SUPPORTING INFORMATION FOR:

Seitfudem, G., Berger, M., Müller Schmied, H., Boulay, A.-B. (2025) The updated and improved method for water scarcity impact assessment in LCA, AWARE2.0. *Journal of Industrial Ecology.*

Summary

This supporting information provides further information on WaterGAP2.2e and its output data used, as well as about the extrapolation approach for water consumption.

Contents

S 1 The WaterGAP2.2e output variables

S 1.1 Input variables to AWARE

Recalculations of AWARE CFs often are not fully comparable because of conceptual differences, e.g., regarding temporal reference periods or the AMD_{world_avg} (Andrade et al., 2020; Ansorge & Beránková, 2017; Lee et al., 2019), or definitions of water availability (Bontinck et al., 2021; Lee et al., 2019). AWARE2.0 aims to improve data availability and thus comparability by using publicly available ISIMIP data (Table S1), which will facilitate future studies and improve traceability of data or assumption differences. Note that this data was post-processed for changes in water consumption as described in S 3. The resulting data is available in the same repository as the AWARE2.0 CFs.

Table S1: WaterGAP2.2e (Müller Schmied et al., 2024) output variables used for the calculation of AWARE2.0. Note that this is the data before the adjustment of the values for recent years (see chapter S 3). The DOI for all data obtained from ISIMIP is: https://doi.org/10.48364/ISIMIP.398165.3 (Gosling et al., 2024), while the area data is to be referenced as https://doi.org/10.25716/gude.0tny-kjpg (Müller Schmied, Trautmann, et al., 2023)

Variable and link to file	description	used for	reference period	spatial extent
continentalarea https://gude.uni-frankfurt.de/bitstreams/0ba40ee1-4e40-481b-9ffe-811b3e786597/download	land area per grid cell	Area values for calculation of basin area	-	global grid cells
dis_default https://data.isimip.org/files/b9e69096-2ccd-4107-9cf4-23b036d412fb/	river discharge or streamflow	$ActAvail$	1990 – 2019	outflow cell
		IN_{sink}	1990 – 2019	inflows to sink
dis_nowatermgt https://data.isimip.org/files/e73fca83-7ef5-451b-8616-db8911660af5/	river discharge or streamflow (naturalized)	$NatAvail$	1960 – 2010	outflow cell
		IN_{sink} (for EWRs)	1960 – 2010	inflows to sink
qtot_nowatermgt https://data.isimip.org/files/9325a486-516a-47de-911b-23ae773ca8ec/	total runoff as sum of runoff from soil and groundwater outflow	RO_{sink} (for EWRs)	1960 – 2010	sink cell
		RO_{sink}	1990 – 2019	sink cell
atotuse (actual consumptive use) https://data.isimip.org/files/8f4e007d-1db2-4df8-a87b-a0b01f8f2003/	Actual consumptive water use as sum of all sectors (considering water availability)	AC_{sink}	1990 – 2019	sink cell
		HWC	2019	entire basin
pirruse https://data.isimip.org/files/5d3dcadf-36ed-456c-92c5-94354ca78568/ pdomuse https://data.isimip.org/files/a00ad2fd-143e-4969-bfe6-e0b8b7423e82/ pelecuse https://data.isimip.org/files/58ebe0	potential consumptive water use in the irrigation, domestic, thermal electricity, manufacturing, and livestock sectors	basis for extrapolation and scaling (chapter S 3)	1990 – 2019	entire basin

d9-83d4-4e7b-a25c-e7e7bea48952/ pmanuse https://data.isimip.org/files/c17b3586-d454-412e-8621-7137cac0a9f5/ pliveuse https://data.isimip.org/files/703ab85f-a023-49b2-9c72-6ebd7bf98839/	after extrapolation and scaling: weights for aggregations	2019	entire basin

S 1.2 GHM FAQ

For researchers less familiar with hydrological modeling, an FAQ about WaterGAP2.2e is provided here. The questions are based on frequent questions to the authors about AWARE input data.

Q: What is the difference between naturalized and actual (anthropogenic) discharge in the WaterGAP2.2e data?
A: In contrast to actual discharge, in a naturalized setup no water use and no reservoirs are considered, representing river discharge without direct human impacts.

Q: What climate data is used in WaterGAP2.2e?
A: As climate forcing, gswp3-w5e5 (Lange et al., 2022) was used for calibration and simulation with WaterGAP2.2e. It is an observation-based dataset including data from 1901 to 2019 and in daily resolution.

Q: How is water consumption calculated in WaterGAP2.2e?
A: In WaterGAP, five sectoral water use sectors (irrigation, domestic, manufacturing, thermoelectric, livestock) are considered by individual models. In the sub-model GWSWUSE, the source of the water is distinguished in groundwater or surface water, and return flows are considered; referring to "potential" withdrawal water use and consumptive water use. Those time series are the input to the WaterGAP Global Hydrology Model. Whereas water abstractions from groundwater can always be satisfied, under limited availability in rivers, lakes and reservoirs (surface water resources) only a part of water abstractions can be satisfied. In this case, actual water consumption differs from potential water consumption (Müller Schmied et al., 2021, 2024; Müller Schmied, Flörke, et al., 2023).

Q: How is the existence of dams and reservoirs respected in WaterGAP2.2e and is there a way to find out which ones are included?
A: The water balance of reservoirs including the reservoir management are calculated in the outflow cell of the reservoirs. There is a total of 1181 reservoirs and 86 regulated lakes with a storage capacity of > 0.5 km^3. Smaller reservoirs (in total 5722) do not consider an explicit reservoir management but are included in the lake storage. Both reservoir types are excluded in a naturalized run. A spatial dataset considering all reservoirs > 0.5 km^3 in WaterGAP2.2e including their attributes

is published here: https://doi.org/10.5281/zenodo.8147625 (Müller Schmied et al., 2021; Müller Schmied & Trautmann, 2023).

Q: To what extent does WaterGAP2.2e include water transfers?
A: Water transfers are considered implicitly only. In the case water abstractions from surface water cannot be met by a grid cell, water use is tried to be satisfied by the direct neighboring cell with highest water availability (Müller Schmied et al., 2021, Section 4.8).

Q: How is calibration used in WaterGAP2.2e? What is its implication on the accuracy of monthly long-term averaged discharge (anthropogenic and naturalized) used in AWARE?
A: The calibration procedure is described in (Müller Schmied et al., 2021, Section 4.9). In WaterGAP 2.2e, the data base for calibration has been updated to a total of 1509 stations. WaterGAP is calibrated to match long-term mean annual observed river discharge which leads to a realistic representation of observed water resources in the anthropogenic run of WaterGAP2.2e.

Q: Does WaterGAP2.2e model changes in land use, dams & reservoirs, water consumption… explicitly for each year? To what degree are changing population numbers included? Is this relevant to long-term averaged discharge data used in AWARE2.0?
A: Land use is determined to be constant except for varying irrigation areas. Reservoirs are included according to their year of commission. Water consumption is simulated either on monthly (irrigation) or yearly (all other water use sectors) time step (more details in (Müller Schmied et al., 2021; Müller Schmied, Flörke, et al., 2023)). Changing population is considered in manufacturing and domestic water use sectors. Consideration of direct human impacts such as reservoir management and water use affects long term average discharge especially in regions with high water use and downstream of large reservoirs (Müller Schmied et al., 2016). On global scale, long-term average river discharge to the oceans or inland sinks is lower when reservoirs and water use are considered (Müller Schmied et al., 2014).

S 1.3 Major adjustments between WaterGAP2.2d and WaterGAP2.2e

The following adjustments between WaterGAP2.2e, used for AWARE2.0, and its predecessor WaterGAP2.2d (Müller Schmied et al., 2021) might be relevant to AWARE (Müller Schmied et al., 2024):

- New handling of inland sinks: a) no focused groundwater recharge below surface water bodies, b) surface runoff and groundwater outflow are routed to the surface water bodies (no fractional routing), c) simulated streamflow of inland sinks is added to actual evapotranspiration in model output, streamflow is set to zero.
- Reservoir input data has been updated to GRanD version 1.3 plus 4 reservoirs from Kansas State University, resulting in total 1181 reservoirs and 86 regulated lakes where

the reservoir algorithm is being used and the remaining as local lakes (Müller Schmied & Trautmann, 2023).

- Small reservoirs (<0.5 km³ storage capacity) are no longer considered in naturalized runs (apart from local lakes)
- Calibration data base was updated to in total 1509 stations from a merge of three databases (*BfG - The GRDC*, n.d.; Do et al., 2018; Gudmundsson et al., 2018; Tramblay et al., 2021). The final calibration database is available at https://doi.org/10.5281/zenodo.7255968 (Müller Schmied & Schiebener, 2022).
- Update of industrial (manufacturing and thermoelectric) water uses

S 2 Actual and potential human water consumption

Following adjustment of the aHWC data for the calculation of $AMD_{world\ avg}$ was required: WaterGAP2.2e calculates aHWC as a balance of extractions (withdrawal) and return flows for every grid cell (Figure S1). aHWC therefore is the net water consumption which considers that there are return flows to the environment. If part of that water is supplied by basins nearby and "replenishes" local flows, the net water consumption in a grid cell can be smaller than the amount of water actually consumed (Müller Schmied et al., 2021). Even when summing up grid cell aHWC over a basin, the resulting values can be zero or negative, indicating that there is no net water consumption in this basin (Figure S2). Vice versa, there are months where aHWC > pHWC, implying that more water was consumed from the basin than required internally (Figure S3). In basins where aHWC was negative, it was set to zero for AWARE2.0 (Figure S4).

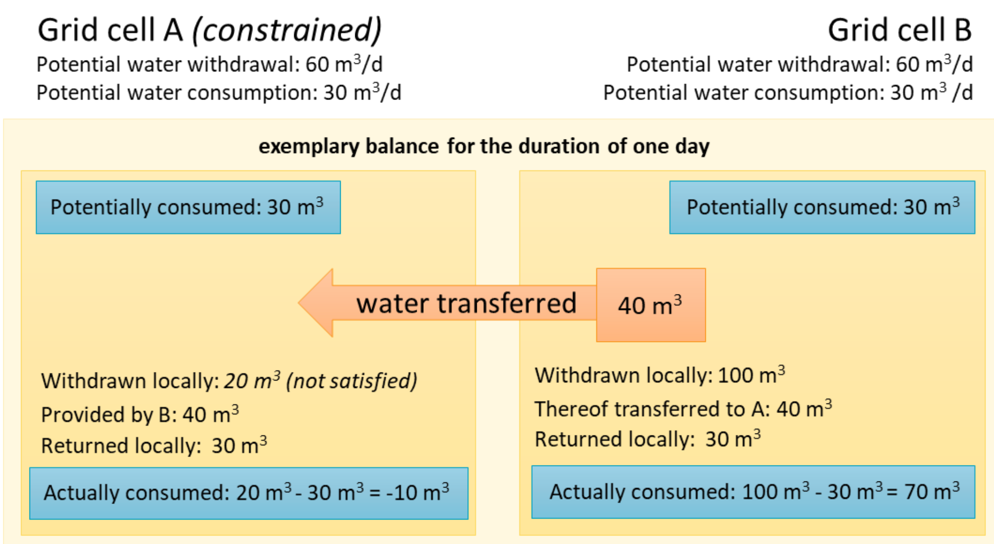

Figure S1: The reason for negative aHWC in WaterGAP2.2e (simplified). Both grid cells A and B have the same water demand, but A cannot satisfy it on its own. Therefore, it receives water from neighboring grid cell B, where it counts as consumed water, while part of it returning to the environment in A (the return flow) counts as a credit for A and leads to a negative aHWC. As mentioned in the FAQ (S 1.2), water transfers only happen in case of a surface water deficit. Note: The relevant variables in WaterGAP2.2e are flows in m³/d

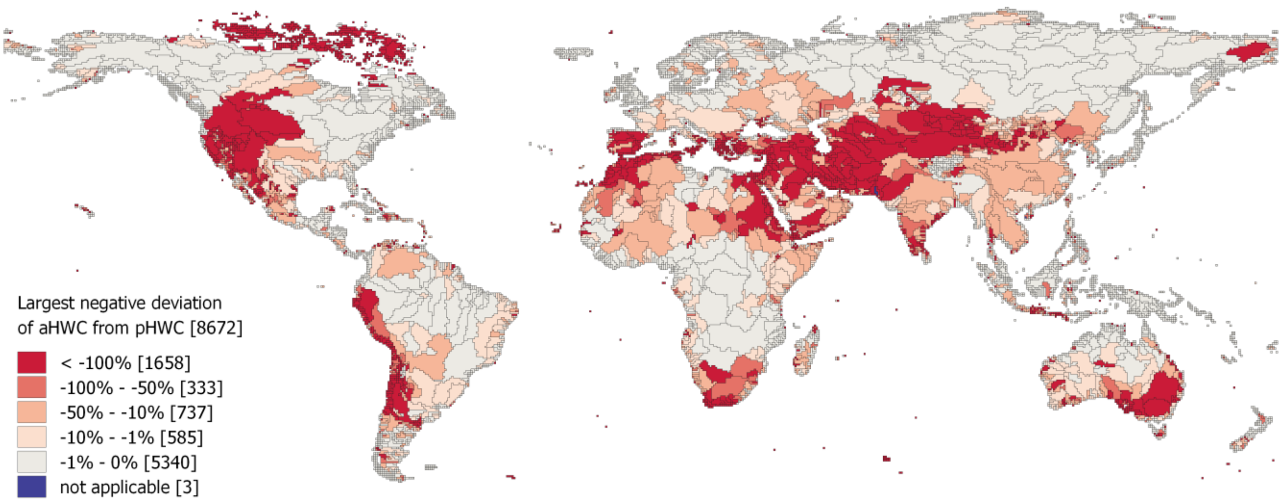

Figure S2: Largest negative deviation of long-term monthly actual human water consumption (aHWC) from potential human water consumption (pHWC). Note: This is before applying the extrapolation and scaling approach described in chapter S3.

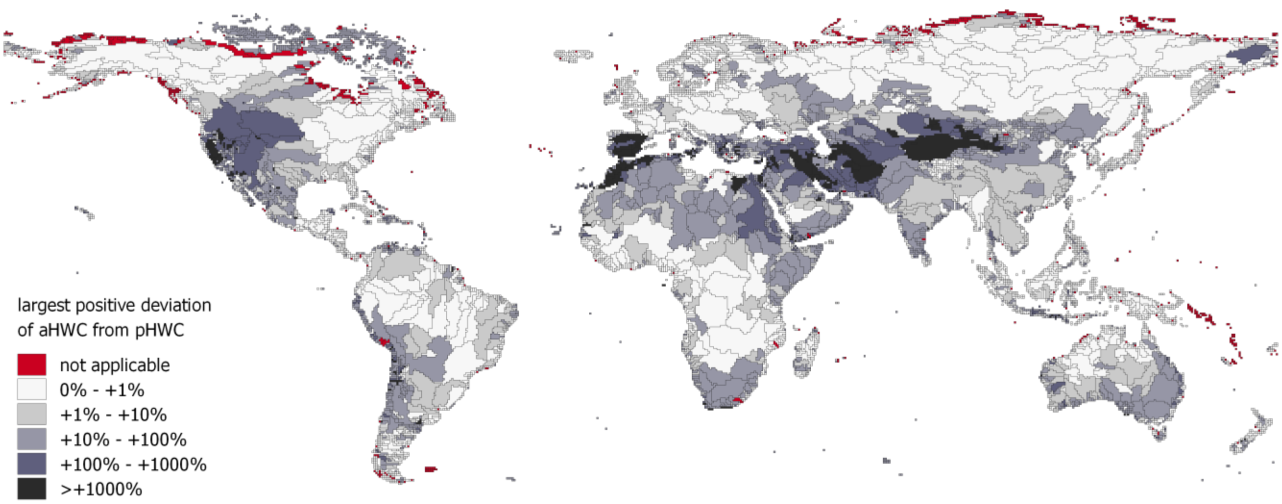

Figure S3: Largest positive deviation of long-term monthly actual human water consumption (aHWC) from potential human water consumption (pHWC). Note: This is before applying the extrapolation and scaling approach described in chapter S3.

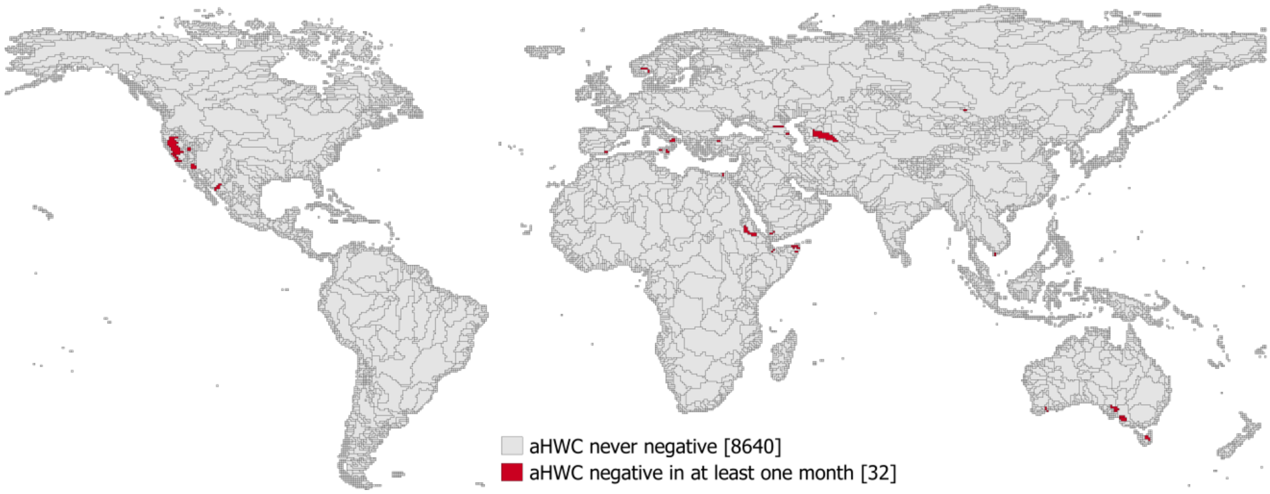

Figure S4: Basins at least affected once by setting negative aHWC to zero for the AMD_{world_avg}.

S 3 Adjustment of WaterGAP2.2e output variables for recent years

S 3.1 Motivation

The WaterGAP2.2e model runs used for AWARE do not model all water use sectors dynamically for every year of the AWARE2.0 reference period 1990-2019. Furthermore, the temporal coverage of explicit, year-dependent sector data differs between sectors (**Error! Reference source not found.**). The world total of consumptive water demand seems to have stopped in its trend after approximately 2008 (Figure S5). Water consumption is a relevant variable for AWARE2.0 since the global inventory is used to calculate the AMD_{world_avg} and to weigh individual watersheds in the aggregation of characterization factors. Depending on the basin, it is also relevant to the AMD values, since they are based on long-term discharge which is subject to long-term water consumption. To approximate water consumption patterns in 2019 and adjust the WaterGAP2.2e output data to potential changes in water demand, an extrapolation and scaling approach was used, described below.

Table S2: Temporal limitations in explicit modeling of water demands

sector	temporal coverage	number of years affected
irrigation	irrigated areas are held constant after 2008. For some countries (not specified) after 2005	minimum 11
domestic	water demand is held constant after 2010	9
manufacturing	water demand is held constant after 2016	3
livestock	water demand is held constant after 2011	8
thermoelectric	water demand is held constant after 2017	2

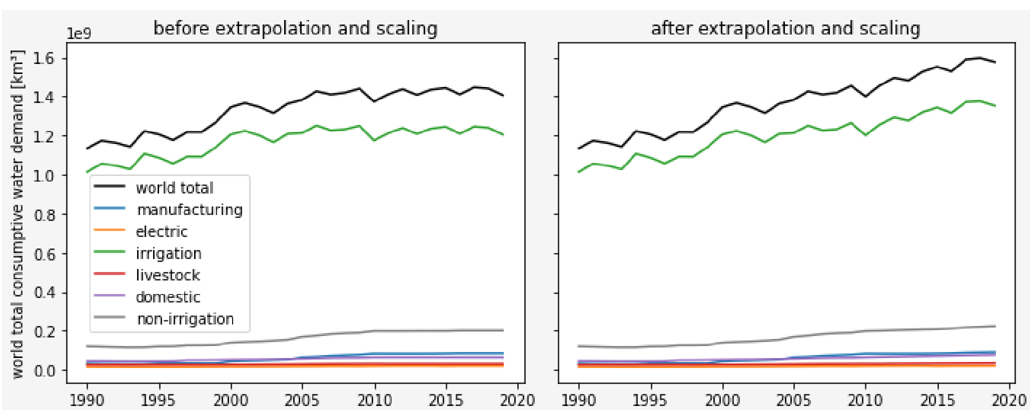

Figure S5 World total consumptive demand before and after extrapolation and scaling approach. Shown is the 30-year reference period used to calculate *ActAvail.*

S 3.2 Extrapolation and scaling approach

The calculation of actual water consumption in WaterGAP2.2e is based on potential water demand and actual water availability for each grid cell. Sector-wise data is only provided as potential water demand but the satisfied demand per sector is not specified, since partitioning the actually consumed water into different sectors would require a prioritization of water users which without region-specific data on this partitioning would require substantial subjective judgement. Consequentially, the adjustment of actual water consumption and corresponding long-term discharge first determines the potential change in demand, then detects whether this change can be satisfied on grid cell level and, lastly, adds the changed demand to the actual consumption value that was calculated by WaterGAP2.2e. The procedure is detailed in Figure S6.

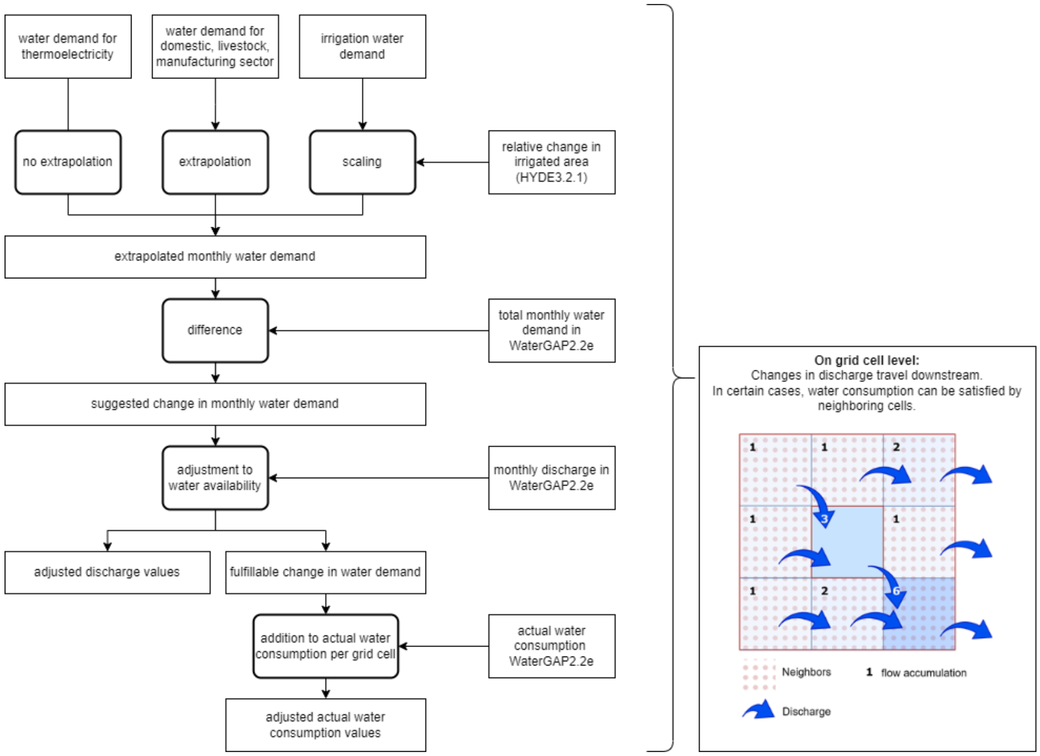

Figure S6 Process for adjusting actual consumption and longterm discharge with extrapolated/scaled water demands.

Water demand for thermoelectricity was not extrapolated due to its small relevance to river discharge compared to the other sectors, the difficulty to reason for a linear trend in thermoelectric water consumption on grid cell level (capped capacity of a power plant) and the fact that it was explicitly modeled until 2017. For the other **non-irrigation** sectors, i.e. domestic, livestock, manufacturing water use, a linear regression was performed for the ten years before the time frame to be extrapolated, using the *linregress()* function of the Python library *scipy*. In some grid cells, the water demand data for these sectors showed relatively large jumps, which would lead to unreasonable regression results. Therefore, limits for relative changes in water demand between years were defined based on the overall distribution of relative changes between years. Where the inter-annual change exceeded the limit, the regression starts with the first year after the exceedance. Where an exceedance happens between two of the last five years, no regression is performed (Figure S8).

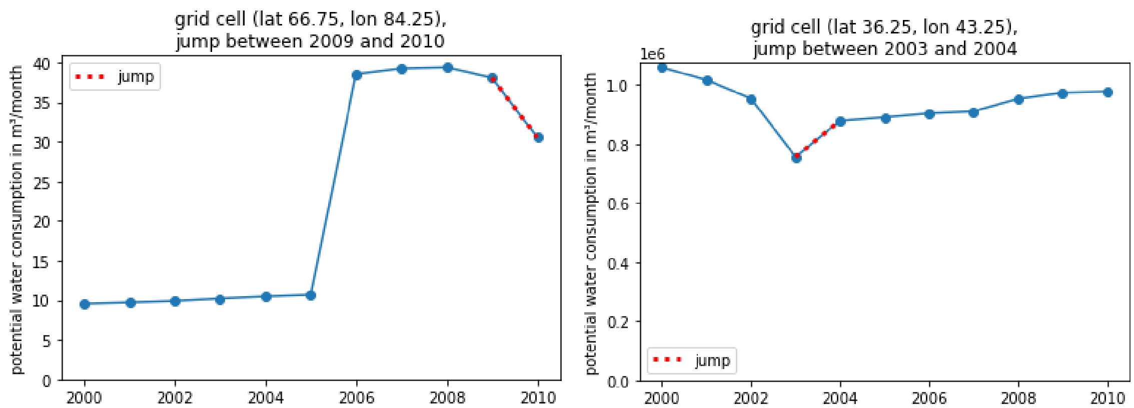

Figure S7 Examples of grid cells with jumps identified in potential domestic water consumption. Left: Jump between last two years. No extrapolation performed for 2011-2019. Right: Jump between 2003 and 2004. Extrapolation was performed based on a regression of 2004 – 2010.

The **irrigation** scaling is based on the relative change in irrigated area in HYDE3.2.1 (Klein Goldewijk et al., 2017), a land use dataset reaching until 2017 in its most recent update (https://easy.dans.knaw.nl/ui/datasets/id/easy-dataset:74467/tab/2). Absolute irrigated area per 5'x5' grid cells (one value per year) were combined to absolute irrigated area per 0.5°x0.5° grid cells. Relative change in irrigated area compared to 2008 was calculated for every grid cell. This scaling factor then was multiplied with the potential irrigation water consumption data of WaterGAP2.2e in the respective year, limited to following rules:

- To cut off outliers and extremes, for each year the size of scaling factors was limited to the 99.9th percentile of all scaling factors of that year. This affects 10 grid cells per year.
- Grid cells without irrigated area in 2008 but showing irrigated area afterwards were not scaled (they were assigned a scaling factor of 1).
- Irrigated areas for 2018 and 2019 were obtained by linear extrapolation of the area change from the previous ten years, but limited to grid cells where irrigated area was > 0 km² during 2009 – 2017.

S 3.3 Adjustment to water availability

Based on the calculated changes in water demand in the period 2009 – 2019, the variables actual consumption (*aHWC* in main publication) and discharge at the outflow cells (*ActAvail* in main publication) were adjusted. A simple algorithm was developed, illustrated in Figure S8.

Application to all flow accumulation levels, starting with lowest flow accumulation, i.e., grid cells without any inflow from upstream

1. For every grid cell: calculate the change in water demand (extrapolated minus non-extrapolated)
2. If changed water demand can not be satisfied by the available discharge of a cell as modeled in WaterGAP:
   - satisfy as much as possible (until discharge = 0)
   - check for neighbors where still discharge is left and "remember" them
3. For all cells that still have discharge left:
   - collect information about neighbors that still require water after using up their own discharge
   - satisfy their requirements, starting with the grid cell that has the lowest cumulative discharge around themselves. Satisfaction of demands of downstream basins is not allowed, since this would implicate a recursive function
4. Adjust outflow of all grid cells and, respectively, the capacity of downstream grid cells to satisfy water consumption

=> As in WaterGAP2.2e, water availability due to changed consumption is forwarded until final grid cell of the basin, except if a river runs dry on the way.

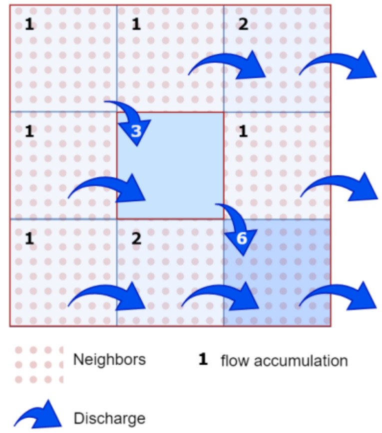

Figure S8 Left: Algorithm for adjustment of changed water demand to actual water availability. Right: Exemplary grid cell with a flow accumulation of 3, shown with its eight neighbor cells.

S 3.4 Impact of adjustment

The adjustment of *aHWC* and *ActAvail* affects the final CFs via *AMD* and the AMD_{world_avg}. Because of using the extrapolation approach, the AMD_{world_avg} increases by 3.95%. Consequently, CFs of most basins are about 3.95% higher than without extrapolations, which results from the use of AMD_{world_avg} as normalization value.

For most of the watersheds, the adjustment does not change the overall order of magnitude of CFs throughout the year (Figure S9). The rank correlation coefficient (RCC) for annual arithmetic average CFs as defined in the article applied to this comparison equals 0.9997. The change in CFs can be assessed with the Difference-To-Mean (DTM) between the monthly CFs (Boulay et al., 2021). 6.8% of basins at least in one month exceed a DTM of ±0.1. Together, they represent 36.3% of the global water consumption in 2019. The strongest CF increases are mainly found in the Middle East and South Asia (Figure S10).

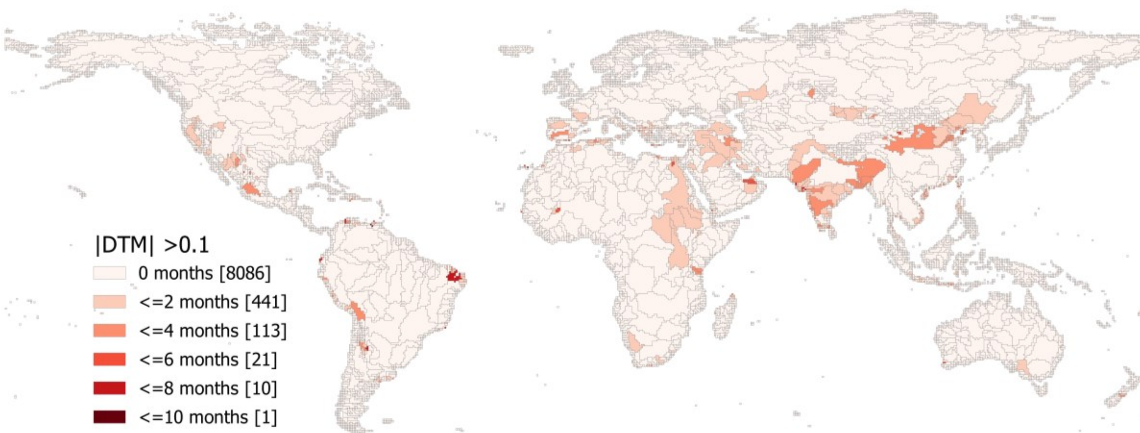

Figure S9 Number of months with a Difference-To-Mean (DTM) exceeding ± 0.1. The DTM was calculated from monthly CFs with and without adjustment.

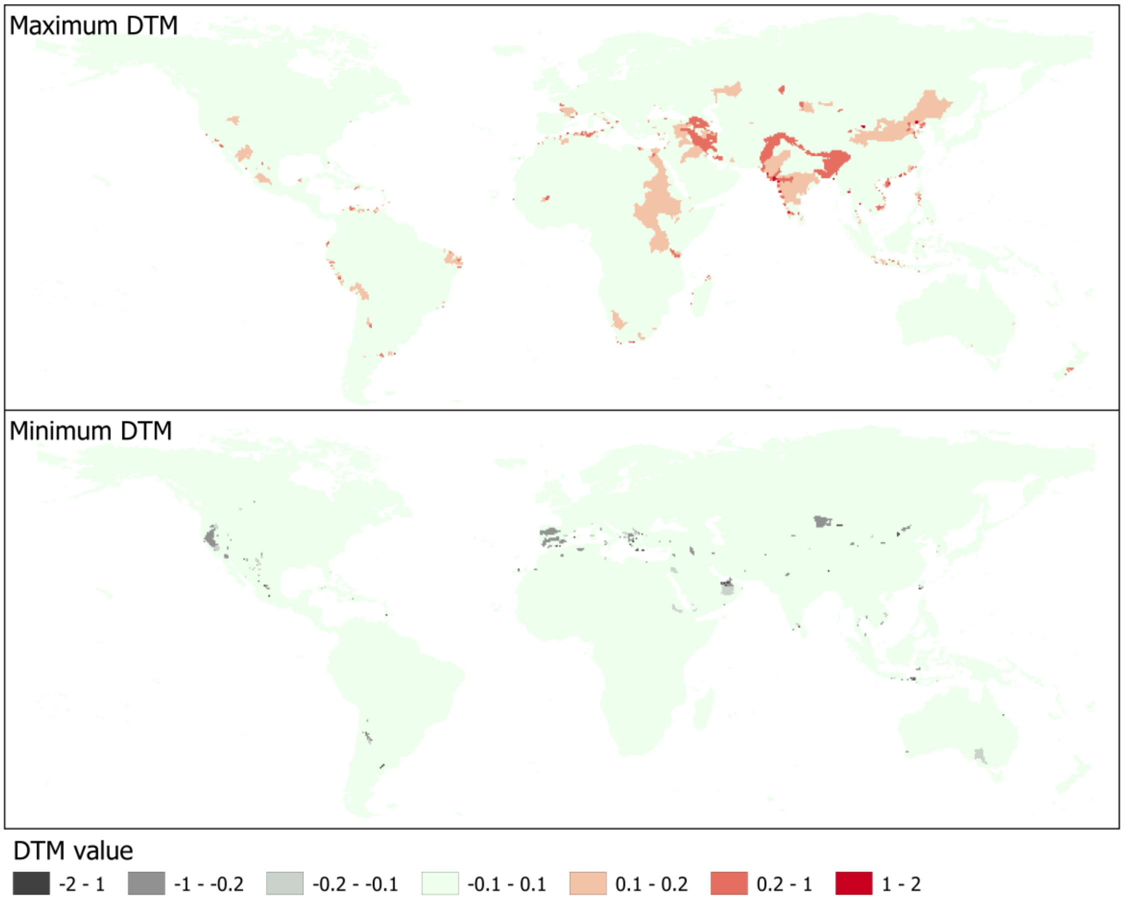

Figure S10 Maximum and minimum DTM per basin. Positive (red) values indicate higher CFs with the extrapolation. A DTM of 0.2 (1) indicates an increase by 22% (200%), a DTM of -0.2 (-1) a decrease by 18% (67%).

S 3.5 Limitations

The approach used here for retrospective adjustment of the discharge and consumption data has several limitations, of which the main one is the scaling of irrigation water consumption. This is because recent trends in irrigated area can only partially be covered, especially if the HYDE dataset and WaterGAP2.2e do not agree on the intensity of irrigation in the base year 2008. Furthermore, since HYDE describes actual land use, it already includes information on the water availability in a certain year in the calculation of the irrigated area, reducing irrigated areas where water availability is too low. WaterGAP2.2e additionally adjusts actual irrigation water consumption to water availability, which means that scaled irrigation demand in regions with insufficient water availability might be underestimated. On the other hand, the scaling does not consider technological progress and increases in irrigation efficiency, which could lead to overestimations of water consumption. A comparison of the scaled potential irrigation water consumption with the global dataset for 175 crops in (Mialyk et al., 2024) showed that WaterGAP probably misrepresents the decadal trend of the irrigation water consumption calculated with the Theil-Sen slope estimator in some watersheds

(Table S3, Figure S11). However, the variables compared here are conceptually different and only for a few of the studied watersheds (<5%, see Figure S12) the trend in Mialyk et al. (2024) is significant. As an example: For the Pearl River basin, the scaling by change in irrigated area leads to a divergence in irrigation water consumption trends (Figure S13): Scaled, irrigation water consumption seems to increase, while non-scaled the irrigation water consumption seems to decrease. Therefore, it is not straightforward to draw conclusions on the performance of the irrigation scaling approach on a global scale, except that it probably neither improves nor worsens irrigation water consumption data accuracy significantly.

Table S3: Comparison of potential irrigation water consumption with blue water irrigation consumption for 175 crops in Mialyk et al. (2024). Note that the bias to larger values could be a result of Mialyk et al. focusing on a set of 175 crops, while WaterGAP aims for representing all agricultural irrigation.

	% of basins with positive trend	**% of basins with negative trend**	**2019: % of basins with higher value than Mialyk et al. (2024)**
Mialyk et al. (2024)	17.9	82.1	------
Potential irrigation water consumption in this study	25.5	74.5	79.0
Potential irrigation water consumption in this study - scaled	26.3	73.7	78.3

Additional uncertainty is introduced by the extrapolation of domestic, manufacturing and livestock water uses, which might in some places not represent the factual trends. However, these sectors in most cases are less influential on AWARE characterization factors than irrigation is: The AMDs where non-irrigation sectors have a high share in the overall water demand, tend to be less influenced by human water demand in the first place (Figure S14).

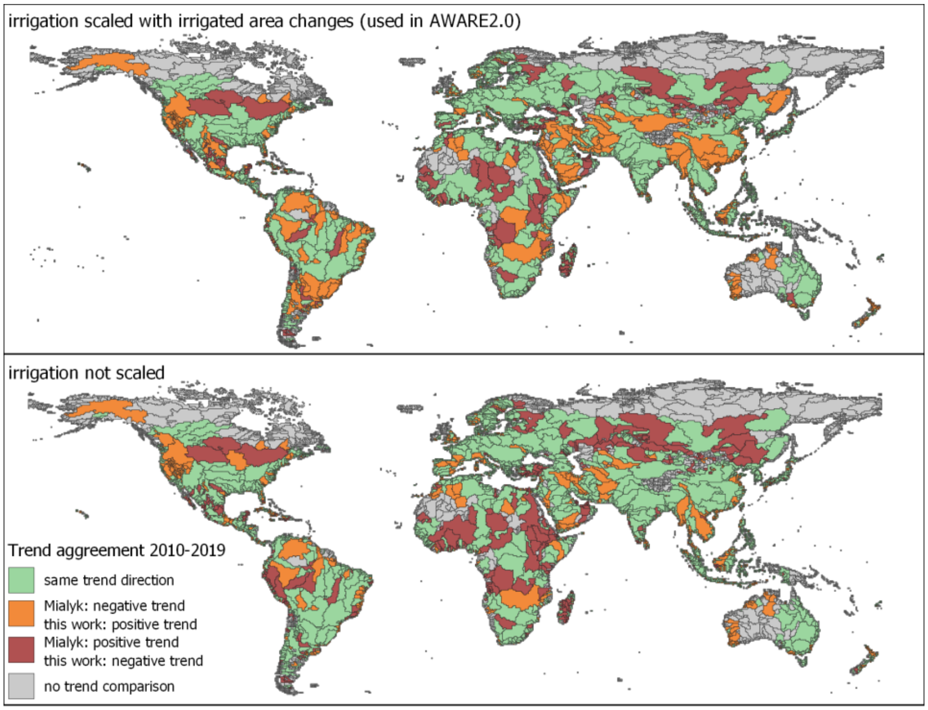

Figure S11 The agreement in short-term trend of potential irrigation water consumption from 2010 to 2019 between (Mialyk et al., 2024) and the data used in this work. Trends were calculated from annual totals using the Theil-Sen slope estimator. No evaluation of trend significance included. No trend comparison where Theil-Sen estimator not defined.

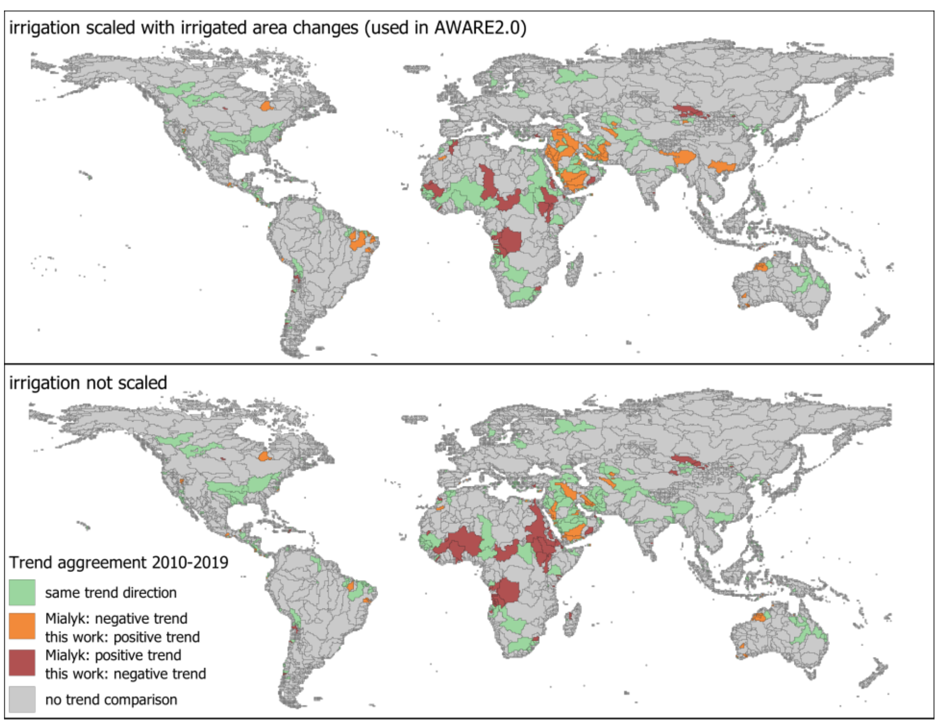

Figure S12 The agreement in short-term trend of potential irrigation water consumption from 2010 to 2019 between (Mialyk et al., 2024) and the data used in this work. Same figure as Figure S11, but with basins excluded where the Mann-Kendall Test (α=0.05) indicates no trend significance.

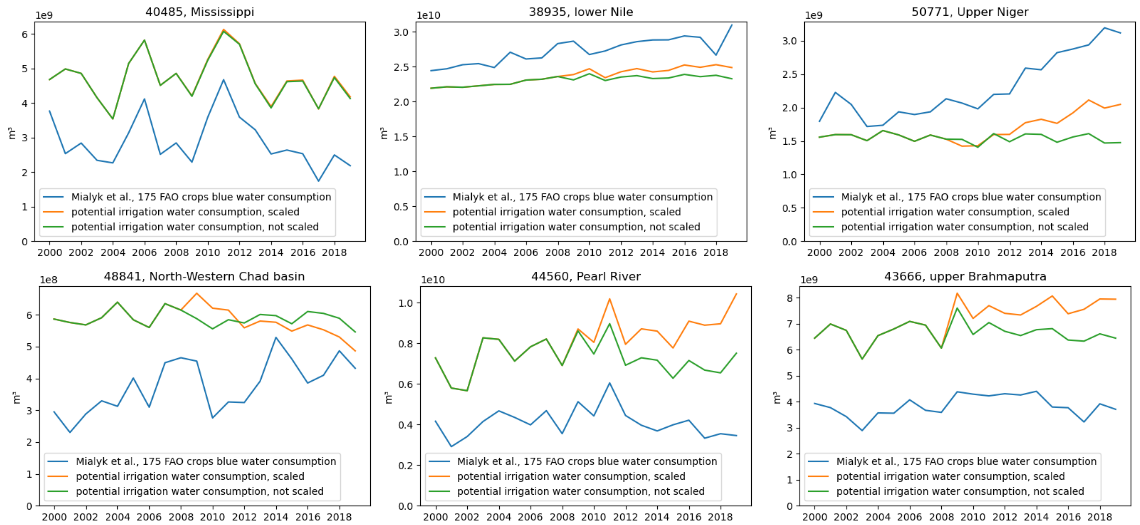

Figure S13 Examples of matching (Mississippi, lower Nile, upper Niger) and of diverging (North-Western Chad basin, Pearl River, upper Brahmaputra) trends in irrigation water consumption after scaling potential irrigation water consumption by irrigated area changes.

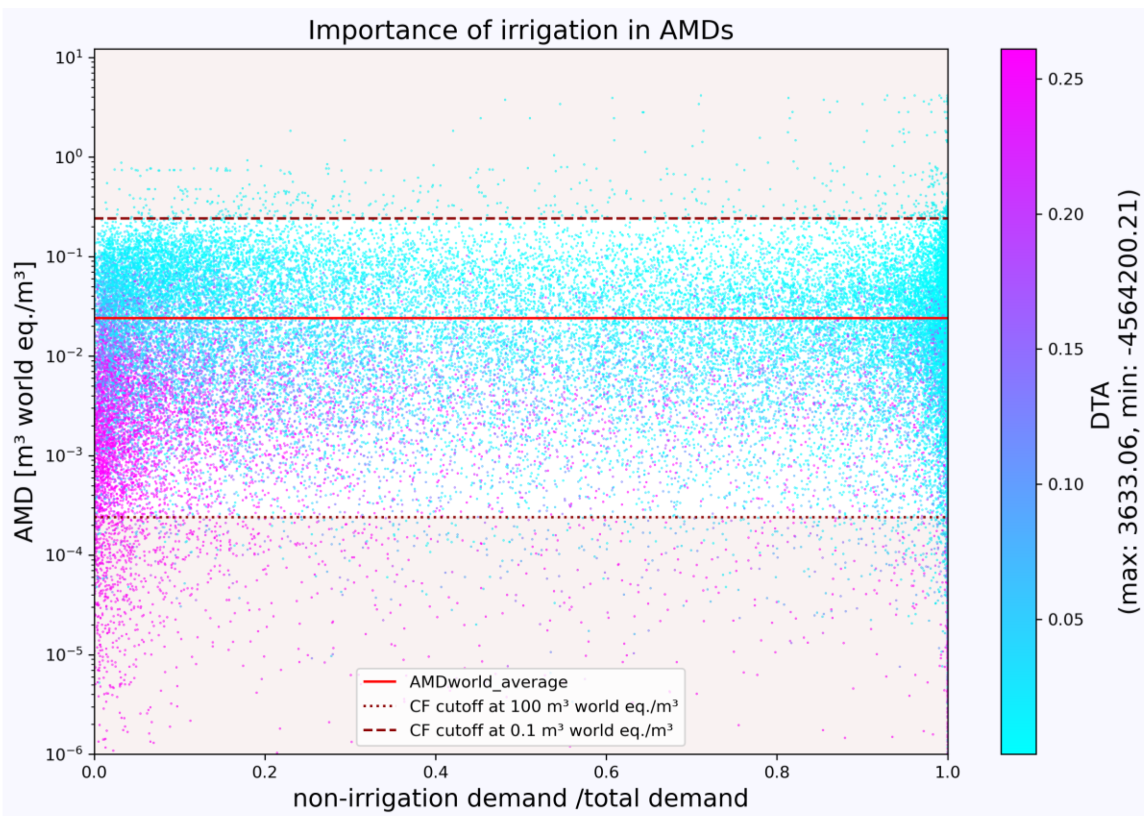

Figure S14 Importance of irrigation in AMDs. Where non-irrigation sectors have a high share in water demand, demand-to-availability (DTA, here: water demand compared to availability for human water consumption after the EWR is already satisfied) is rather low. Low DTAs indicate low influence of overall water demand on available water remaining. Therefore, where non-irrigation sectors are most important to the overall water consumption, the water consumption in general is

less relevant to the AMDs. Lower AMDs are rather found where irrigation represents a large part of the total water demand.

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