SUPPORTING INFORMATION

Modeling the impact of salinity variations on aquatic environments: including negative and positive effects in life cycle assessment

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The Supporting information contains 20 pages and 5 Sections, with 4 tables and 7 figures.

SECTION SI. General water bodies classification

Table S1. Salt concentration in aquatic environments according to their salt concentration and biome distribution[1,2].

According to biome distribution		According to salt concentration	
Waterbody Category	Characteristics and subcategories	Waterbody Category	Concentration (g salts*/L)
Rivers and streams	Freshwater	Freshwater	< 0.5
Lakes	Salt lakes (from oligohaline to hyperhaline), freshwater lakes, oases and springs (normally fed with fresh ground water).	Oligohaline	0.5 – 4.0
Palustrine wetlands	Highly biodiverse, non-riverine and non-tidal freshwater ecosystems. Include tropical flooded and peat forests, subtropical/temperate forested wetlands, permanent marshes, seasonal floodplain marshes, episodic arid floodplains, boreal, temperate and montane peat bogs, and boreal and temperate fens.	Mesohaline	5.0 – 18.0
Transitional waters	Combined marine and freshwater sources, varying from oligohaline to euhaline. It includes estuaries and bays, coastal inlets or fjords, and intermittently closed and open lagoons and lakes	Polyhaline	18.0 – 30.0
Brackish tidal systems	Intersection of marine, terrestrial, and freshwater processes, usually euhaline. They include deltas, intertidal forests and shrublands and saltmarshes.	Euhaline	30.0 – 40.0
Subterranean waterbodies	Freshwater	Hyperhaline	> 40.0
Oceanic	Euhaline (averaging 35 g/L)		
Artificial wetlands	Freshwater		

* Salinity is defined by the concentration of several ions (Na^+, Ca^{2+}, Mg^{2+}, K^+, Cl^-, SO_4^{2-} CO_3^{2-}, NO_3^- and HCO_3^-), where the main considered substance is NaCl. However, to accurately measure it, the sum of the concentrations of all these ions needs to be considered.

SECTION SII. Effect factor calculation assuming an exponential approximation.

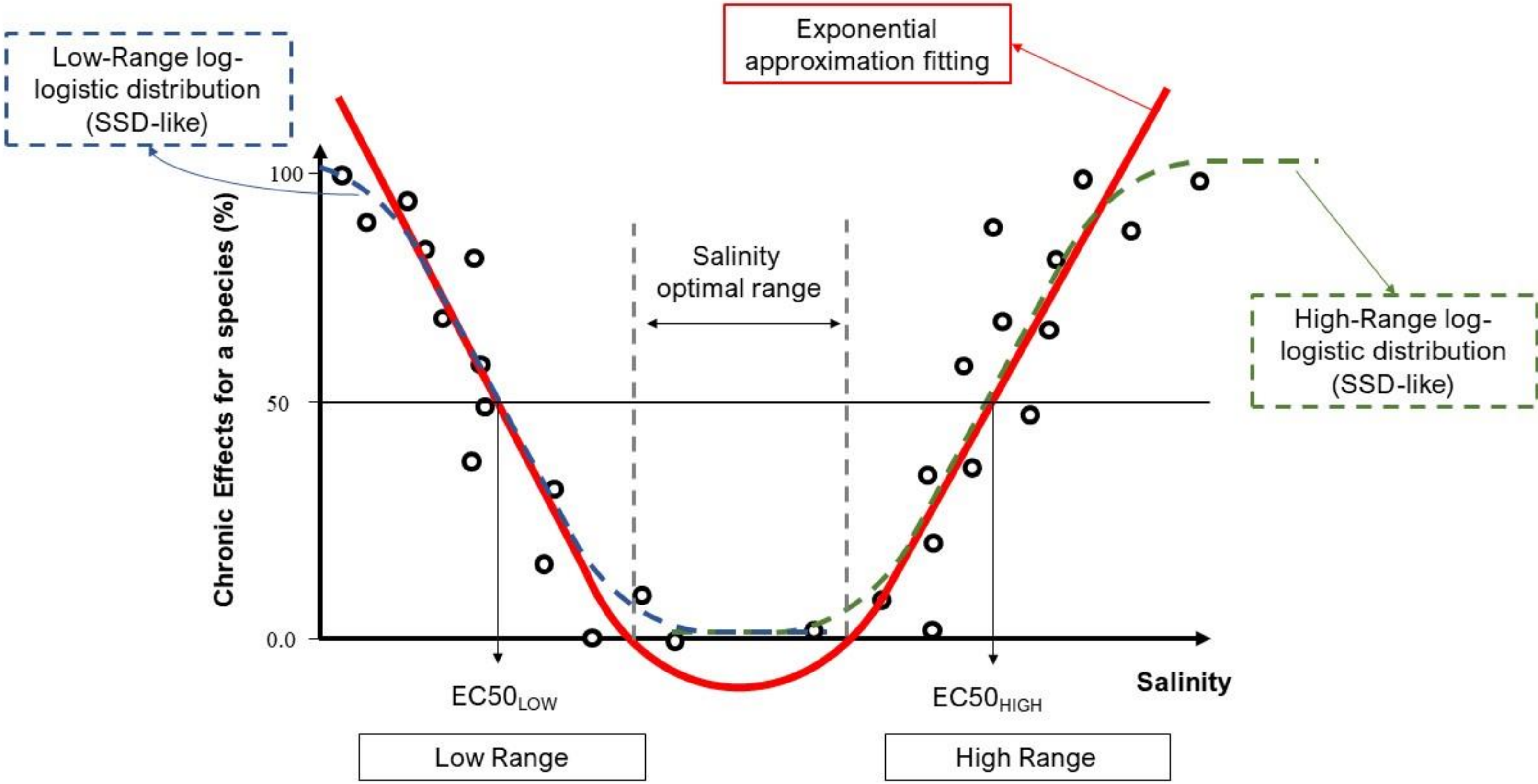


Figure S1. Quadratic approximation to quantify EC50s (power function).

SECTION SIII. Fate Factor calculation for *Arousa ría*

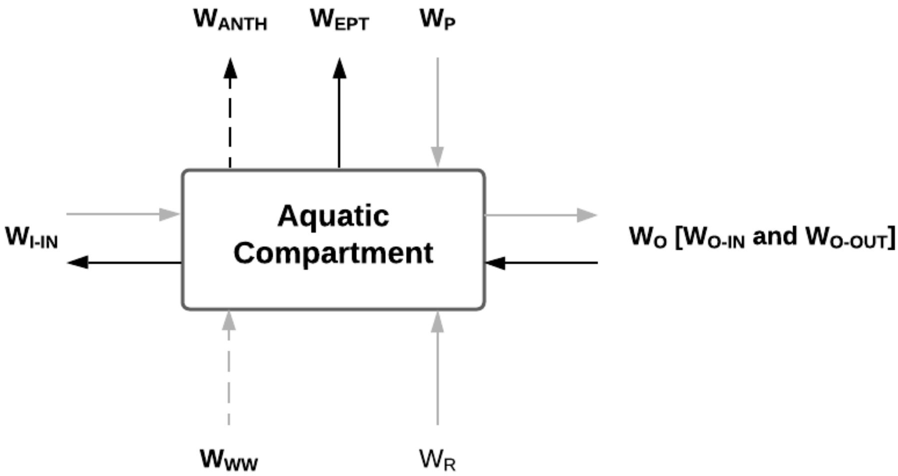


Figure S2. Scheme of the streams considered to solve the mass balances necessary to calculate the *Arousa* regional FF.

Table S2. Distribution of the shellfish and seafood captures along the year, calculated as an average of the monthly captures of three of the most representative captures (cockle, clam, and octopus)[3].

Month	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Distribution (%)	7.5	6.8	7.9	5.4	4.8	3.7	8.0	6.9	8.0	12.0	14.5	14.6

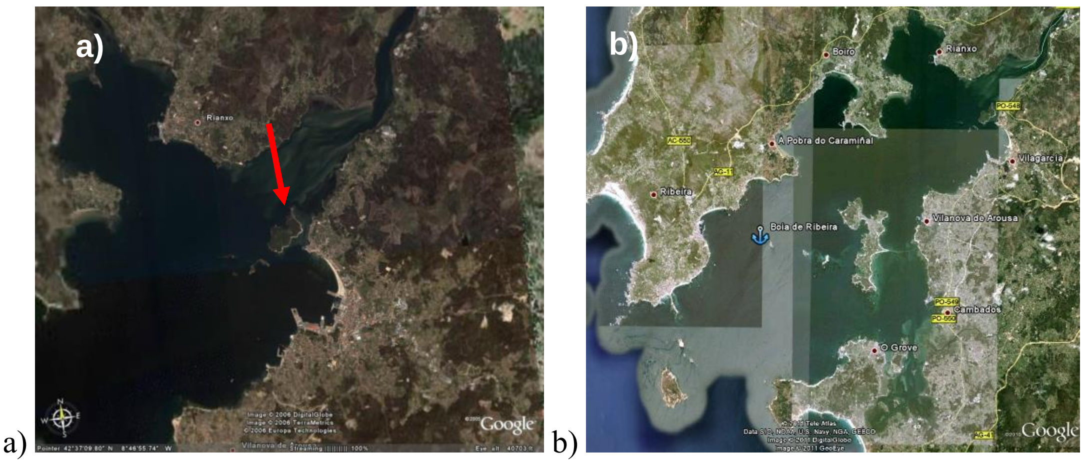


Figure S3. Location of the two buoys measuring salinity in *Arousa ría*. a) Cortegada buoy, location (-8° 47,03'; 42° 37,54') is marked with a red arrow. b) Ribeira buoy, location (-8° 56,87'; 42° 32,98') is marked with a blue anchor. Both pictures were provided by the Galician meteorological services[4].

Table S3. Quantification of system flows and the salt concentration of streams with yearly variable salinity for the time frame selected.

	YEAR							
	2011	2012	2013	2014	2015	2016	2017	2018
Stream	Stream flow (m^3/year)							
$W_{I\text{-}IN}$	$1.81\cdot10^{9}$	$1.28\cdot10^{9}$	$2.55\cdot10^{9}$	$3.16\cdot10^{9}$	$1.64\cdot10^{9}$	$2.96\cdot10^{9}$	$1.20\cdot10^{9}$	$2.20\cdot10^{9}$
W_{WW}	$1.06\cdot10^{8}$	$1.06\cdot10^{8}$	$1.08\cdot10^{8}$	$1.02\cdot10^{8}$	$1.07\cdot10^{8}$	$1.07\cdot10^{8}$	$1.03\cdot10^{8}$	$1.12\cdot10^{8}$
$W_{WW\text{-}SALT}$	$9.69\cdot10^{7}$	$9.68\cdot10^{7}$	$9.94\cdot10^{7}$	$9.43\cdot10^{7}$	$9.44\cdot10^{7}$	$9.45\cdot10^{7}$	$9.41\cdot10^{7}$	$9.42\cdot10^{7}$
$W_{WW\text{-}FRESH}$	$8.89\cdot10^{6}$	$9.33\cdot10^{6}$	$8.29\cdot10^{6}$	$7.77\cdot10^{6}$	$1.25\cdot10^{7}$	$1.26\cdot10^{7}$	$8.39\cdot10^{6}$	$1.78\cdot10^{7}$
W_{ANTH}	$7.27\cdot10^{7}$	$7.26\cdot10^{7}$	$7.45\cdot10^{7}$	$7.07\cdot10^{7}$	$7.08\cdot10^{7}$	$7.09\cdot10^{7}$	$7.06\cdot10^{7}$	$7.07\cdot10^{7}$
W_{EPT}	$9.37\cdot10^{6}$	$9.58\cdot10^{6}$	$4.75\cdot10^{6}$	$4.86\cdot10^{6}$	$5.22\cdot10^{6}$	$4.97\cdot10^{6}$	$5.31\cdot10^{6}$	$4.62\cdot10^{6}$
W_{P}	$2.42\cdot10^{8}$	$2.82\cdot10^{8}$	$3.86\cdot10^{8}$	$4.70\cdot10^{8}$	$2.56\cdot10^{8}$	$3.39\cdot10^{8}$	$2.24\cdot10^{8}$	$3.40\cdot10^{8}$
W_{R}	$1.72\cdot10^{8}$	$1.72\cdot10^{8}$	$1.72\cdot10^{8}$	$1.72\cdot10^{8}$	$1.72\cdot10^{8}$	$1.72\cdot10^{8}$	$1.72\cdot10^{8}$	$1.72\cdot10^{8}$
$W_{O\text{-}IN}$	$9.69\cdot10^{9}$	$8.94\cdot10^{9}$	$1.24\cdot10^{10}$	$9.84\cdot10^{9}$	$6.75\cdot10^{9}$	$1.06\cdot10^{10}$	$7.97\cdot10^{9}$	$5.09\cdot10^{9}$
$W_{O\text{-}OUT}$	$1.19\cdot10^{10}$	$1.07\cdot10^{10}$	$1.55\cdot10^{10}$	$1.36\cdot10^{10}$	$8.81\cdot10^{10}$	$1.41\cdot10^{10}$	$9.56\cdot10^{9}$	$7.80\cdot10^{9}$
$\mathbf{W_{IN}}$	$\mathbf{1.21\cdot10^{10}}$	$\mathbf{1.08\cdot10^{10}}$	$\mathbf{1.56\cdot10^{10}}$	$\mathbf{1.37\cdot10^{10}}$	$\mathbf{8.92\cdot10^{9}}$	$\mathbf{1.42\cdot10^{10}}$	$\mathbf{9.66\cdot10^{9}}$	$\mathbf{7.92\cdot10^{9}}$
$\mathbf{W_{OUT}}$	$\mathbf{1.20\cdot10^{10}}$	$\mathbf{1.07\cdot10^{10}}$	$\mathbf{1.56\cdot10^{10}}$	$\mathbf{1.37\cdot10^{10}}$	$\mathbf{8.88\cdot10^{9}}$	$\mathbf{1.42\cdot10^{10}}$	$\mathbf{9.63\cdot10^{9}}$	$\mathbf{7.88\cdot10^{9}}$
	Salinity (kg/m^3)							
$S_{WW\text{-}SALT}$	22.75	23.01	21.39	20.67	20.67	21.94	22.93	18.03
$S_{O\text{-}OUT}$	30.17	30.52	28.35	27.40	27.40	29.08	30.40	23.88
	Corrected value of $W_{O\text{-}OUT}$ ($W^*_{O\text{-}OUT}$)							
$W^*_{O\text{-}OUT}$	$1.20\cdot10^{10}$	$1.07\cdot10^{10}$	$1.56\cdot10^{10}$	$1.37\cdot10^{10}$	$8.84\cdot10^{10}$	$1.41\cdot10^{10}$	$9.59\cdot10^{9}$	$7.95\cdot10^{9}$

Due to the quantification procedure (solving mass balances for a situation as natural as possible and then summing the anthropogenic flows, where $W_{WW} > W_{ANTH}$), the total inlet flow is sometimes slightly higher than the total outlet flow ($W_{IN}>W_{OUT}$, see Table S3). Therefore, $W_{O\text{-}OUT}$ was recalculated monthly ($W^*_{O\text{-}OUT}$) to fit the steady state assumption ($W_{IN}=W_{OUT}$).

To calculate $W^*_{O\text{-}OUT}$, the total inlet and outlet flows (W_{IN} and W_{OUT}, respectively) are calculated summing each stream of Fig. S2 (being anthropogenic also included). At this point, as the volume of wastewater is higher than the withdrawals, $W_{IN} > W_{OUT}$. Therefore, $W_{O\text{-}OUT}$ was recalculated monthly to fit steady state assumption according to Eq. (S1).

$$W^*_{O-OUT} = W_{WW} + W_R + W_{I-IN} + W_{O-IN} - W_{EPT} - W_{ANTH} \quad \text{(S1)}$$

Finally, to quantify the FF, F_{IN} and F_{OUT} are calculated as stablished in Eq. (4), where *Arousa ría* salinity ($\bar{S}$) was considered as seasonal or yearly averages. Finally, as ocean height varies widely due to the tidal (≈ 5 m), the volume of the estuary also changes seasonally and yearly. To acknowledge this, average volume (4.34 km^3 of water) and area (230 km^2) of *Arousa ría*[5] was used to estimate an average depth of 18.9 m. Then, data of sea height variability (monthly averages) were directly taken from the buoy located in Vilagarcía de Arousa[6] (depth = 2.23 ± 0.09 m). Monthly data of sea height were used to estimate the proportion in which depth deviated from the average, and that proportion was used to estimate volume variations (considering a height of 18.9 m). Finally, data were processed to obtain seasonal and yearly volume averages.

SECTION SIV. Effect Factor calculation for Arousa *ría*

It is necessary to determine the cutoff point that will define the high and low effect factors, knowing that the concentration–response relationships for essential substances in aquatic environments might be modeled as a quadratic function. This means that there will be a range of concentration for which no effects will exist, or effects will be minimal. In this sense, the uncertainty of modeling a whole ecosystem can be very high, so we tested several approaches as shown below.

A) Optimal concentration point defined as the range of salt concentration where no effects are observed.

When plotting all the effect- related data (Figure S4), there is an intermediate concentration of NaCl for which no effects are observed (the experiments yielded a mortality of 0%). This range is 28 – 35 NaCl/L. The central point of this interval is 31.5 g/L, which is the value of the optimal (environmental) point of salt concentration derived after this estimation approach.

B) Optimal concentration point defined as the intersection point of two linear fittings defining low and high range of concentration.

Guided by the interval defined in the previous approach, it is possible to define a dot cloud for the high concentration, and another one for the low concentration (Figure S5). The cutoff point of these two linear fits is the value of the environmental concentration obtained by this estimation approach, i.e., 32.5 g NaCl/L. The need of previously establishing the boundary that divides low and high regions (in this case, the preliminary estimation based on ranges with no effect: 31.5 g/L) is in our opinion the main weakness of this approach. In fact, as the goal of this fitting is precisely to provide a value for this cutoff, the initial hypothesis for the fitting is already partially defining the result, so this approach is not recommended for being applied individually.

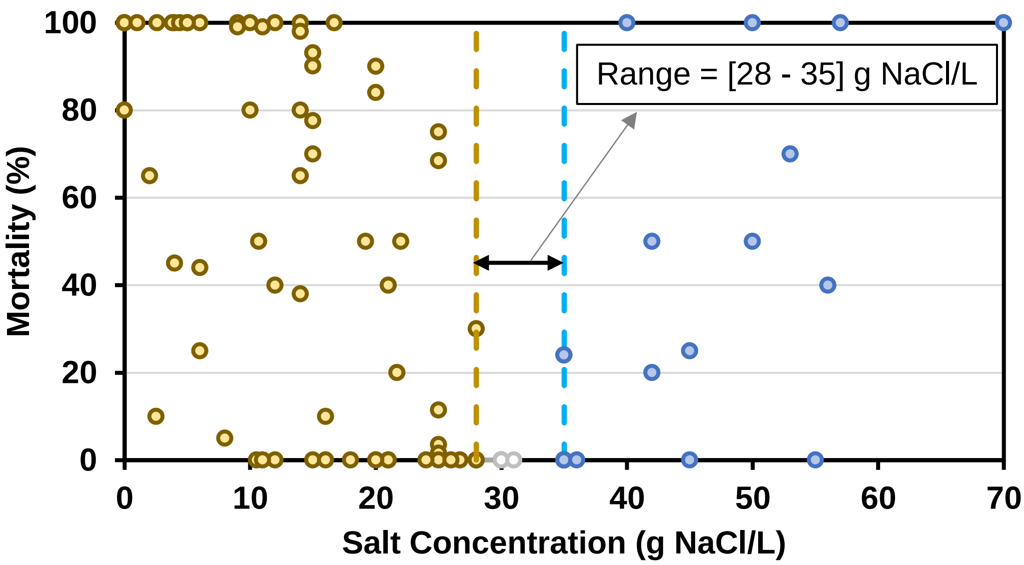


Figure S4. Approximation for the optimal (environmental) salinity of the aquatic ecosystem based on the observed range with no effects.

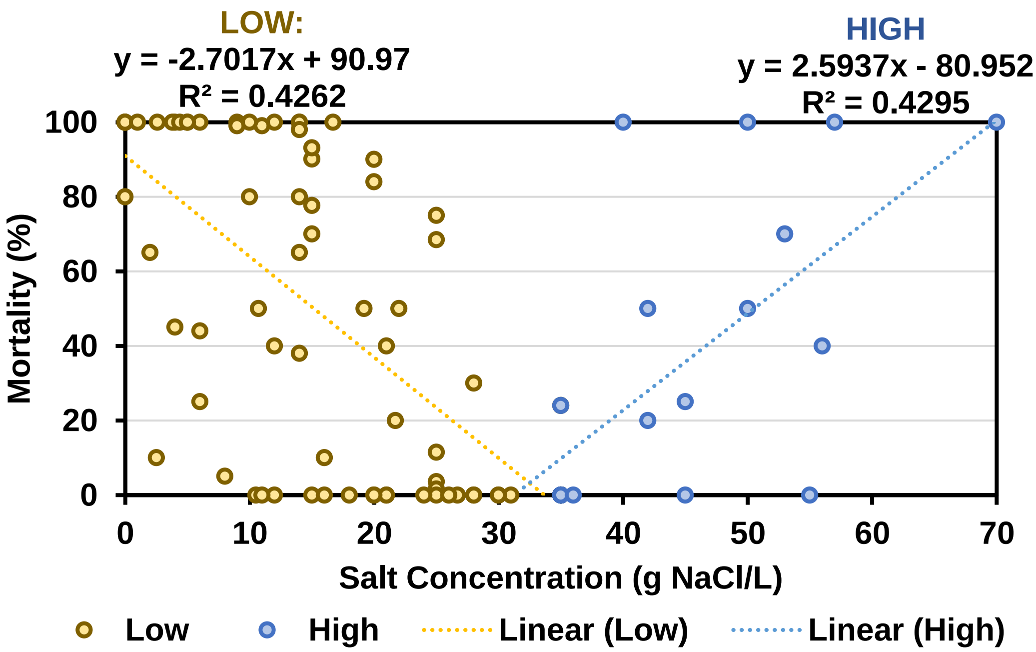


Figure S5. Approximation for the optimal (environmental) salinity of the aquatic ecosystem based on the cutoff point of two linear fittings.

C) Optimal concentration point defined as the minimum value of a quadratic function.

One of the core assumptions of the present work is that, for elemental substances, impacts cannot be measured considering a normal distribution, as it is necessary to acknowledge that different ecosystems will have a range of salinity that is optimal for the biota living in that environment, and therefore effects are observed below and above that range. Consequently, the application of a quadratic fitting appropriately represents the ecosystem under this approach (Figure S6), which yields a minimum value of 33.8 g NaCl/L.

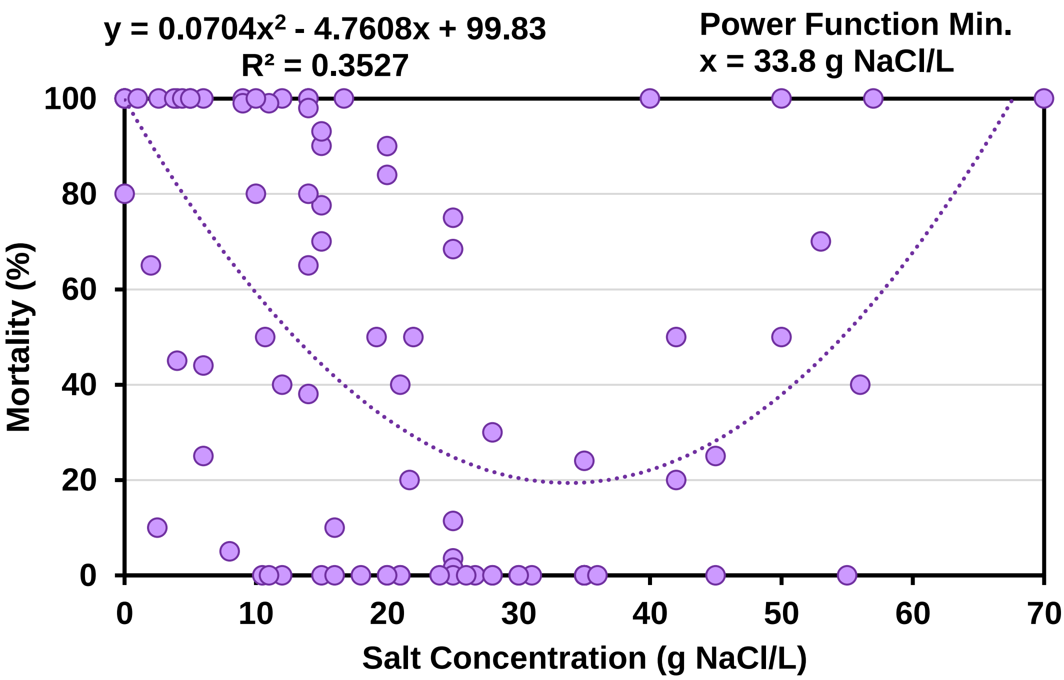


Figure S6. Approximation for the optimal (environmental) salinity of the aquatic ecosystem based on the minimum point of a quadratic fitting.

Although this strategy is useful because acknowledges the nature of the element studied (an essential substance, not a pollutant), it presents an important drawback. The minimum value obtained corresponds with an effect of 20%, while for the fitting to be completely accurate this effect should be around 0%. The reason behind this might be linked to the spatial approximation performed, as salt concentration varies along with depth as well as with the proximity to the river mouth. However, salt concentration of the estuary was considered as an average of measurements taken in several locations at several depths. This quadratic function disregards the fact that some marine species can move and redistribute, and that the species distribution might affect salinity tolerance (for example, biota living near the river mouth could better tolerate lower salinities). Therefore, that observed effect of 20% when applying the quadratic approach acknowledges the uncertainty linked to the chosen estimation strategy.

D) Optimal concentration point defined as a range of the minimal values for two opposite sigmoidal curves.

Sigmoidal curves define the classic Species Sensitivity Distribution (SSD) approach for concentration–response relationships in aquatic ecosystems, so it makes sense to have two opposite sigmoidal curves (for both positive and negative effects) where the optimal (environmental) value corresponds to the range where the two functions overlap (i.e., at their lower values). Note that the two curves do not have to be necessarily mirrored (Figure S7), as the effects of exposure to low and high salt concentrations do not necessary affect the ecosystems in the same way (which is also a drawback affecting the quadratic approximation C explained above).

For the double-sigmoidal approach (Figure S7), a range of 24 – 36 g NaCl/L, with a central point of 32.3 g/L (i.e., the optimal (environmental) concentration) is obtained. Also note that this approximation presents a similar problem than approximation B, as it also requires to previously define the range of data used for the high and for the low ranges (again fixed as the value obtained by approximation A: 31.5 g/L), so the outcome of this strategy is also partially pre-defined as occurred with the double linear fitting approach.

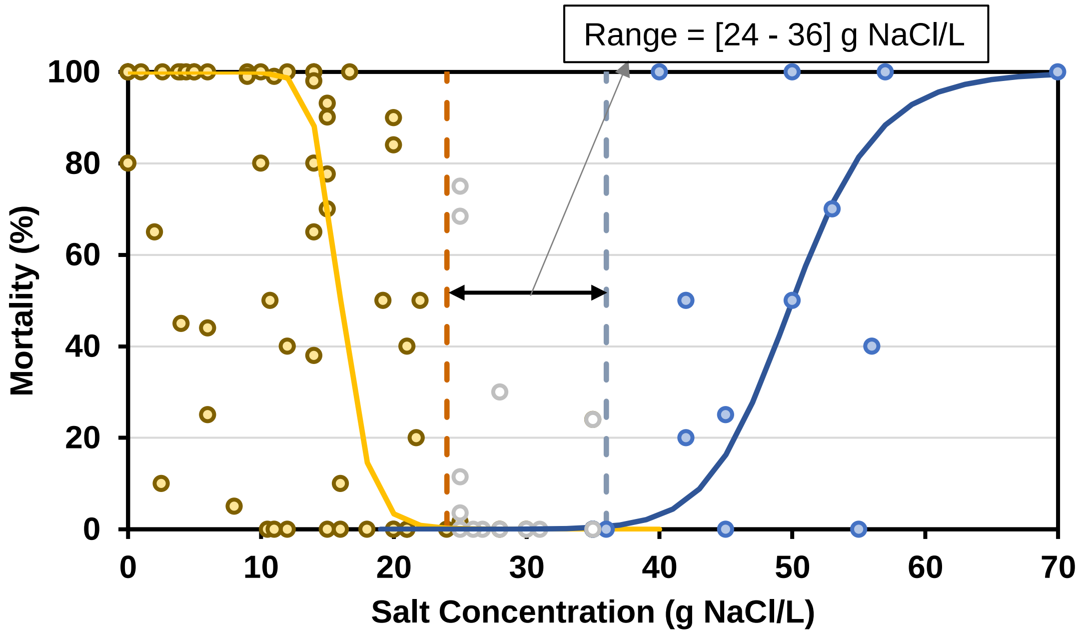
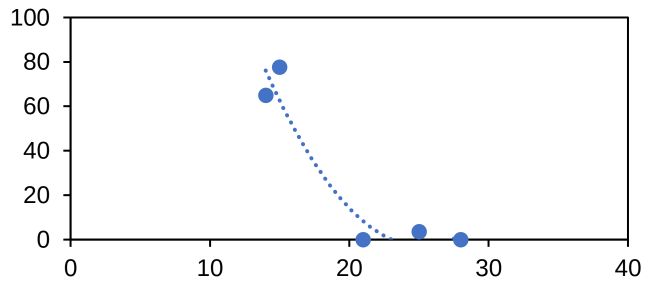
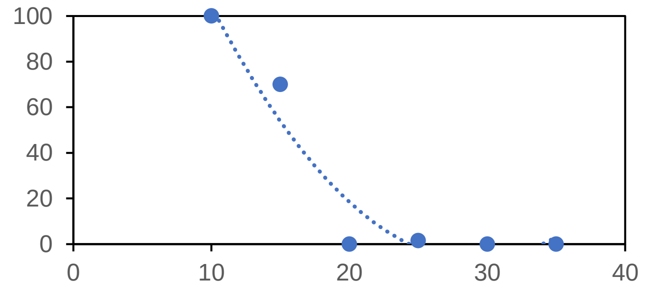


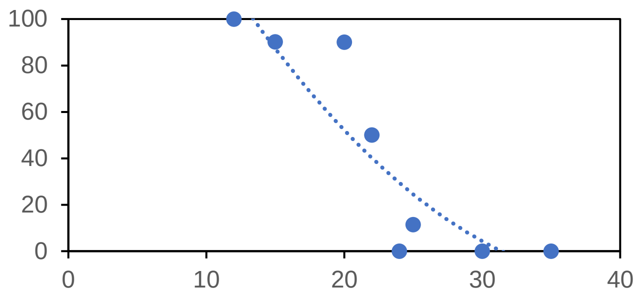
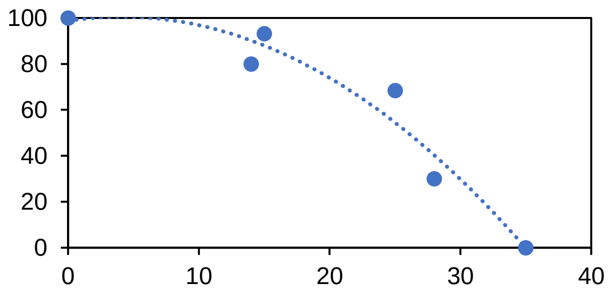
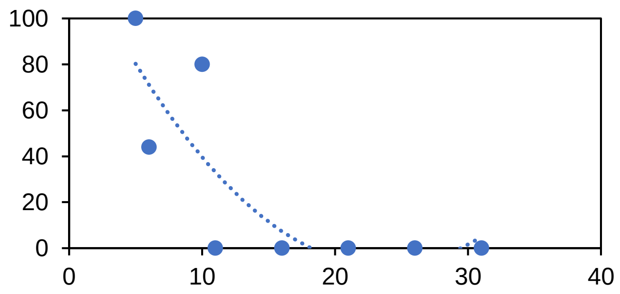
Figure S7. Approximation for the optimal (environmental) salinity of the aquatic ecosystem based on the coincident points of two sigmoidal curves.

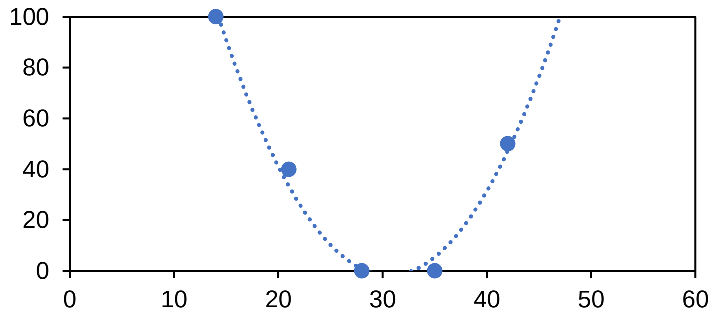
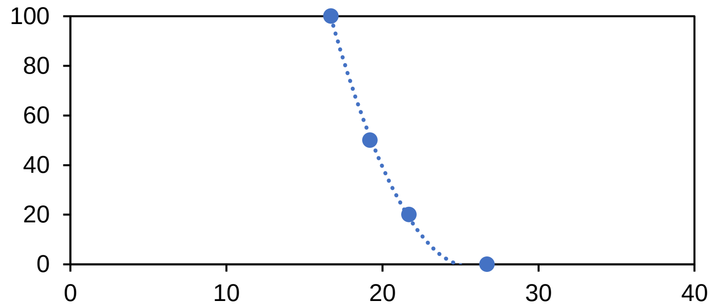
- **Optimal concentration point definition**

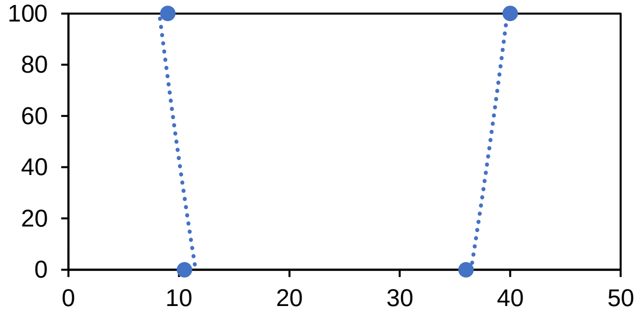
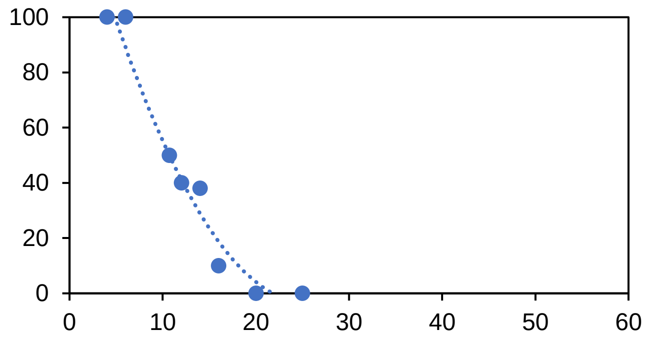
As observed, results might vary by applying each of the proposed approaches, and the recommendation is to test several approximations and generate an average optimal value out of this testing, acknowledging the uncertainty linked to this type of studies. For the present case, the average optimal (environmental) salt concentration is 31.9 ± 1.4 g NaCl/L, calculated as the average value brought by each proposed fitting. Therefore, this value will be the cutoff point to calculate the low and high effect factors.

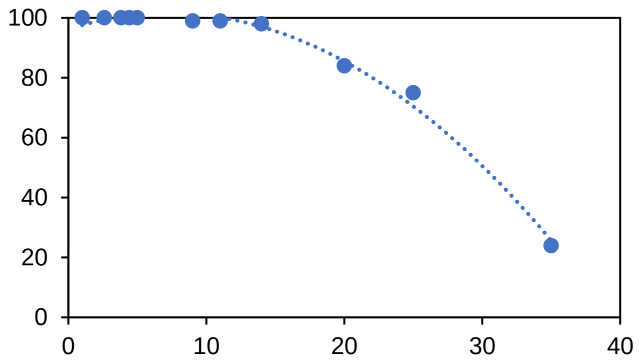
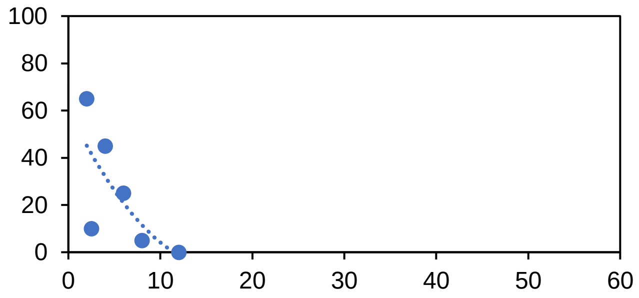
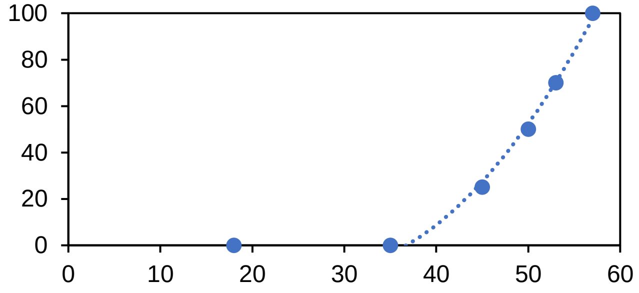
Table S4. Data used to calculate the EFs. For each graphic, the y-axis represents Mortality (%), and the x-axis represents the salt concentration. The literature from which data was acquired are indicated in the references section.

Species	Chronic data (Mortality (%) vs. Salt concentration (g/L))	Notes
Ruditapes philipinarium (Manila clam)[7,8]		Function: $y = 0.6275 \cdot x^2 - 31.653 \cdot x + 396.27$ $R^2 = 0.923$ $EC50_{LOW} = 16.0$ g/L, $EC50_{HIGH} = 34.4$ g/L
Ruditapes decussatus[7,9] (Grooved carpet shell)		Function: $y = 0.3027 \cdot x^2 - 17.668 \cdot x + 250.83$ $R^2 = 0.931$ $EC50_{LOW} = 15.5$ g/L, $EC50_{HIGH} = 42.9$ g/L

Cerastoderma edule (Common cockle)[7,10]		Function: $y = 0.1493 \cdot x^2 - 12.248 \cdot x + 237.42$ $R^2 = 0.803$ $EC50_{LOW}$ = 20.4 g/L, $EC50_{HIGH}$ = 61.7 g/L
Vanerupis corrugata[7,8] (Pullet carpet shell)		Function: $y = -0.1056 \cdot x^2 + 0.8701 \cdot x + 98.721$ $R^2 = 0.9434$ $EC50_{LOW}$ = 21.7 g/L To calculate $EC50_{HIGH}$, the inverse function was used, being: Function: $y_{HIGH} = (x - 30.7)^2$ $EC50_{LOW}$ = 37.8 g/L
Saccharina latissima[11,12] (Sea belt, brown algae)		Function: $y = 0.2485 \cdot x^2 - 11.842 \cdot x + 133.27$ $R^2 = 0.668$ $EC50_{LOW}$ = 8.6 g/L, $EC50_{HIGH}$ = 39.1 g/L

Diopatra neapolitana (Polychaete)[13]		The chronic data provided information for both ranges of the curve, fitting an exponential profile. Function: $y = 0.379 \cdot x^2 - 23.224 \cdot x + 354$ $R^2 = 0.987$ $EC50_{LOW}$ = 19.0 g/L, $EC50_{HIGH}$ = 42.3 g/L
Donax trunculus (Wedge clam)[14]		Function: $y = 1.2364 \cdot x^2 - 63.585 \cdot x + 816.52$ $R^2 = 0.999$ $EC50_{LOW}$ = 19.3 g/L, $EC50_{HIGH}$ = 32.1 g/L

Mytilus galloprovincialis (Mediterranean Mussel)[15]		Information provided by other studies reveal that the Mediterranean mussel adapts worse to salinities around 11 (non-lethal effects observed), but mortality only increases to 10%, while it adapts good for salinity of 37[16]. This is in concordance with the lethal effects observed for M. edulis (blue mussel, not found in Galicia), as mortality sharply increases for salt concentrations of about 9 and 40 g/L. Therefore, we assumed that both mytilids present the same salt tolerance. The chronic data provided information for both ranges of the curve, fitting an exponential profile. Function: $y = 1.074 \cdot x^2 - 51.534 \cdot x + 451.16$ $R^2 = 0.832$ $EC50_{LOW}$ = 9.8 g/L, $EC50_{HIGH}$ = 38.2 g/L
Scrobicularia plana[10] (Peppery furrow shell)		Function: $y = 0.2414 \cdot x^2 - 12.349 \cdot x + 154.57$ $R^2 = 0.966$ $EC50_{LOW}$ = 10.7 g/L, $EC50_{HIGH}$ = 40.4 g/L

Saccorhiza polyschides (Furbellow, brown algae)[17]		Function: $y = -0.1056 \cdot x^2 + 0.8701 \cdot x + 98.721$ $R^2 = 0.9434$ $EC50_{LOW} = 30.1$ g/L To calculate $EC50_{HIGH}$, the inverse function was used, being: Function: $y_{HIGH} = (x - 39.36) \cdot (x + 24.8)$ $EC50_{LOW} = 40.1$ g/L
Zostera noltei (Dwarf eelgrass, seagrass)[18,19]		The functions provided a better fitting if they were adjusted separately for each range. Functions: $y_{LOW} = 0.2402 \cdot x^2 - 8.003 \cdot x + 60.199$ $R^2 = 0.499$ $y_{HIGH} = 0.1249 \cdot x^2 - 6.8814 \cdot x + 84.254$ $R^2 = 0.996$ $EC50_{LOW} = 1.3$ g/L, $EC50_{HIGH} = 49.6$ g/L

SECTION SV. Data requirements and information sources for fate and effect factors and for the characterization factor application

- **FATE FACTOR**

- W_I ($W_{I\text{-}IN}$ and $W_{I\text{-}OUT}$) and W_O ($W_{O\text{-}IN}$ and $W_{O\text{-}OUT}$) refer to the main inlet and outlet stream, respectively, and the calculation of these streams recognize that possible infiltrations or returns can take place in the system. Some of these stream flows can be available through local governments websites and reports (for example, it is common that river flows are measured for monitoring and control). Nevertheless, some of these streams cannot be quantified (like oceanic flows), and mass balances (in steady state or transient) will be needed to estimate them.

- W_P and W_G represent the precipitations and the groundwater, respectively, and they are generally measured and provided by local administrations.

- W_{EPT} is the evaporation. Although some information can be found in the literature and in some meteorological databases, it is recommended to calculate this parameter using the references provided in the manuscript[20,21] and that are low data demanding.

- W_R is the runoff. If no specific datum is available, general databases can be employed[22].

- W_{ANTH} and W_{WW} are the anthropogenic outflows and inflows in the system, respectively. The exact values of these parameters are hard to estimate. In this case, the availability of data is determined by the control and monitoring of the effluents and of the agricultural activity in the studied area. If data are not available, estimations can be performed considering the local characteristics of the studied system. For example, if irrigation is an important activity, the amount of water used for this purpose can be estimated by knowing the main crops cultivated and the water demand of each of them, as previously performed in other works[23,24].

- The salinity of each stream only can be obtained by direct measurements, mass balances, or specific studies. However, it can be estimated using the values provided in Table S1.

- **EFFECT FACTOR**

Data gathering for effect factor calculation is a heavy task. The first step is to identify representative species for the aquatic ecosystem studied. Some scientific databases, like the World Register of Marine Species (WORMS) can be used as a starting point to determine the most common species. After that, other search engines, like Scopus, can be employed to search for studies where the tolerance of the representative species to different salinities is tested. A minimum number of three species from three different trophic levels is recommended.

- **CHARACTERISATION FACTOR APPLICATION**

Ideally, the LCA practitioner shall know the salt concentration of the environment where the salt release occurs in order to apply either CF_{LOW} or CF_{HIGH}. However, this is rarely the case. In such cases, average estimates depending on e.g. the type of water body (see Table S1) and spatial salinity datasets such as GEMstat[25], which contains more than 3.5 million measurements of salt concentration for rivers, lakes, reservoirs, wetlands and groundwater systems worldwide, can be used to guide the selection of the CF (low or high) to apply.

References

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