ELECTRONIC SUPPLEMENTARY INFORMATION:

Techno-economic analysis of capacitive and intercalative water deionization

Michael Metzger,*[a] Münir Besli,[a] Saravanan Kuppan,[a] Sondra Hellstrom,[a] Soo Kim,[b] Elias Sebti,[c] Chinmayee V. Subban,[c] and Jake Christensen[a]

[a] *Robert Bosch LLC, Research and Technology Center, Sunnyvale, California 94085, United States*

[b] *Robert Bosch LLC, Research and Technology Center, Cambridge, Massachusetts 02139, United States*

[c] *Energy Storage and Distributed Resources Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States*

Supplementary Materials

1. Intercalation module design and operation

Depending on the requirements, an IDI stack can be designed in monopolar arrangement (favors high current since cells are in parallel and individual currents add up, see Fig. S1a) or bipolar arrangement (favors high voltage since cells are in series and individual voltages add up, see Fig. S1b). A counter-flow design with opposite flow directions for the two water streams could lead to better reactant distribution than co-flow. In Fig. S1 and Fig. S2 we assume counter-flow without evaluating it in detail, since stack optimization is not in the scope of this analysis. As nomenclature for the "state of charge" (SOC) we adopt the convention for batteries and refer to intercalation electrodes as being at a "high SOC" when they are mostly empty (salt cations deintercalated and vacancies in the intercalation host lattice). Vice versa, they are at a "low SOC" when they are mostly filled (salt cations intercalated).

Since the IDI concept has only recently been introduced in literature[2–4] and is more complex than the well-described mCDI concept, we want to provide a brief description of the operating principle of an IDI module (see Fig. S2). During charge (Fig. S2a) feed water of salt concentration c_{in} flows at a velocity $\dot{V}_{charge}$ through a water distributor at stack inlet (similar to a gas distribution manifold in a fuel cell stack) and is directed to the negatively polarized electrodes in the stack (indicated by "-" sign). Simultaneously, feed water is also directed to the positively polarized electrodes (marked with a "+" sign) at a lower flow rate $\dot{V}_{brine}$ ($\dot{V}_{brine} < \dot{V}_{charge}$ in order to achieve the water recovery target).

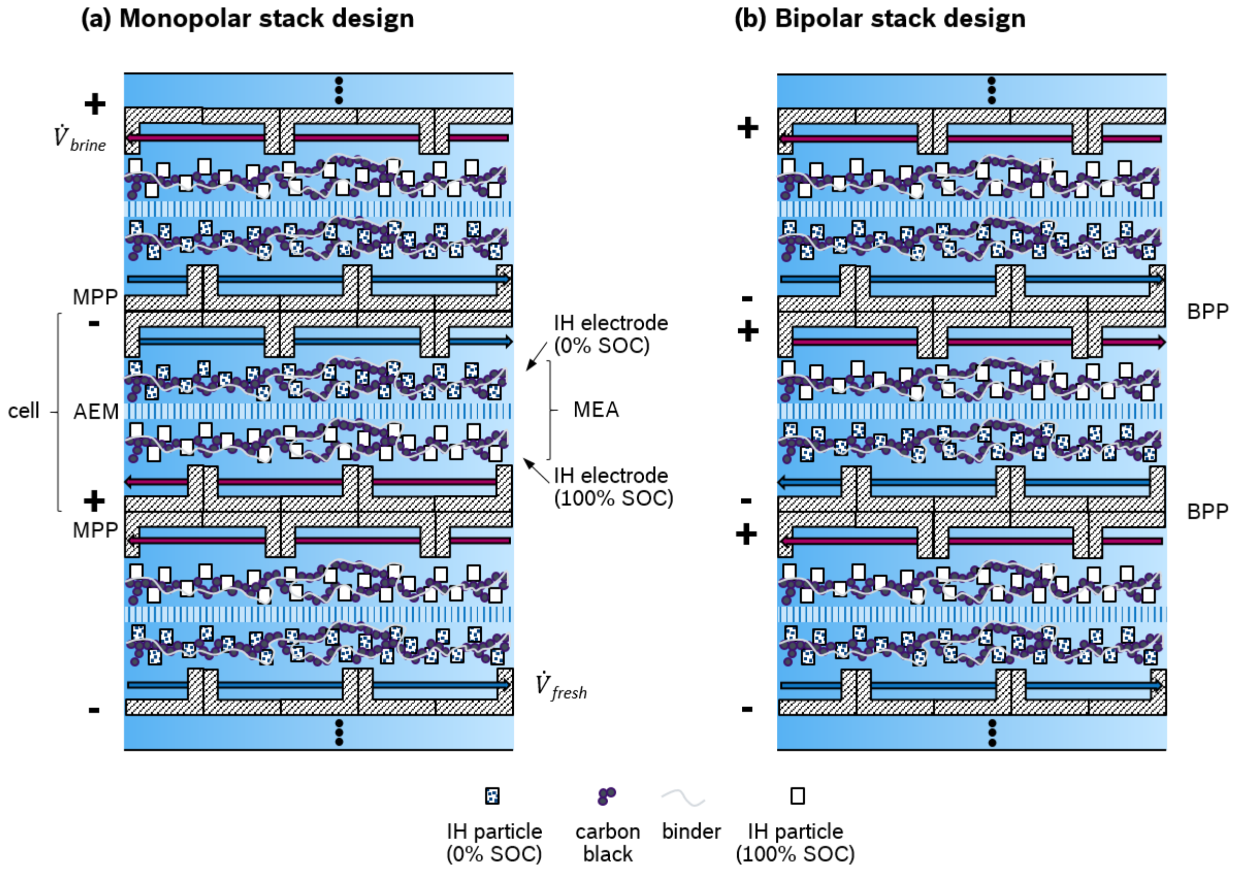

Fig. S1. Design of an electrode stack in a module for intercalative water deionization (IDI) in monopolar (a) and bipolar (b) arrangement. Monopolar design favors high current (cells in parallel, currents add up), bipolar design favors high voltage operation (cells in series, voltages add up). Blue and red arrows indicate freshwater streams and brine streams, respectively, in counter-flow configuration. Intercalation electrodes consist of intercalation host (IH) material, carbon black and binder. Depending on the polarity of the mono-/bipolar plates (MPPs/BPPs) the IH electrodes are either at low state of charge (SOC, salt cations intercalated) or high SOC (cation vacancies in the IH lattice). Anion exchange membranes (AEM) separate the IH electrodes and permit anions to cross between the water streams. A pair of IH electrodes and AEM can be called “membrane electrode assembly” (MEA) in analogy to the respective component in a fuel cell stack. The repeating unit that comprises the stack is labeled “cell”.

The negatively polarized electrodes get charged by intercalating cations from the feed water stream, corresponding counter anions cross the AEM to maintain charge neutrality, and pair with cations expelled from the positively polarized electrode. The resultant freshwater stream ($c_{out} << c_{in}$) can be directly applied or collected for the intended use, while the brine ($c_{brine} >> c_{in}$) has to be drained or collected for disposal. In the subsequent half-cycle, the polarity of the electrodes is reversed, e.g., by drawing a current from the stack, the flow rates are adjusted and what originally was the freshwater stream now becomes the brine stream and vice versa. The IDI concept allows to generate a continuous freshwater output in contrast to mCDI and HCDI, where a single water stream alternately transports either freshwater or brine. Accordingly, IDI would in principle not require a storage tank, as freshwater can be uninterruptedly provided on demand.

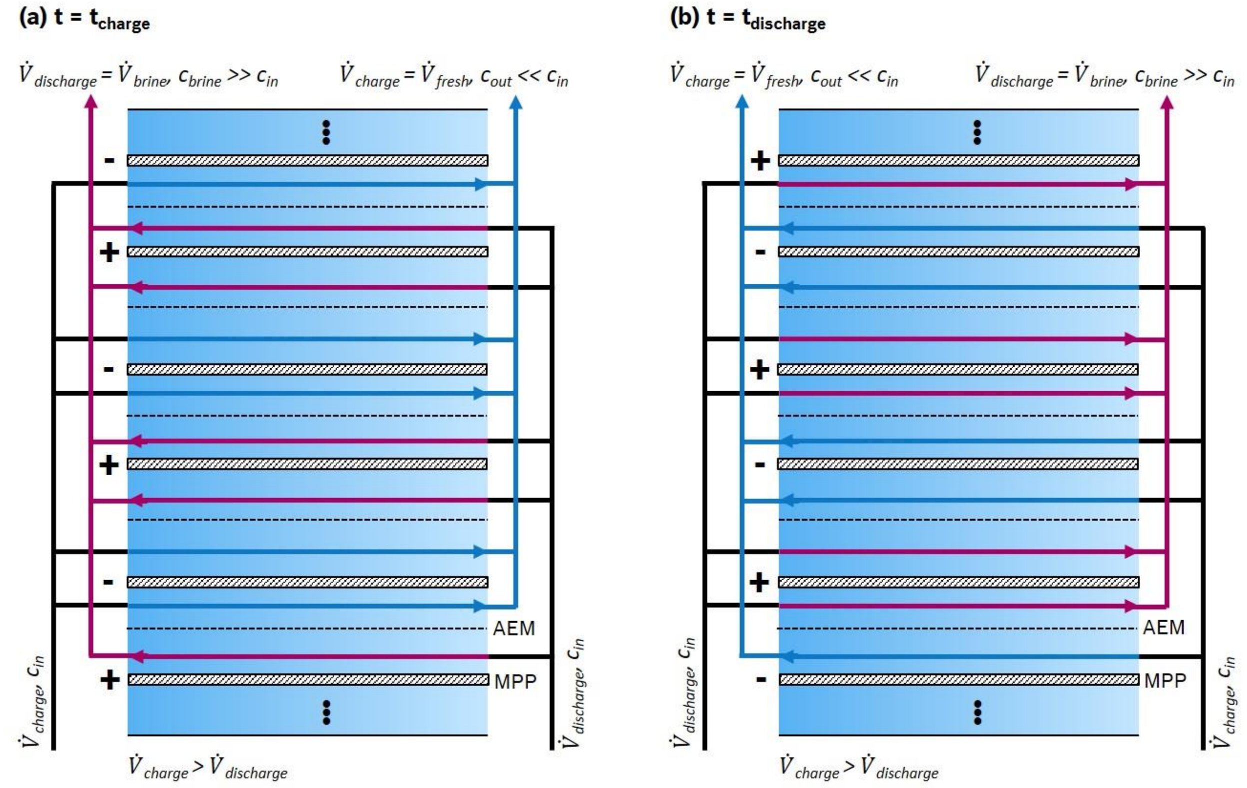

Fig. S2. IDI module operation in monopolar configuration with black arrows indicating feed water, blue arrows indicating freshwater streams and red arrows indicating brine streams. Flows are sketched in counter-flow design. Depending on the electrode polarity, i.e., whether current is applied to or drawn from the stack, either freshwater is directed to the right-hand exhaust ($c_{out} << c_{in}$) and brine to the left-hand exhaust ($c_{brine} >> c_{in}$) or vice versa. In order to achieve the water recovery target the flow rate of the brine water stream is lower than the flow rate of the freshwater stream ($\dot{V}_{discharge} = \dot{V}_{brine} < \dot{V}_{fresh} = \dot{V}_{charge}$).

2. Complete deduction of performance metrics

Based on the parameters we introduce in the main article, we calculate several performance metrics that can be grouped into the categories (i) cycle time and water volumes, (ii) salt load and specific capacity, (iii) number of cells and C-rates, (iv) total surface area and residence times, (v) module volume and mass, as well as (vi) module cost. The following section shows the equations for the IDI concept, calculations for mCDI and HCDI follow the same principle (see section 4 of the SI for the full set of equations incl. conversion factors).

Cycle time and water volumes – The cycle time is defined as the total duration of the charge and discharge step. We choose a symmetric cycle with a typical duration of 4 min (2 min charge, 2 min discharge).

$$t_{cyc} = t_{charge} + t_{discharge} \tag{1}$$

For the analysis at hand, we select the same cycle time for, both, the capacitive and intercalative concept. The volume of freshwater produced in one cycle can be calculated from the charge time and the corresponding flow rate.

$$V_{fresh,cyc} = t_{charge} \cdot \dot{V_{charge}} \cdot 2 \tag{2}$$

In order to achieve the water recovery target, the flow rate during discharge is reduced from $\dot{V}_{charge}$ to $\dot{V}_{discharge}$.

$$\dot{V_{discharge}} = \frac{\left(\dot{V_{charge}} \cdot t_{charge}\right)}{t_{discharge}} \cdot (1 - WR) \tag{3}$$

Given a certain water throughput per day, V_{day}, we can derive the required number of cycles in a given day.

$$n_{cyc,day} = \frac{\frac{V_{day} \cdot WR}{V_{fresh,cyc}}}{t_{cyc} \cdot \dot{V_{charge}} \cdot 2} \tag{4}$$

With the example parameters in this study, the device is balanced such that it performs ~15 cycles a day, each treating ~6 liters of water. Note that IDI produces freshwater in the charge *and* discharge step, such that the freshwater output per cycle is twice as high as for mCDI or HCDI at the same flow rate. The total run time is ~1 h/day. Extrapolated to a device life of 10 years, the cycle life requirement would be around 54,750 cycles and the total run time would amount to ~3,650 h. The device would deliver 90 liters of freshwater a day, with 10 liters/day of brine. A comparable mCDI or HCDI system would do twice as many cycles over its lifetime.

Salt load and specific capacity – The fundamental quantity that determines the design point of a water deionization systems is the salt load that needs to be removed in any given half-cycle, i.e., the grams of salt when expressed in gravimetric terms or the Coulombs of charge associated with the salt ions when expressed in electronic terms. In order to derive this fundamental quantity, we have to look at salt concentrations, c, and flow rates, $\dot{V}$. The salt load increases the higher the delta in salt concertation, Δc, between influent and effluent water streams.

$$\Delta c = c_{in} - c_{out} \tag{5}$$

Here, the salt concentration of the influent and effluent water is c_{in} and c_{out}, respectively. Given the concentrations in Table I, a salt removal efficiency, e_{cyc}^{salt}, of 91% is achieved.

$$e_{cyc}^{salt} = 1 - \frac{c_{out}}{c_{in}} \tag{6}$$

The salt load also increases the higher the flow rate during the ion removal step (charge). The gravimetric salt load per half-cycle is defined as follows.

$$m_{cyc}^{salt} = \Delta c \cdot t_{charge} \cdot \dot{V}_{charge} \tag{7}$$

In order to express the salt load in electronic terms we have to take into account the valence and molecular weight of the salt species.

$$Q_{cyc}^{salt} = \frac{m_{cyc}^{salt}}{M} \cdot z \cdot F \tag{8}$$

As we can see from Equations 7 and 8, the salt load per half-cycle, Q_{cyc}^{salt}, depends on the delta in TDS as well as charge time, flow rate and type of ion (valence and molecular weight). A current, I_{charge}, flows across the deionization stack when the salt load is removed within a given half-cycle.

$$I_{charge} = \frac{\Lambda^{-1} \cdot Q_{cyc}^{salt}}{t_{charge}} \tag{9}$$

Since the charge efficiency, Λ, is always below unity (see Table I), a higher current than what would be derived just from salt load and charge time is required to remove the entire salt load in the given time. During discharge a current of opposite sign is drawn from the deionization stack. Ultimately, the salt load will need to be balanced by the electrode capacity. We can calculate the specific capacity of the intercalation electrode, $\hat{C}_{IH,SIC}$, from the respective salt intercalation capacity (SIC_{IH} in $\mathrm{mg_{salt}/g_{IH}}$, see Table II). The specific electrode capacity is given in units of $\mathrm{mAh/g_{IH}}$.

$$\hat{C}_{IH,SIC} = \frac{SIC_{IH}}{M} \cdot z \cdot F \tag{10}$$

Number of cells and C-rates – For IDI, the term "cell" refers to a pair of positive and negative electrodes separated by an ion exchange membrane and enclosed on both sides with the respective half of a flow plate (see Fig. S1). For mCDI and HCDI, which do not require separation of water streams, it is simply a pair of electrodes that is separated by a porous, electrically insulating separator sheet. In order to calculate the required number of cells for a module that fulfills the parameter targets in Table I-III (see main article), we first need to calculate the electrode volume from electrode area, A_{el}, and thickness, $d_{el,IH}$.

$$V_{el,IH} = A_{el} \cdot d_{el,IH} \tag{11}$$

The active material mass can then be deduced using electrode porosity, active material volume fraction and density.

$$m_{el,IH} = V_{el,IH} \cdot (1 - P_{el,IH}) \cdot \varepsilon_{IH} \cdot \rho_{IH} \tag{12}$$

Using the previously derived specific capacity of the intercalation host material (see Equation 10), we can calculate the electrode capacity.

$$C_{el,IH} = m_{el,IH} \cdot \hat{C}_{IH,SIC} \tag{13}$$

The number of cells then follows from the salt load per half-cycle, Q_{cyc}^{salt}, and the limited utilization, χ, of the intercalation electrode.

$$n_{cells} = \frac{Q_{cyc}^{salt}}{\chi \cdot C_{el,IH}} \tag{14}$$

From Equations 11-14 it becomes obvious that the number of cells is inversely proportional to the active geometric area of the electrodes. For the analysis at hand we assume an active area of 100 cm^2. For further analysis it is practical to break down the salt load that each electrode pair in the module has to carry.

$$Q_{cyc,el}^{salt} = \frac{Q_{cyc}^{salt}}{n_{cells}} \tag{15}$$

Fig. S3 shows that a mCDI module removing a salt load of ~700 mAh/half-cycle would require ~250 cells with 100 cm^2 each. The same number of cells would be required for HCDI, since the capacity per cell in HCDI is limited by the capacitive electrode (intercalated capacity in PBA electrode cannot exceed adsorbed capacity at carbon electrode due to charge neutrality). In contrast, IDI can utilize the full potential of the intercalation host's higher intrinsic salt removal capacity and thus only requires ~65 cells with 100 cm^2 each to remove the same amount of charge per half-cycle.

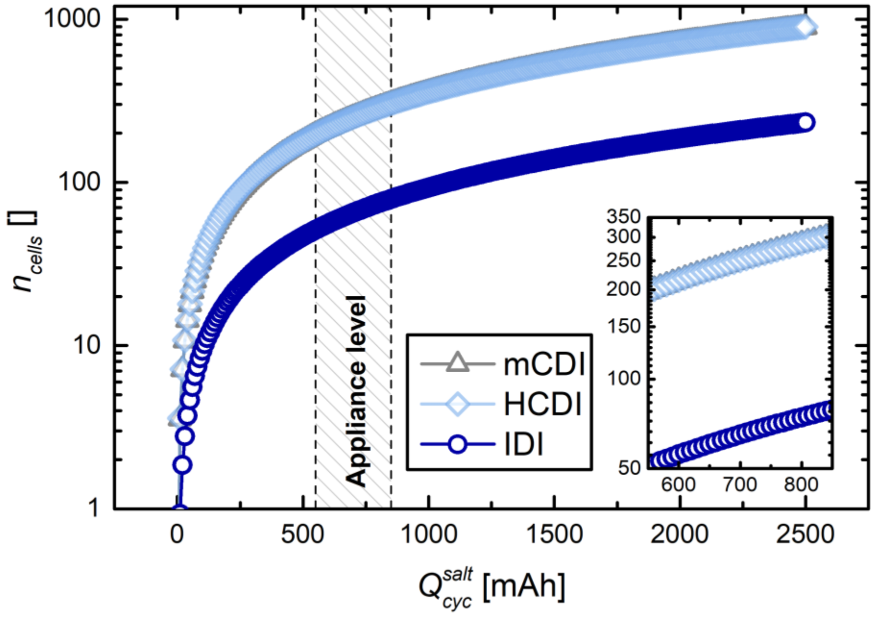

Fig. S3. Required number of cells as a function of salt load per half-cycle. Since the data is presented on the basis of salt load, it is applicable for different combinations of salt concentrations, flow rates and cycle times. Dashed area and inset show typical parameters for appliance level modules.

Analogous to batteries, we can define a C-rate for the intercalation electrodes. "C-rate" refers to the inverse time in hours to complete a full charge or discharge (xC means full charge takes 1/x hours). It implies a current density that is needed to achieve the desired salt removal within the half-cycle time. For IDI the C-rate is calculated by comparing the charge that is associated with the salt load per half-cycle and electrode, $Q_{cyc,el}^{salt}$, with the electrode capacity $C_{el,IH}$ and referencing it to the half-cycle time (charge or discharge time) in hours.

$$r_{charge} = \frac{\frac{Q_{cyc,el}^{salt}}{C_{el,IH}}}{\frac{t_{charge}}{60}} \tag{16}$$

For the inputs in Table I-III, the resultant C-rate during charge and discharge (we assumed symmetric cycles) is 25.5C. Prussian blue analogs have been reported to possess outstanding rate capability. In their HCDI system with activated carbon and $Fe_2(CN)_6$, Guo et al. demonstrated high salt removal capacities of 50 and 30 mg/g at C-rates of 20C and 40C, respectively.[5]

Total surface area and residence times – Given mCDIs problems with scaling, fouling and oxidation the total microscopic surface area available in the device is of high importance. The total active material surface area in the module directly follows from the active material mass in the electrode (see Equation 12), BET surface area of the material (see Table III) and the number of cells per module.

$$A_{mod,IH}^{BET} = 2 \cdot m_{el,IH} \cdot A_{IH}^{BET} \cdot n_{cells} \tag{17}$$

Fig. S4 compares total surface area per module for mCDI, HCDI, and IDI. The calculation of A_{mod}^{BET} is similar for mCDI and IDI, but since the BET surface area of the activated carbon used for the capacitive electrodes is more than 10x larger than the BET surface area of PBA (here, 600 vs. 52 m^2/g, see Table III), the resultant surface area in mCDI and HCDI modules is much larger than for IDI.

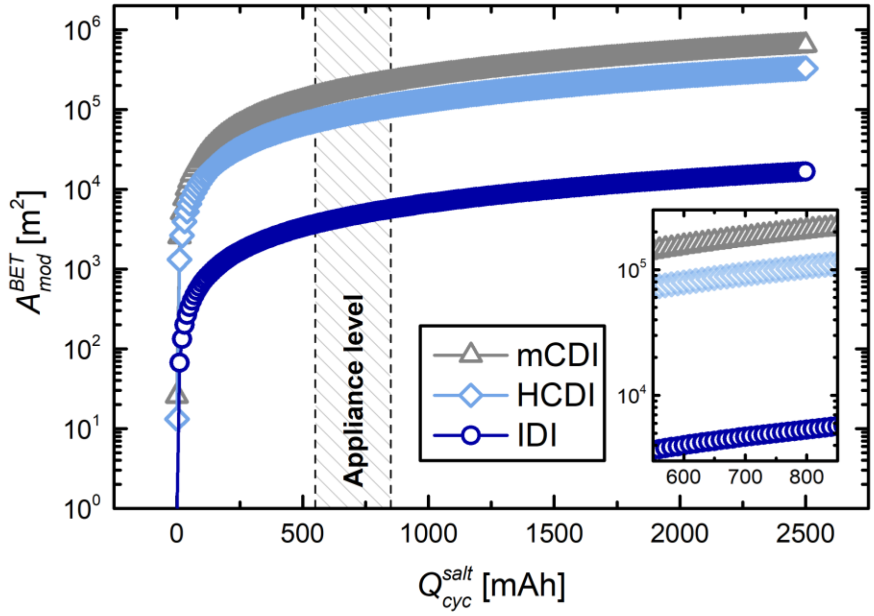

Fig. S4. Total surface area of active material in module as a function of salt load per half-cycle. Since the data is presented on the basis of salt load, it is applicable for different combinations of salt concentrations, flow rates and cycle times. Dashed area and inset show typical parameters for appliance level modules.

Similar to the interaction area, the interaction time, i.e., the residence time of water in the module could be correlated to cell aging. If contaminants have a long residence time in the device the chance of detrimental reactions with cell components might be higher. To calculate the residence time, we first need to derive the void volume that is filled with water during operation. For the intercalation electrodes, the electrode void volume is given by electrode volume and porosity.

$$V_{el,IH}^{void} = V_{el,IH} \cdot P_{el,IH} \tag{18}$$

The void volume fraction of channels in the flow plate, ε_{FP}, allows to calculate the flow plate void volume.

$$V_{FP}^{void} = A_{el} \cdot d_{BPP} \cdot \varepsilon_{FP} \tag{19}$$

As can be seen from Fig. S1, these are the only void volumes to be filled by water in the IDI device concept, assuming negligible porosity of ion exchange membranes (IEMs). Thus, the residence time during charge or discharge can be derived by considering the respective flow rate ($\dot{V}_{charge}$ or $\dot{V}_{brine}$) and the number of cells.

$$t_{res,charge} = \frac{\left(2 \cdot V_{el,IH}^{void} + V_{FP}^{void}\right) \cdot n_{cells}}{\dot{V}_{charge}} \tag{20}$$

For mCDI and HCDI, several other void volumes have to be considered, e.g., the pores in the separator and the carbon electrode. With the parameters given in Tables I and II, the residence times during charge for IDI, HCDI, and mCDI are 26, 33 and 59 s, respectively.

Module volume and mass – For the volume of the intercalation module we need to sum up all component volumes per cell and multiply them with the number of cells. We need to consider twice the electrode volume, the volume of the ion exchange membrane between the electrodes and the flow plate volume plus an additional endplate (see Fig. S1 for a schematic of the stack). Flow plates are assumed to have channels on both sides, so only one plate per cell needs to be counted.

$$V_{stack} = \left(2 \cdot V_{el,IH} + A_{el} \cdot d_{BPP} + A_{el} \cdot d_{IEM}\right) \cdot n_{cells} + A_{el} \cdot d_{BPP} \tag{21}$$

Obviously, the three device concepts have different contributors to the overall cell volume (separators or flow plates, one or two IEMs per cell, different electrode thicknesses, etc.). The thickness of the cell stack in the IDI module simply depends on the form factor, i.e., the chosen electrode area.

$$d_{stack} = \frac{V_{stack}}{A_{el}} \tag{22}$$

In order to provide a realistic assessment of the module volume we cannot simply use the volume of the cell stack, but have to account for casing as well. Thus, we assume a typical packaging factor, ψ, of 1.3 to derive the module case volume.

$$V_{mod} = V_{stack} \cdot \psi \tag{23}$$

Fig. S5 displays the module case volume as a function of salt load per cycle.

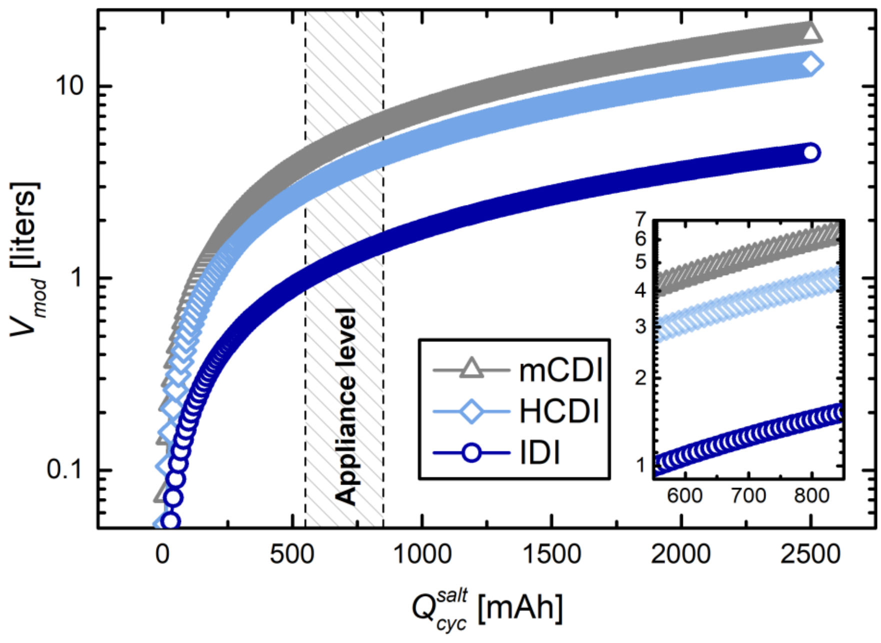

Fig. S5. Volume of module casing as a function of salt load per half-cycle. Since the data is presented on the basis of salt load, it is applicable for different combinations of salt concentrations, flow rates and cycle times. Dashed area and inset show typical parameters for appliance level modules.

The mass of the intercalation host module can be calculated by summing up all individual components using their volume and the respective density (see Table III). For the case of IDI we have to account for PBA active material (already determined in Equation 12), binder, and conductive carbon additive in the electrodes as well as ion exchange membranes, flow plates, and the mass of the module case. There are two intercalation electrodes per IDI cell.

$$m_{mod,IH} = 2 \cdot m_{el,IH} \cdot n_{cells} \tag{24}$$

For the mass of the other electrode components we assume that the electrode volume fraction not filled with PBA active material is evenly split into binder and conductive carbon. The mass of binder can thus be calculated as follows.

$$m_{mod,b} = 2 \cdot V_{el,IH} \cdot (1 - P_{el,IH}) \cdot 0.5 \cdot (1 - \varepsilon_{IH}) \cdot \rho_b \cdot n_{cells} \tag{25}$$

The mass of carbon black is calculated analogously. In IDI there is only one IEM sheet per cell.

$$m_{mod,IEM} = A_{el} \cdot d_{IEM} \cdot \rho_{IEM} \cdot n_{cells} \tag{26}$$

We assume the same density for graphite current collector sheet and graphite flow plate. The total number of flow plates is $n_{cells} + 1$ to account for the endplates.

$$m_{mod,FP} = A_{el} \cdot d_{FP} \cdot (1 - \varepsilon_{FP}) \cdot \rho_{cc} \cdot (n_{cells} + 1) \tag{27}$$

Finally, we assume 1 cm thick walls of the polypropylene case and assume the case is rectangular.

$$m_{mod,case} = (A_{el} \cdot 1 \cdot 2 + \frac{V_{case}}{A_{el}} \cdot \sqrt{A_{el}} \cdot 1 \cdot 4) \cdot \rho_{case} \tag{28}$$

Consequently, the total mass of the IDI module can be written as the sum of all components.

$$m_{mod} = (m_{mod,IH} + m_{mod,IEM} + m_{mod,b} + m_{mod,cb} + m_{mod,FP} + m_{mod,case}) \tag{29}$$

Fig. S6 shows the module mass for the mCDI, HCDI, IDI.

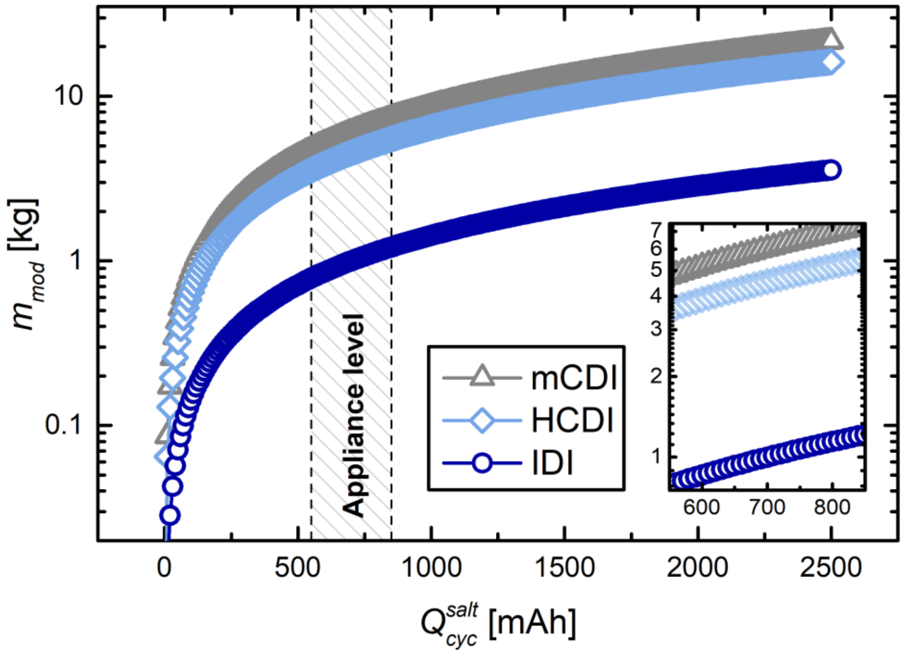

Fig. S6. Module mass as a function of salt load per half-cycle. Since the data is presented on the basis of salt load, it is applicable for different combinations of salt concentrations, flow rates and cycle times. Dashed area and inset show typical parameters for appliance level modules.

Module cost – In order to derive the module cost, arguably the most important metric, we estimate the cost of each individual element based on the material and component costs presented in Tale IV. For weight-based costs, e.g., the intercalation host material, we can use the already calculated masses. Note that intercalation host material has to be counted twice per cell for IDI.

$$\kappa_{mod,IH} = 2 \cdot \kappa_{IH} \cdot m_{el,IH} \cdot n_{cells} \tag{30}$$

The costs of binder and conductive carbon follow analogously. For an area-based cost, e.g., the IEMs, we have to consider the electrode area.

$$\kappa_{mod,IEM} = \kappa_{IEM} \cdot A_{el} \cdot n_{cells} \tag{31}$$

Adding costs for flow plates (counted n_{cells} + 1 times to account for end plates) and module case we can write the total module cost as follows.

$$\kappa_{mod} = \kappa_{mod,IH} + \kappa_{mod,IEM} + \kappa_{mod,b} + \kappa_{mod,cb} + \kappa_{mod,FP} + \kappa_{mod,case} \tag{32}$$

Fig. S7 shows that intercalative approaches allow to eliminate considerable costs, since PBAs are inexpensive and fewer ion exchange membranes are needed. The module cost does not take into account auxiliary system components like pumps, electronics or storage tanks. However, one can argue that performance requirements for pumps and other components should be alleviated for smaller purification modules, thereby strengthening the case for IDI over mCDI.

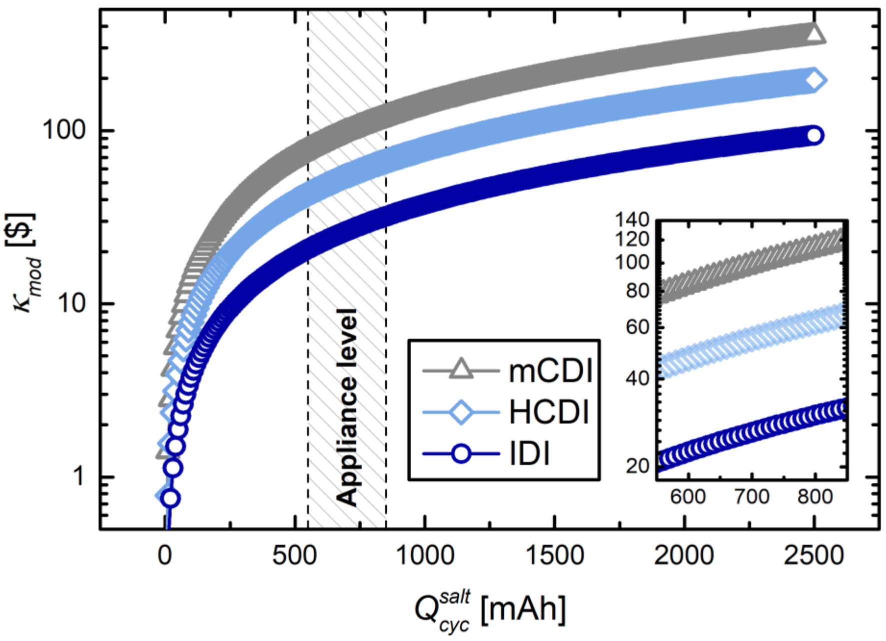

Fig. S7. Cost of module as a function of salt load per half-cycle. Since the data is presented on the basis of salt load, it is applicable for different combinations of salt concentrations, flow rates and cycle times. Dashed area and inset show typical parameters for appliance level modules.

3. Carbon footprint of different desalination technologies

The carbon footprint of mCDI, HCDI and IDI is estimated with reference to the currently installed reverse osmosis capacity for brackish water desalination and seawater desalination.

Carbon intensity of industry energy consumption – We begin by extracting the carbon intensity of the industry energy consumption in different world regions of interest from the database of the International Energy Agency (IEA).[7] This quantity refers to the amount of CO_2 released into the atmosphere per unit of energy consumed by a countries industry (typically in units of tons_{CO2}/MJ). It is thus a good measure to assess the carbon footprint of desalination technologies, as a desalination plant requires energy just like any other industrial facility. Fig. S8 summarizes the carbon intensities as taken from the IEA database for major countries in the world regions of interest.[7] We use these to form an average carbon intensity per region.

Carbon footprint of electrochemical desalination – Next the share of reverse osmosis in the total desalination capacity for brackish water and seawater needs to be deduced, since we use RO as a reference to the electrochemical technologies investigated in the analysis. We rely on a recent review by E. Jones et al. that details the total installed desalination capacity in the world regions of interest and use the published values for the share of brackish water reverse osmosis (BW-RO, 19%) and seawater reverse osmosis (SW-RO, 34%) to estimate the absolute desalination capacity in 10^6 m^3/day (see Table SI).[8]

Table SI. Global shares of brackish water reverse osmosis (BW-RO) and seawater reverse osmosis (SW-RO) in total desalination capacity for different world regions.[8]

Region	Total desalination capacity [10^6 m^3/day]	Share BW-RO [10^6 m^3/day]	Share SW-RO [10^6 m^3/day]
Middle East and North Africa	45.32	8.61	15.41
East Asia and Pacific	17.52	3.33	5.96
North America	11.34	2.15	3.86
Western Europe	8.75	1.66	2.98
Latin America and Caribbean	5.46	1.04	1.86
Southern Asia	2.94	0.56	1.00
Eastern Europe and Central Asia	2.26	0.43	0.77
Sub-Saharan Africa	1.78	0.34	0.61

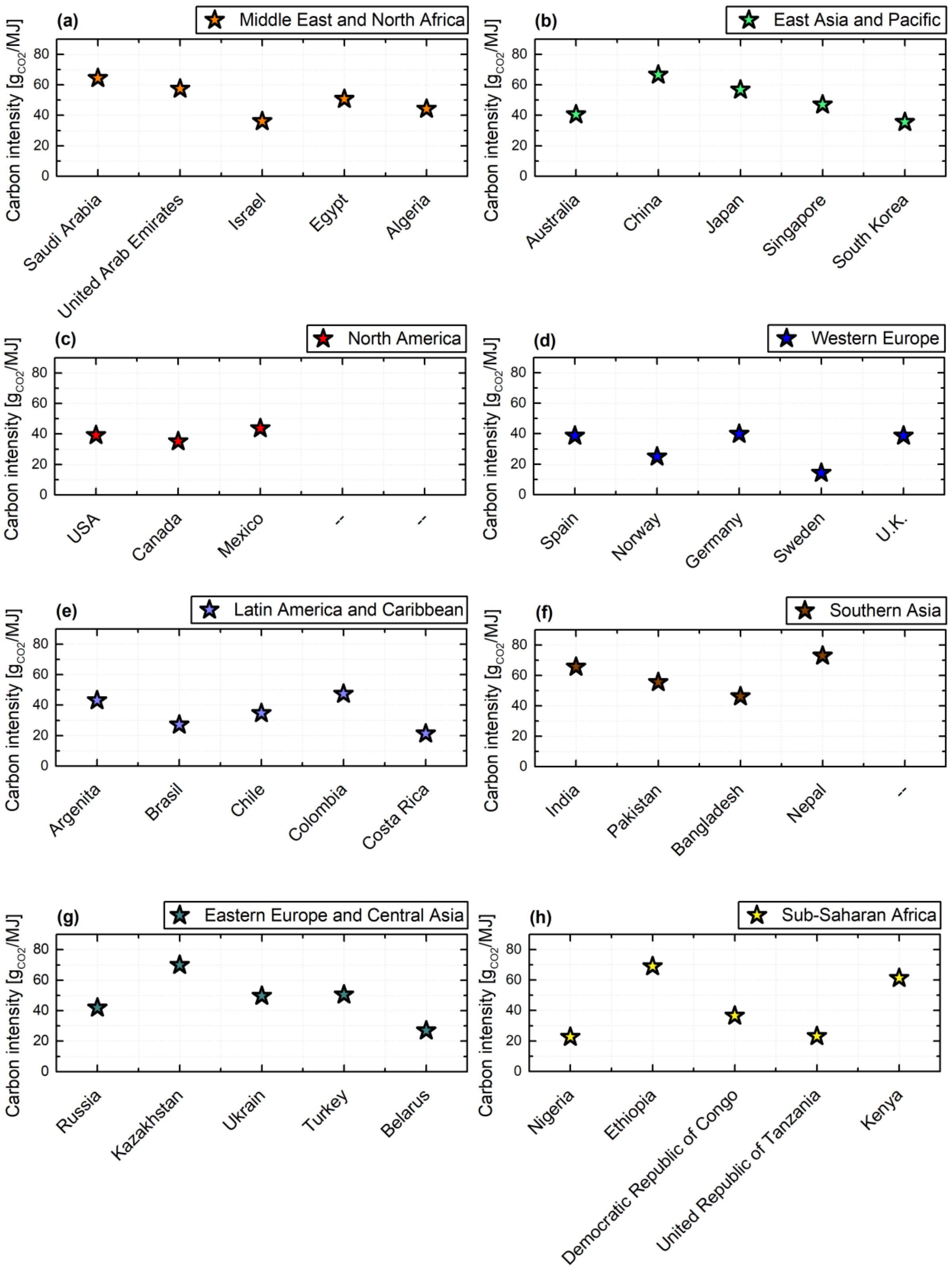

Fig. S8. Carbon intensity of industry energy consumption in major countries of selected world regions as extracted from the International Energy Agency database for the year 2017.[7]

The carbon footprint for mCDI, HCDI, and IDI now follows from combining the previously derived energy efficiencies incl. energy recovery benefits (see Fig. 6b of the main article) with the average carbon intensity per region and applying the result to the installed capacity in these regions (Table SI). Fig. S9 summarizes the resulting difference in carbon dioxide release (tons$_{CO2}$/day) for a hypothetical transition from RO to the respective electrochemical desalination technology in the various regions of interest. The data in Fig. S9a is calculated for a brackish water salinity of 3,000 ppm, the data in Fig. S9b for a seawater salinity of 3.5%. We can observe that a considerable reductions in the carbon footprint of brackish water desalination can be achieved by replacing RO with IDI, e.g., -130 tons$_{CO2}$/day in the "Middle East and North Africa" region (see Fig. S9a). mCDI with energy recovery also leads to a negative delta in carbon dioxide release, so a smaller carbon footprint. However, a transition from RO to HCDI would actually increase the carbon footprint of brackish water desalination. For seawater desalination IDI offers slight CO_2 savings compared to RO, the other techniques increase the carbon footprint substantially (Fig. S9b).

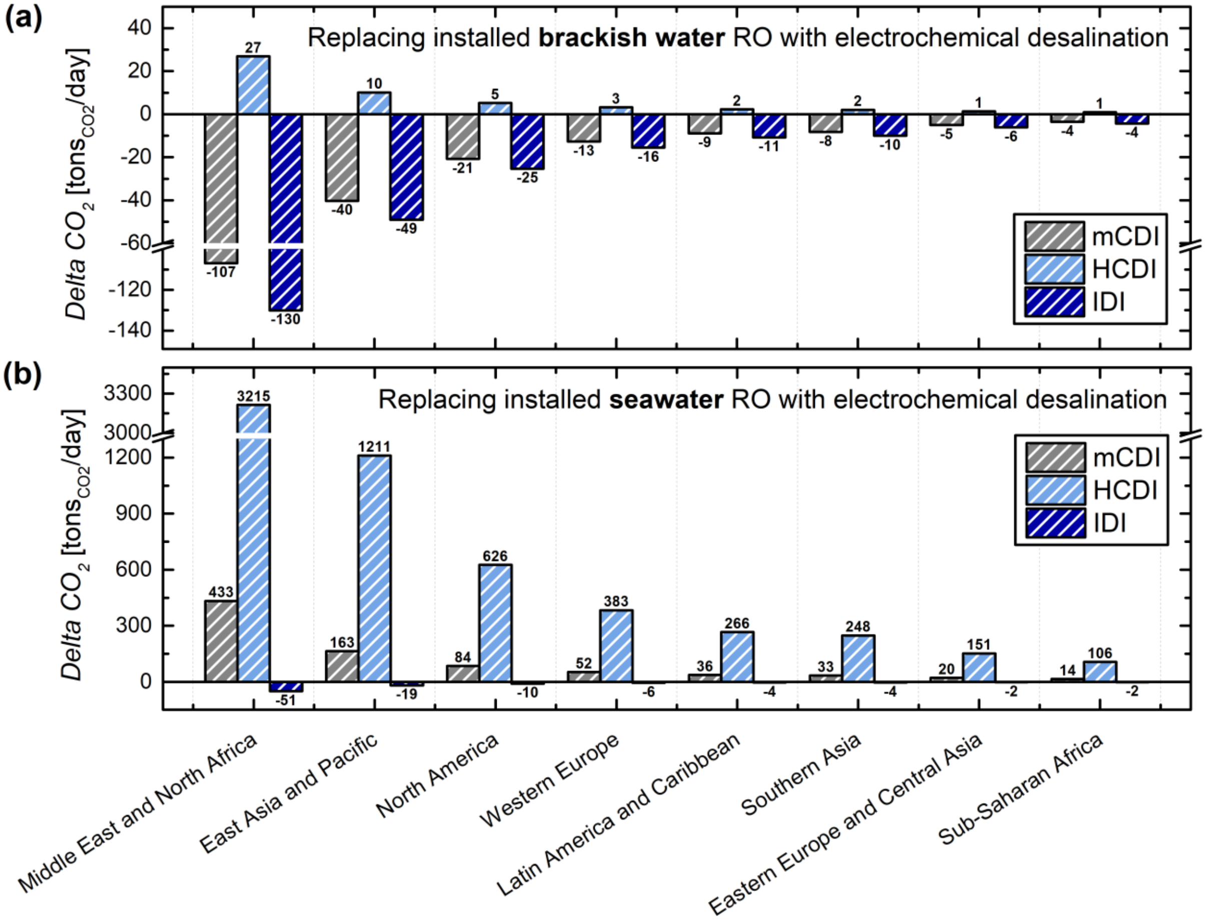

Fig. S9. Differences in carbon footprint of water desalination in different world regions for a hypothetical replacement of all installed reverse osmosis capacity for (a) brackish water desalination and (b) seawater desalination with electrochemical deionization based on mCDI (gray), HCDI (light blue), or IDI (dark blue). Energy recovery benefits are included in the analysis.

Carbon footprint of Electrodialysis (ED) – Finally, we can do the same carbon footprint analysis for brackish water electrodialysis (BW-ED), another emerging membrane based desalination technology, by relying on the published energy consumption of 0.86 Wh/liter$_{H2O}$ at 3,000 ppm NaCl from K. Chehayeb et al.[9] Fig. S10 shows that a hypothetical replacement of the installed BW-RO capacity with BW-ED can lead to smaller carbon footprints, however, current ED technology does not quite achieve the same reduction as IDI or advanced mCDI with energy recovery. That said, combining IDI and ED holds great promise for providing a low energy desalination technology that combines the advantages of both approached, as demonstrated in pioneering work by T. Kim et al.[3]

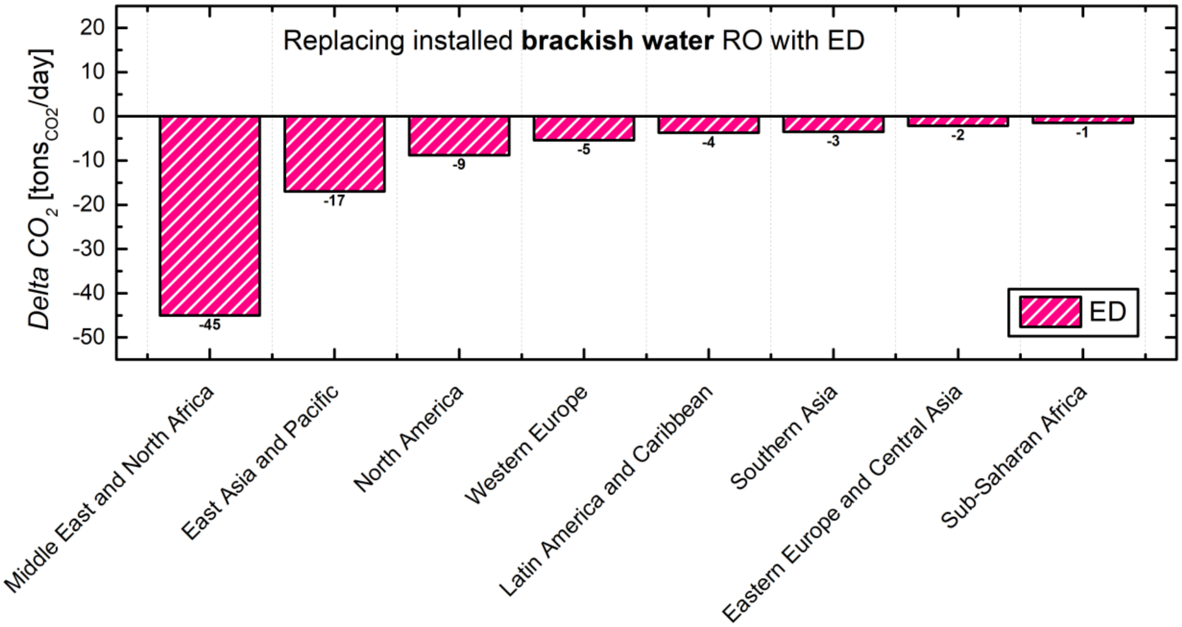

Fig. S10. Differences in carbon footprint of water desalination in different world regions for a hypothetical replacement of all installed reverse osmosis capacity for brackish water desalination with electrodialysis (ED).

4. Full set of equations incl. conversion factors

In the main article and chapter 2 of the supplementary information conversion factors have been omitted in the equations for clarity. This chapter summarizes the full set of equations and conversion factor used to compute the performance metrics for mCDI, HCDI and IDI.

Membrane capacitive deionization (mCDI) – Full set of equations for mCDI:

t_cyc = t_charge + t_discharge
dV_dt_discharge = (dV_dt_charge * t_charge) * (100 - x_recovery) / 100 / t_discharge
V_cyc = t_charge * dV_dt_charge
n_cyc = V_day * x_recovery / 100 / V_cyc
t_day = n_cyc * t_cyc / 60
V_day_clean = V_cyc * n_cyc
V_day_brine = V_day * (100 - x_recovery) / 100
n_cyc_lifetime = n_cyc * 365 * t_lifetime
delta_c = c_in - c_out
e_TDS = 100 - c_out / c_in * 100
m_salt_load_cyc = delta_c * 10 ^ (-6) * t_charge * dV_dt_charge * 1000
Q_salt_load_cyc = (m_salt_load_cyc) / M_W * z_ion * F * 1000 / 3600
Q_SAC_c = SAC_c / 1000 / M_W * (z_ion * F) * 1000 / 3600
V_el_c = A_el * d_el_c / 10000
m_el_c = V_el_c * (100 - P_c) / 100 * r_c * rho_c
Q_el_c = m_el_c * Q_SAC_c
n_cells = Q_salt_load_cyc / (U_el / 100 * Q_el_c)
Q_salt_load_cyc_el = Q_salt_load_cyc / n_cells
BET_c_el = BET_c * m_el_c
BET_c_mod = 2 * BET_c_el * n_cells
V_void_c = V_el_c * P_c / 100
V_void_sep = (A_el * d_sep / 10000) * P_sep / 100
t_res_charge_CDI_mod = ((2 * V_void_c + V_void_sep) * n_cells) / (dV_dt_charge * 1000) * 60
t_res_discharge_CDI_mod = ((2 * V_void_c + V_void_sep) * n_cells) / (dV_dt_discharge * 1000) * 60
I_1C_el_c = Q_el_c / 1
I_salt_load_charge = Q_salt_load_cyc_el / (t_charge / 60)
I_salt_load_discharge = Q_salt_load_cyc_el / (t_discharge / 60)
C_rate_charge = (Q_salt_load_cyc_el / Q_el_c) / (t_charge / 60)
C_rate_discharge = (Q_salt_load_cyc_el / Q_el_c) / (t_discharge / 60)
V_CDI_mod = (2 * V_el_c + 1 * A_el * d_sep / 10000 + 2 * A_el * d_cc / 10000 + 2 * A_el * d_IEM / 10000) * n_cells
d_CDI_mod = V_CDI_mod / A_el
V_case_CDI_mod = V_CDI_mod * Pf / 1000
m_c_CDI_mod = (2 * m_el_c) * n_cells
m_IEM_CDI_mod = 2 * A_el * d_IEM / 10000 * n_cells * rho_IEM
m_sep_CDI_mod = 2 * A_el * d_sep / 10000 * (1 - P_sep / 100) * n_cells * rho_sep
m_b_CDI_mod = V_el_c * (100 - P_c) / 100 * (1 - r_c) * rho_b * 2 * n_cells
m_cc_CDI_mod = 2 * A_el * d_cc / 10000 * rho_cc * n_cells

m_case_CDI_mod = (A_el * 1 * 2 + V_case_CDI_mod * 1000 / A_el * (A_el) ^ 0.5 * 1 * 4) * rho_case
m_CDI_mod = (m_c_CDI_mod + m_IEM_CDI_mod + m_sep_CDI_mod + m_b_CDI_mod + m_cc_CDI_mod + m_case_CDI_mod) / 1000
K_c_CDI_mod = K_c / 1000 * (2 * m_el_c) * n_cells
K_IEM_CDI_mod = A_el / (10 ^ 4) * n_cells * 2 * K_IEM
K_sep_CDI_mod = A_el / (10 ^ 4) * n_cells * K_sep
K_b_CDI_mod = K_b / 1000 * m_b_CDI_mod
K_cc_CDI_mod = m_cc_CDI_mod * K_cc / 1000
K_case_CDI_mod = m_case_CDI_mod * K_case / 1000
K_CDI_mod = K_c_CDI_mod + K_IEM_CDI_mod + K_sep_CDI_mod + K_b_CDI_mod + K_cc_CDI_mod + K_case_CDI_mod

Hybrid capacitive deionization (HCDI) – Full set of equations for HCDI:

t_cyc = t_charge + t_discharge
dV_dt_discharge = (dV_dt_charge * t_charge) * (100 - x_recovery) / 100 / t_discharge
V_cyc = t_charge * dV_dt_charge
n_cyc = V_day * x_recovery / 100 / V_cyc
t_day = n_cyc * t_cyc / 60
V_day_clean = V_cyc * n_cyc
V_day_brine = V_day * (100 - x_recovery) / 100
n_cyc_lifetime = n_cyc * 365 * t_lifetime
delta_c = c_in - c_out
e_TDS = 100 - c_out / c_in * 100
m_salt_load_cyc = delta_c * 10 ^ (-6) * t_charge * dV_dt_charge * 1000
Q_salt_load_cyc = (m_salt_load_cyc) / M_W * z_ion * F * 1000 / 3600
Q_SAC_c = SAC_c / 1000 / M_W * (z_ion * F) * 1000 / 3600
Q_SIC_IH = SIC_IH / 1000 / M_W * (z_ion * F) * 1000 / 3600
V_el_c = A_el * d_el_c / 10000
m_el_c = V_el_c * (100 - P_c) / 100 * r_c * rho_c
Q_el_c = m_el_c * Q_SAC_c
n_cells = Q_salt_load_cyc / (U_el / 100 * Q_el_c)
Q_salt_load_cyc_el = Q_salt_load_cyc / n_cells
m_el_IH = Q_el_c / Q_SIC_IH
V_el_IH = m_el_IH / (100 - P_IH) * 100 / r_IH / rho_IH
d_el_IH_act = V_el_IH / A_el * 10000
BET_c_el = BET_c * m_el_c
BET_IH_el = BET_IH * m_el_IH
b_c_IH = BET_c_el / BET_IH_el
BET_IH_c_mod = (BET_c_el + BET_IH_el) * n_cells
V_void_c = V_el_c * P_c / 100
V_void_IH = V_el_IH * P_IH / 100
V_void_sep = (A_el * d_sep / 10000) * P_sep / 100
t_res_charge_HCDI_mod = ((V_void_c + V_void_IH + V_void_sep) * n_cells) / (dV_dt_charge * 1000) * 60

t_res_discharge_HCDI_mod = ((V_void_c + V_void_IH + V_void_sep) * n_cells) / (dV_dt_discharge * 1000) * 60
I_1C_el_c = Q_el_c / 1
I_salt_load_charge = Q_salt_load_cyc_el / (t_charge / 60)
I_salt_load_discharge = Q_salt_load_cyc_el / (t_discharge / 60)
C_rate_charge = I_salt_load_charge / I_1C_el_c
C_rate_discharge = I_salt_load_discharge / I_1C_el_c
V_HCDI_mod = (1 * V_el_IH + 1 * V_el_c + 1 * A_el * d_sep / 10000 + 2 * A_el * d_cc / 10000 + 1 * A_el * d_IEM / 10000) * n_cells
d_HCDI_mod = V_HCDI_mod / A_el
V_case_HCDI_mod = V_HCDI_mod * Pf / 1000
m_c_HCDI_mod = m_el_c * n_cells
m_IH_HCDI_mod = m_el_IH * n_cells
m_IEM_HCDI_mod = 1 * A_el * d_IEM / 10000 * n_cells * rho_IEM
m_sep_HCDI_mod = 1 * A_el * d_sep / 10000 * (1 - P_sep / 100) * n_cells * rho_sep
m_b_HCDI_mod = ((V_el_c * (100 - P_c) / 100 * (1 - r_c)) + (V_el_IH * (100 - P_IH) / 100 * 0.5 * (1 - r_IH))) * rho_b * n_cells
m_cb_HCDI_mod = (V_el_IH * (100 - P_IH) / 100 * 0.5 * (1 - r_IH)) * rho_cb * n_cells
m_cc_HCDI_mod = 2 * A_el * d_cc / 10000 * rho_cc * n_cells
m_case_HCDI_mod = (A_el * 1 * 2 + V_case_HCDI_mod * 1000 / A_el * (A_el) ^ 0.5 * 1 * 4) * rho_case
m_HCDI_mod = (m_c_HCDI_mod + m_IH_HCDI_mod + m_IEM_HCDI_mod + m_sep_HCDI_mod + m_b_HCDI_mod + m_cb_HCDI_mod + m_cc_HCDI_mod + m_case_HCDI_mod) / 1000
K_c_HCDI_mod = (K_c / 1000 * m_el_c) * n_cells
K_IH_HCDI_mod = (K_IH / 1000 * m_el_IH) * n_cells
K_IEM_HCDI_mod = A_el / (10 ^ 4) * 1 * K_IEM * n_cells
K_sep_HCDI_mod = A_el / (10 ^ 4) * K_sep * n_cells
K_b_HCDI_mod = K_b / 1000 * m_b_HCDI_mod
K_cb_HCDI_mod = K_cb / 1000 * m_cb_HCDI_mod
K_cc_HCDI_mod = m_cc_HCDI_mod * K_cc / 1000
K_case_HCDI_mod = m_case_HCDI_mod * K_case / 1000
K_HCDI_mod = K_c_HCDI_mod + K_IH_HCDI_mod + K_IEM_HCDI_mod + K_sep_HCDI_mod + K_b_HCDI_mod + K_cb_HCDI_mod + K_cc_HCDI_mod + K_case_HCDI_mod

Intercalative deionization (IDI) – Full set of equations for IDI:

t_cyc = t_charge + t_discharge
dV_dt_brine = (dV_dt_charge * t_charge) * (100 - x_recovery) / 100 / t_discharge
V_cyc = t_charge * dV_dt_charge * 2
n_cyc = V_day * x_recovery / 100 / V_cyc
t_day = n_cyc * t_cyc / 60
V_day_clean = V_cyc * n_cyc
V_day_brine = V_day * (100 - x_recovery) / 100
n_cyc_lifetime = n_cyc * 365 * t_lifetime
delta_c = c_in - c_out

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e_TDS = 100 - c_out / c_in * 100
m_salt_load_cyc = delta_c * 10 ^ (-6) * t_charge * dV_dt_charge * 1000
Q_salt_load_cyc = (m_salt_load_cyc / (1)) / M_W * z_ion * F * 1000 / 3600
Q_SIC_IH = SIC_IH / 1000 / M_W * (z_ion * F) * 1000 / 3600
V_el_IH = A_el * d_el_IH / 10000
m_el_IH = V_el_IH * (100 - P_IH) / 100 * r_IH * rho_IH
Q_el_IH = m_el_IH * Q_SIC_IH
n_cells = Q_salt_load_cyc / (U_el / 100 * Q_el_IH)
Q_salt_load_cyc_el = Q_salt_load_cyc / n_cells
BET_IH_el = BET_IH * m_el_IH
BET_IH_mod = 2 * BET_IH_el * n_cells
V_void_IH = V_el_IH * P_IH / 100
V_void_BPP = (A_el * d_BPP / 10000) * r_BPP_c_l
t_res_charge_IDI_mod = ((V_void_IH + V_void_IH + V_void_BPP) * n_cells) / (dV_dt_charge * 1000) * 60
t_res_discharge_IDI_mod = ((V_void_IH + V_void_IH + V_void_BPP) * n_cells) / (dV_dt_brine * 1000) * 60
I_1C_el_IH = Q_el_IH / 1
I_salt_load_charge = Q_salt_load_cyc_el / (t_charge / 60)
I_salt_load_discharge = Q_salt_load_cyc_el / (t_discharge / 60)
C_rate_charge = (Q_salt_load_cyc_el / Q_el_IH) / (t_charge / 60)
C_rate_discharge = (Q_salt_load_cyc_el / Q_el_IH) / (t_discharge / 60)
V_IDI_mod = (2 * V_el_IH + 1 * A_el * d_BPP / 10000 + 1 * A_el * d_IEM / 10000) * n_cells + 1 * A_el * d_BPP / 10000
d_IDI_mod = V_IDI_mod / A_el
V_case_IDI_mod = V_IDI_mod * Pf / 1000
m_IH_IDI_mod = 2 * m_el_IH * n_cells
m_IEM_IDI_mod = 1 * A_el * d_IEM / 10000 * n_cells * rho_IEM
m_b_IDI_mod = V_el_IH * (100 - P_IH) / 100 * 0.5 * (1 - r_IH) * rho_b * 2 * n_cells
m_cb_IDI_mod = V_el_IH * (100 - P_IH) / 100 * 0.5 * (1 - r_IH) * rho_cb * 2 * n_cells
m_BPP_IDI_mod = A_el * (d_BPP) / 10000 * (1 - r_BPP_c_l) * (n_cells + 1) * rho_cc
m_case_IDI_mod = (A_el * 1 * 2 + V_case_IDI_mod * 1000 / A_el * (A_el) ^ 0.5 * 1 * 4) * rho_case
m_IDI_mod = (m_IH_IDI_mod + m_IEM_IDI_mod + m_b_IDI_mod + m_cb_IDI_mod + m_BPP_IDI_mod + m_case_IDI_mod) / 1000
K_IH_IDI_mod = K_IH / 1000 * m_el_IH * n_cells * 2
K_IEM_IDI_mod = A_el / (10 ^ 4) * n_cells * 1 * K_IEM
K_sep_IDI_mod = A_el / (10 ^ 4) * n_cells * K_sep
K_b_IDI_mod = K_b / 1000 * m_b_IDI_mod
K_cb_IDI_mod = K_cb / 1000 * m_cb_IDI_mod
K_BPP_IDI_mod = (n_cells + 1) * K_BPP / 10000 * A_el
K_case_IDI_mod = m_case_IDI_mod * K_case / 1000
K_IDI_mod = K_IH_IDI_mod + K_IEM_IDI_mod + K_b_IDI_mod + K_cb_IDI_mod + K_BPP_IDI_mod + K_case_IDI_mod
```

List of symbols

A_{el}	geometric electrode area [cm^2]
c	salt concentration [ppm]
C	capacity [mAh]
$\hat{C}$	specific capacity of active material [mAh/g]
Δc	difference in salt concentration [ppm]
d	thickness [µm]
e	efficiency [%]
E	energy [Wh]
$\hat{E}$	energy density [Wh/liter or Wh/kg]
E_{cell}	cell voltage [V]
ER	energy recovery [%]
F	Faraday's constant
m	mass [g]
M	molar mass [g/mol]
n_{cells}	number of cells in module
n_{cyc}	number of cycles
P	porosity [%]
Q	charge [mAh]
r	C-rate
R	resistivity [$\Omega\cdot cm^2/mm$]
SAC	salt adsorption capacity [mg/g]
SIC	salt intercalation capacity [mg/g]
t	time [s]
V	volume [cm^3]
$\dot{V}$	flow rate [ml/min]
WR	water recovery [%]
z	valence
Greek	
ε	active material volume fraction [%]
η	overpotential [V]
κ	material cost [\$/kg or \$/m^2]
Λ	charge efficiency [%]
ρ	density [g/cm^3]
χ	utilization of electrode capacity [%]
ψ	packaging factor
Subscripts	
b	binder property
c	activated carbon property
FP	flow plate property (mono- or bipolar plate)
$brine$	referring to brine (stream)
$case$	property of casing around module
cc	current collector property
cb	conductive carbon black property
$charge$	referring to charge, also adsorption, intercalation, or operation step
cyc	(half-)cycle based quantity
day	referring to daily basis

discharge	referring to discharge, also desorption, de-intercalation, or regeneration step
el	electrode property
fresh	referring to freshwater (stream)
IEM	ion exchange membrane property
IH	intercalation host property
mod	module property
salt	salt property
sep	separator property
stack	property of desalination stack
void	void property
Superscripts	
BET	referring to microscopic surface area according to Braun-Emmett-Teller method
salt	salt property

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