are still large, mainly due to data gaps and assumptions made. Nevertheless, we regard our results as useful for the development of national monitoring, where water quality has so far been underrepresented, in identifying and monitoring points in the supply chain of the German bioeconomy where the greatest water pollution takes place. Due to the low spatial resolution of EXIOBASE regarding the rest-of-world regions Africa, America, Asia-Pacific, Europe and Middle East the results are associated with uncertainties. Did the absolute quantities of agricultural goods that Germany procures from these regions, and the associated virtual dilution volumes, remain broadly the same, information of higher spatial resolution can mean a shift in the hotspots within the related regions. In particular, this could lead to a spatial specification of the hotspots of clean water scarcity Iran and Pakistan. For all other countries, the results are nevertheless directionally reliable, including in particular the greatest hotspots Brazil and the USA in terms of quantity as well as Spain, Turkey, Iran, India and China in terms of high regional clean water stress. The latter is regarded one of the serious issues of the 21st century^{30,31}.

The classification of the magnitude of virtual dilution volumes in comparison with real volumes such as irrigation volumes has shown that reduced water quality can favour clean water scarcity while often fading into the background alongside quantitative water scarcity. Identified hotspots are strong signals that there is a need to monitor the scarcity of clean water, to pay attention to it in decision-making processes and to raise awareness of water pollution associated with consume habits among end users. Against the background of the national aim to promote the bioeconomy in order to achieve climate goals and reduce other environmental impacts in Germany and other countries, this is necessary in order not to promote the emergence and increase of regional scarcity of clean water worldwide.

Based on this, the database and the depth of the analyses can be successively refined in order to enhance resolution, reduce uncertainties, validate results and increase significance and informative value. At this stage, the presented water quality footprint indicator is suitable to supplement the monitoring of the German bioeconomy through identification of hotspots of clean water scarcity from agricultural production and observation of trends over time.

Materials and methods

Preliminary work on the grey water footprint. In the context of this study, grey water footprint refers to the idea of expressing water pollution in water volumes by converting substance loads into the dilution volume that would be required to dilute the pollution below substance-specific limits. Conversely, a substance-specific dilution factor can be derived from this. This idea is basically not new because already in 1974 it has been pointed out that an average dilution factor of 10 for wastewater flows is at least required to “dilute[d] [polluted water] in order that concentrations of pollutants be reduced to an “acceptable” level”, although the approach has not yet been called grey water footprint³². Almost 20 years later, annual freshwater runoffs have

been studied to find out what proportion of Earth's freshwater is actually accessible to humans and a then common dilution factor of 28 litres per second per 1000 people³³ has been used to take into account the amount of dilution required for waste water treatment. While these studies still used average dilution factors to describe human-induced water pollution in principle, a more recent study suggested to use substance-specific dilution factors³⁴, e.g. 100 for N (related to cubic metres) considering a permissible limit of 0.01 kg m^{-3} . Shortly after, the expression grey water footprint has been introduced¹², which has since become common, by defining it as the substance load divided by a specific threshold value that is valid for the receiving water body. Such thresholds can originate from generally applicable national or international water quality standards. In a further study, the authors changed their approach slightly by carrying out the dilution with regionally actually available water, so to speak, and not with demineralised water¹³. Mathematically, this means that the substance load is divided by the difference between threshold and natural background concentration. This can also be understood as the amount of water needed to assimilate pollution through substances¹⁴. However, the authors have emphasized that dilution is not a "free pass" for water pollution, but a method to quantify it volumetrically in order to be able to reduce it. Since then, the grey water footprint has been widely applied in many different contexts creating a large pool of literature, not all of which we can discuss here. In the field of agriculture it was for example used to express the impact of agricultural emissions of N and P on water quality on the global level^{15,16} and it has been further used to reveal the impact of N fertilizer emissions on ecosystems.

As part of a generally critical examination of existing water footprint methods, a concept of the water scarcity footprint for LCA was introduced in order to set a different focus in the area of water footprinting: the water compartments of a catchment are no longer considered separately (e.g. surface water, groundwater, rainwater), but as a hydrological unit in a catchment. This is to take into account the fact that the use of water from any compartment can contribute to regional water scarcity. In the case of the grey water footprint, which is referred to as the qualitative water scarcity footprint and described by the virtual dilution volume within the approach, regional aspects are taken into account by requiring to orient the dilution on the naturally prevailing water quality. For this purpose, the load is divided by the natural, or geogenic background concentration, if not greater than general water quality standards, referred to as target concentration. Subsequently, in the context of global supply chains, dilution is done fairly with demineralised water for all applications. The argument behind this is that a consumer or product should not take advantage of a lower water quality footprint just because regional water is naturally cleaner. On the other hand, naturally already more pre-loaded water can have this effect, too, but here the target concentration is used to mitigate the effect in the case of excessively pre-loaded water. And in the line of reasoning of the approach, a consumer or product cannot be held responsible for the natural state of a water body. Target concentrations, also applied for artificial substances with no geogenic background concentration, are taken from the WHO drinking water standard³⁵ for the reason that water pollution can contribute to scarcity if user's requirements are no longer met. To consider all users we see drinking water standards to be the most appropriate, as this ensures that there is no danger to humans and nature. The approach uses a mathematical case differentiation and has the advantage that no negative values are possible. It is modified in the following to be applicable beyond the LCA context for which it has been originally presented.

Water quality footprint of agriculture. Water pollution from agriculture follows a certain pattern that must be taken into account when calculating water quality footprints: in the beginning, there is the application of fertilisers, manure and pesticides to the field. Part of it is taken up by plants and extracted by harvesting, released into the atmosphere or is washed away with the surface runoff, the latter referred to as emission to surface water here. What remains is absorbed by the soil or as solution in the soil and is basically available for interaction with groundwater. In fact, however, only a small part of it, the emission to groundwater, actually reaches groundwater depending on substance-specific impact pathways that contain effects such as attachment to soil particles or degradation. Impact pathways are highly substance-specific, very complex and dependent on spatial and temporal conditions (e.g. Siebert et al.³⁶, Borggaard & Gimsing³⁷, Batjes et al.³⁸, Sattari et al.³⁹, Wick et al.⁴⁰, Papadopoulos et al.⁴¹). The water quality footprint of agriculture summarises the emission to surface water and to groundwater. Existing approaches usually use leaching-run-off-rates to calculate the share of the application that ends up in water bodies¹⁶, referred to as loads. It is also common practice⁴² to translate loads into water volumes by dividing the loads by a certain concentration, e.g. substance-related geogenic background. In this way, water quality footprints can also be expressed in terms of water volume, i.e. the volume necessary to dilute the pollution down to the reference concentration, and can be used in the same way and in addition to quantitative water footprints of water withdrawals or consumption.

Substance-specific features. Within this study, water pollution from agricultural application of N, P, and G is considered. N and P are the most important plant macronutrients in terms of quantity (e.g. FAOSTAT Database), that are discharged to a large extent into inland and coastal water bodies¹⁹. The third macronutrient, potassium, often accounts for only a fraction of the total nutrients applied (e.g. FAOSTAT Database) and is therefore neglected in this work, as are micronutrients. The second source of agricultural water pollution are pesticides which comprise chemicals or microorganisms used to destroy or inhibit organisms or viruses that are harmful to crop growth. Due to the large number of pesticides, not all can be considered here. Based on its global importance²⁰, G is chosen to demonstrate the approach and present first results. In the following, relevant characteristics of N, P and G are described and evaluated for the calculation approach.

N contributes to many different pools in the atmosphere, biosphere and hydrosphere and in soils in different chemical forms. Atmospheric N is in the form of inert, elemental N_2 gas. Next to it there are different reactive forms of N, such as ammonia $[\text{NH}_3]$ and ammonium $[\text{NH}_4^+]$, nitric oxide $[\text{NO}]$, nitrogen dioxide $[\text{NO}_2]$, nitrous oxide $[\text{N}_2\text{O}]$, nitrate $[\text{NO}_3^-]$ and nitrite $[\text{NO}_2^-]$ ⁴³, which have strongly increased due to biological fixation of N_2 through leguminous crops, combustion of fossil fuel and, in particular, production of synthetic fertilizer⁴³. For plant nutrition, ammonium $[\text{NH}_4^+]$ or nitrate $[\text{NO}_3^-]$ are required. Also, organic N-nitroso compounds (R-N=O) are present in the environment. The following points are important to balance agricultural N applications: next to mineral fertilizer input, manure as well as biological fixation and atmospheric deposition contribute to the N input, whereas extraction by plants and denitrification, which is the anaerobic conversion of nitrate to N_2 , or N_2O by soil bacteria and subsequent release into the atmosphere, are relevant for the output³⁶. Additionally, emission to surface water by runoff and soil loss are considered in a

balance⁴⁴. The remaining quantity is either adding to the stock of N in the soils or is emitted to groundwater. Stock addition can be neglected due to high water solubility and low adsorption of N compounds. Hence, the remaining quantity can be considered as emission to groundwater. However, it is still important to note that during the residence time of the groundwater, some of the N is denitrified, which is taken into account in the calculation. In principle, all listed N compounds are water soluble and can contribute to the total N content of water bodies. Throughout this study, N in water is always reported as total dissolved inorganic N. The water quality footprint consists of the sum of emission to surface water and groundwater minus denitrification.

As regards P, monophosphine, PH_3 , is the only gaseous form of P, which can be neglected with regard to the whole P cycle. In the absence of an atmospheric cycle, plants can obtain P only from the soil³⁸. There P can occur inorganically in primary P minerals, dissolved in the form of H_2PO_4^- or HPO_4^{2-} or organically in various forms. Plants must make bound P available as H_2PO_4^- in order to be able to absorb it. Harvesting removes P from the soil indirectly, while surface runoff (emission to surface water) and soil loss remove it directly, which together would result in a negative P balance without external supply. Addition of P through manure or mineral fertiliser would avoid that the P is mined from the soil. Depending on their specific soil characteristics, P is easily available for plants or not and whether the soil storage of P is accumulating or not³⁸. These effects are important from an agronomic perspective and have a noteworthy influence on the yield and the amount of P storage in the soil mainly determines the emission to water bodies. Previous work on P leaching to groundwater has concluded that leaching is negligible compared to surface runoff: next to discharge of untreated waste waters, the surface runoff from crop fields and pastures is the globally most important source of excess P in surface water bodies⁴⁵. P leaching may occur in saturated soils, that have faced long-term over-fertilisation⁴⁶, however, application has already been declining since the 1980s in countries with historical over-fertilisation, especially in Europe³⁹. Other studies indicate that P leaching can be important in flat landscapes in the presence of certain subsoil properties^{47,48}. But these are mainly findings from laboratory experiments or specific sites, so that a general indicator for all soil types has not been established yet. Hence, P leaching is neglected in this study and the water quality footprint considers only run-off emission to surface water.

As regards G, it is an artificial substance which means that there are no primarily natural cycles. The mechanisms and effects of G dissipation on certain compartments have variously been studied spatially and temporarily. However, we still know too little about the potential establishment of anthropogenic cycles and interactions (e.g. G as P source⁴⁹). Consequently, inputs from sources other than direct application are neglected in this study. While highly complex and site specific, there are hints that G in general shows a similar behaviour than P with two exceptions: cultivated soils can be saturated with P, which is not likely for G, and G is also degraded by microbes³⁷. To calculate the emission to surface water and groundwater, (bio)degradation, sorption and leaching to groundwater have to be considered as impact pathway.

To account for the complexity and high spatial dependence of the impact pathways, the emission to surface water and groundwater for N, P and G is determined from highly developed models with spatial resolution. These data are also associated with high uncertainties, but represent a suitable state-of-the-art basis that takes substance-specific characteristics into account and is continuously being developed. Our focus here is not the provision of data, but the description of a suitable methodology and representation of water quality footprints with available data.

Application of water scarcity footprint methodology. Agricultural water pollution through N, P and G is expressed in volumes of virtual water to dilute the emission to surface and groundwater. The VDV is calculated with demineralized water VDV_{dem} by dividing the substance-specific load s in a catchment area i by the geogenic background concentration $c_{geo,s}$ in case of naturally occurring substances or the target concentration $c_{target,s}$ in case of anthropogenic substances¹⁸. For the purpose of this study, the calculation is adapted: load s is renamed to $load_{s,em}$ to make it clear that it is the emission to surface and groundwater. VDV's are calculated at country level for the producer countries supplying the German bioeconomy, so that the numerator i stands for the individual countries here and the functional unit (FU) is m^3 per country i . For N and P, the calculation follows Eq. (1), if $c_{geo,s} \leq c_{target,s}$ and Eq. (2), if $c_{geo,s} > c_{target,s}$. For pesticides, the calculation follows Eq. (2):

$$\text{VDV}_{dem,s,i} [\text{m}^3] = \frac{load_{s,em} [\text{kg}]}{c_{geo,s} [\text{kg m}^{-3}]} \quad (1)$$

$$\text{VDV}_{dem,s,i} [\text{m}^3] = \frac{load_{s,em} [\text{kg}]}{c_{target,s} [\text{kg m}^{-3}]} \quad (2)$$

The N load $_{N,em}$ is calculated from a N cropland mass balance with the general equation $m_{t=x+1} = m_{t=x} + dm dt^{-1}$, where m represents a stock, $t=x$ a certain point in time, here the beginning of an agricultural period, and $t=x+1$ a later point in time, here the following agricultural period. The total N storage $N_{stor,t=x+1}$ is the sum of the storage $N_{stor,t=x}$ resulting from the previous agricultural period, the fertilizer input $N_{fert,t=x+1}$, the input from livestock excretions $N_{ex,t=x+1}$, atmospheric deposition $N_{dep,t=x+1}$ and biological N fixation $N_{fix,t=x+1}$ minus N extraction by harvested plant parts $N_{harv,t=x+1}$, ammonia volatilization $N_{vol,t=x+1}$, soil loss $N_{loss,t=x+1}$, denitrification $N_{denit,t=x+1}$ and the $load_{N,res,t=x+1}$. Emission to surface water from runoff and emission to groundwater through leaching are both included in $load_{N,res,t=x+1}$. Converting the formula gives Eq. (3):

$$load_{N,em,t=x+1} = N_{stor,t=x} - N_{stor,t=x+1} + N_{fert,t=x+1} + N_{ex,t=x+1} + N_{dep,t=x+1} + N_{fix,t=x+1} - N_{harv,t=x+1} - N_{vol,t=x+1} - N_{loss,t=x+1} - N_{denit,t=x+1} \quad (3)$$

The global model IMAGE-GNM¹⁹ provides all relevant parameters for the years 1995 and 2020 on grid cell level (0.5 by 0.5 degree, Supplementary Table 1) except for denitrification which cannot be obtained for a single year directly from the current publication of IMAGE-GNM. It is calculated following van Drecht et al.⁵⁰ under the assumption of steady state for every year from 1990 to 2010 (Supplementary Data 5). The average of the years 1990 to 2020 is taken as factor f_{denit} (Supplementary Table 1) to be multiplied with leaching. Country values are aggregated with the help of GIS-based zonal statistics.

The P load $_{P,em}$ corresponds to the emission to surface water here, as emission to groundwater is neglected. It is taken from the global model IMAGE-GNM¹⁹ for the years 1995 and 2020. It is assumed that the surface runoff reaches surface water bodies in the year of application.

The G load $_{G,em}$ is calculated from the gridded application rates according PEST-CHEMGRIDS²⁰ for the year 2020 by multiplication with a mass fraction which is obtained from the USEtox[®] model^{21,22}. The mass fraction is the proportion of G that is emitted into freshwater (surface water and groundwater) after transport, sorption and (bio)degradation in the soil. USEtox[®] provides mass balances for several thousand organic and inorganic substances on different scales considering interactions between indoor compartments, air, agricultural and natural soil, freshwater and coastal marine water by modelling fate and exposure. Actually, these results are further used to derive

characterisation factors for the assessment of the effect of substances on humans and ecosystems in life cycle impact assessment modelling. Here, we use it to describe the impact pathway of G, because we consider it an advanced model for modelling the fate of chemicals that is the consensus method for determining human and ecotoxicity in life cycle impact assessment. As regards spatial resolution, USEtox® considers wind speed, precipitation, groundwater level and runoff on continental and sub-continental level and distinguishes between agricultural and natural soils⁵¹. Input data from IMAGE-GNM and USEtox® have not been validated in the course of this study. IMAGE-GNM has a good validation status on long time series for N and P concentrations in different river basins around the world, but it is not possible to validate the fluxes of surface runoff and groundwater flow^{19,46}.

Country-level geogenic background concentrations $c_{\text{geo},s}$ for N and P are compiled using a literature research (Supplementary Data 6 and 7). Where country-level data are not available, continent-level data are taken, and if also not available, the global median is used. The target concentration $c_{\text{targ},s}$ is taken from the World Health Organisation drinking water standard³⁵ where data from different countries were analysed to determine median values. In case of artificial substances, geogenic background concentrations do not play a role and no regional differences need to be considered. What is important instead is the toxicity to organisms reflected in the global threshold values from the drinking water standard. The drinking water standard is used for surface water and groundwater, because the different water bodies of a catchment are not treated separately from each other, but as a unit¹⁸. The target concentration is also used, if the geogenic background concentration is zero or greater than the target concentration.

The calculated dilution volume is presented in m^3 per inhabitant of Germany and categorised as low ($<4.6 \text{ m}^3$ per German), medium (4.6 to 460) and high (>460) by comparing it with the GDW, the German direct drinking water withdrawal per German inhabitant (127 L d^{-1} in 2020 according to Destatis²⁵, which equals $46 \text{ m}^3 \text{ a}^{-1}$). This classification considers that usually more than 90% of the product water use in general are to be found in the upstream supply⁵². A virtual dilution volume of 460 m^3 per German or smaller, compared to which the GDW of 46 m^3 is one tenth, is consequently still in an acceptable range and marks the border to the category high here. It is important to note, that we compare purely calculated virtual volumes, which are not consumed in reality, to actually used volumes of water, such as the GDW. Thereby, we want to show comparatively how much water would be needed if water pollution were eliminated by dilution to make the extent of water pollution tangible. For comparison purposes, the dilution volumes of the three substances are discussed side by side, but in the overall view for the German bioeconomy, only the largest volume is listed, the so-called critical volume. The largest volume contains the smaller dilution volumes and dilutes all examined substances.

Although recommended, we refrain from using AWARE water stress factors, as the underlying dataset of water availability and water use refers to the year 2010. Instead, the indicator withdrawal-to-availability ratio (WTA), initially presented by Alcamo et al.²³, is used. We use an own calculation of WTA with data from AQUASTAT²⁴ to cover the years both 1995 and 2020 and to receive country level values. They are calculated as the total freshwater withdrawal divided by the total renewable freshwater resources per country (Supplementary Figs. 2, 5). Since the water footprint method presented here is based on an LCA approach, but no LCA is conducted in accordance with the relevant guidelines, we refrain from weighting by multiplication as usually recommended in LCA. Also, routinely performed weighting can be misleading depending on the scope of a study

and is hence not recommended for all applications of the water footprint⁵³. Hence, we conduct the water stress analysis by using a colour scheme⁸ to designate low, middle and high water stress levels besides the calculated virtual dilution volumes, where no water stress corresponds to $0 < \text{WTA} \leq 0.1$, low water stress to $0.1 < \text{WTA} \leq 0.2$, medium water stress to $0.2 < \text{WTA} \leq 0.4$ and high water stress to $\text{WTA} > 0.4$. We have merged the no stress and low stress category to present three categories in total.

Share of the German bioeconomy on agricultural water pollution. Country-level VDV_s are multiplied by the share of the German bioeconomy on the agricultural production in a country. Agricultural production includes the eight primary crop categories paddy rice; wheat; cereal grains nec; vegetables, fruits and nuts; oil seeds; sugar cane, sugar beet; plant based fibres and crops nec. Shares are based on the share of raw material input into the German bioeconomy (RMI, including German domestic consumption and export) in a country's agricultural production EXIOBASE for the years 1995 and 2020⁸, and have been updated meanwhile according to a newer version of EXIOBASE. Shares are predominantly only available at the regional level with five large rest-of-world regions covering a large number of countries. Moreover, the shares refer to production quantities, while the total substance loads are related to area. With the help of agricultural production data according to quantities and areas and the total agricultural area of a country (FAOSTAT), shares of rest-of-world regions are scaled down to country level and all shares are recalculated to area-related shares. To do so, FAOSTAT agricultural data were assigned to the eight primary crop categories of EXIOBASE. As this study supplements an existing monitoring framework for the German bioeconomy with an indicator for water quality, it is calculated with an identical data basis, even though MRIOs with higher resolution are now available. Germany's share of agricultural production in a country is related to the N, P or G emissions of the entire agricultural sector, thus neglecting the actual composition of imports by crop and the effects of crop-specific emission intensities. Disaggregation by crop can make the results bioeconomy-specific, but is not possible with the currently available database, as EXIOBASE only breaks down by eight crop classes and IMAGE-GNM by three, all of which are not bioeconomy-specific (such as biofuels). In the continuation of the monitoring programme, the data basis will be successively refined as planned and results with less uncertainty and higher resolution will be presented.

Data availability

Input data are available from Bringezu et al.⁸ (German share on agricultural production), the IMAGE-GNM model¹⁹, PEST-CHEMGRIDS²⁰, the USEtox® model^{21,22}, FAOSTAT (agricultural production and area) as well as from AQUASTAT²⁴ (total water withdrawal and total renewable water resources per country). All data that were calculated or compiled throughout this study are available in the Supplementary Material, detailed calculations and a README file can be obtained from Mendeley Data⁵⁴.

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Author contributions

A.C.S. is responsible for the conceptual elaboration, carried out the analyses, created the figures, wrote the main paper and compiled the supplementary material. S.B. is responsible for the conceptual elaboration and extensively reviewed the manuscript.

A.W.H.B. provided data based on the IMAGE-GNM model and reviewed the manuscript.

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