PROCESS SYSTEMS ENGINEERING SEMINAR

West Lafayette, Feb 2nd, 2024

Optimizing Reverse Electrodialysis for Salinity-Driven Energy Recovery: A Sustainable Fix for the Water-Energy Nexus.

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PURDUE UNIVERSITY | College of Engineering

A little about me...

Cantabria

Spain

Santander

Dr. Marcos Fallanza

Prof. Raquel Ibáñez

Supervisors

UNIVERSIDAD DE CANTABRIA

Departamento de Ingenierías Química y Biomolecular

Research Groups

SEP	ASP
Sustainable Engineering Processes	Advanced Separation Processes

Ph.D. in
Chemical Engineering, Energy and Processes

01 | SCOPE & OBJECTIVES

Desalination and Water Reuse are on the Rise

The Guardian

Spain

This article is more than **1 month old**

Unprecedented €2.2bn drought response plan approved in Spain

Package of measures will help farmers maintain production and avoid food shortages after hottest April ever

Sam Jones *in Madrid*
@swajones
Thu 11 May 2023 16.55 BST

Drone footage shows Spanish reservoirs dry amid hottest April on record - video

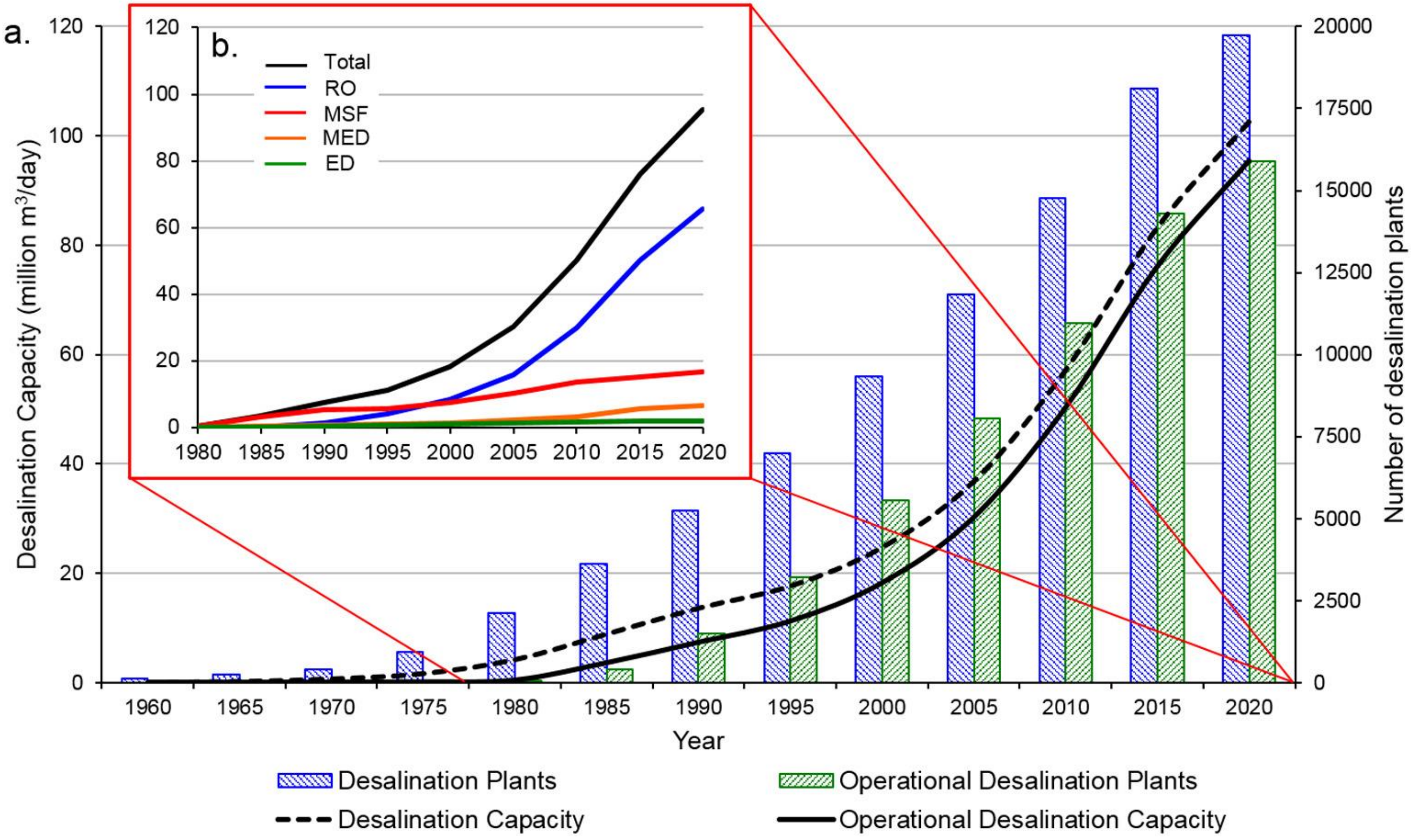
The Spanish government has approved a €2.2bn (£1.9bn) plan to help farmers and consumers cope with an enduring drought that has been exacerbated by the hottest and driest April on record.

The measures, described as unprecedented by the government, were signed off by the cabinet on Thursday. They include €1.4bn of funds from the environment ministry to tackle the drought and increase the availability of water, and €784m from the agriculture ministry to help farmers maintain production and avoid food shortages.

Spain's environment minister, Teresa Ribera, said her department would spend €1.4bn on building new infrastructure such as desalination plants; on doubling the proportion of water that is reused in urban areas from 10% to 20% by 2027; and on subsidising those whose irrigation water supplies would be reduced.

Jones E, Qadir M, van Vliet MTH, et al. Sci Total Environ 2019;657:1343-56.

Desalination and Water Reuse are on the Rise



Desalination Plants

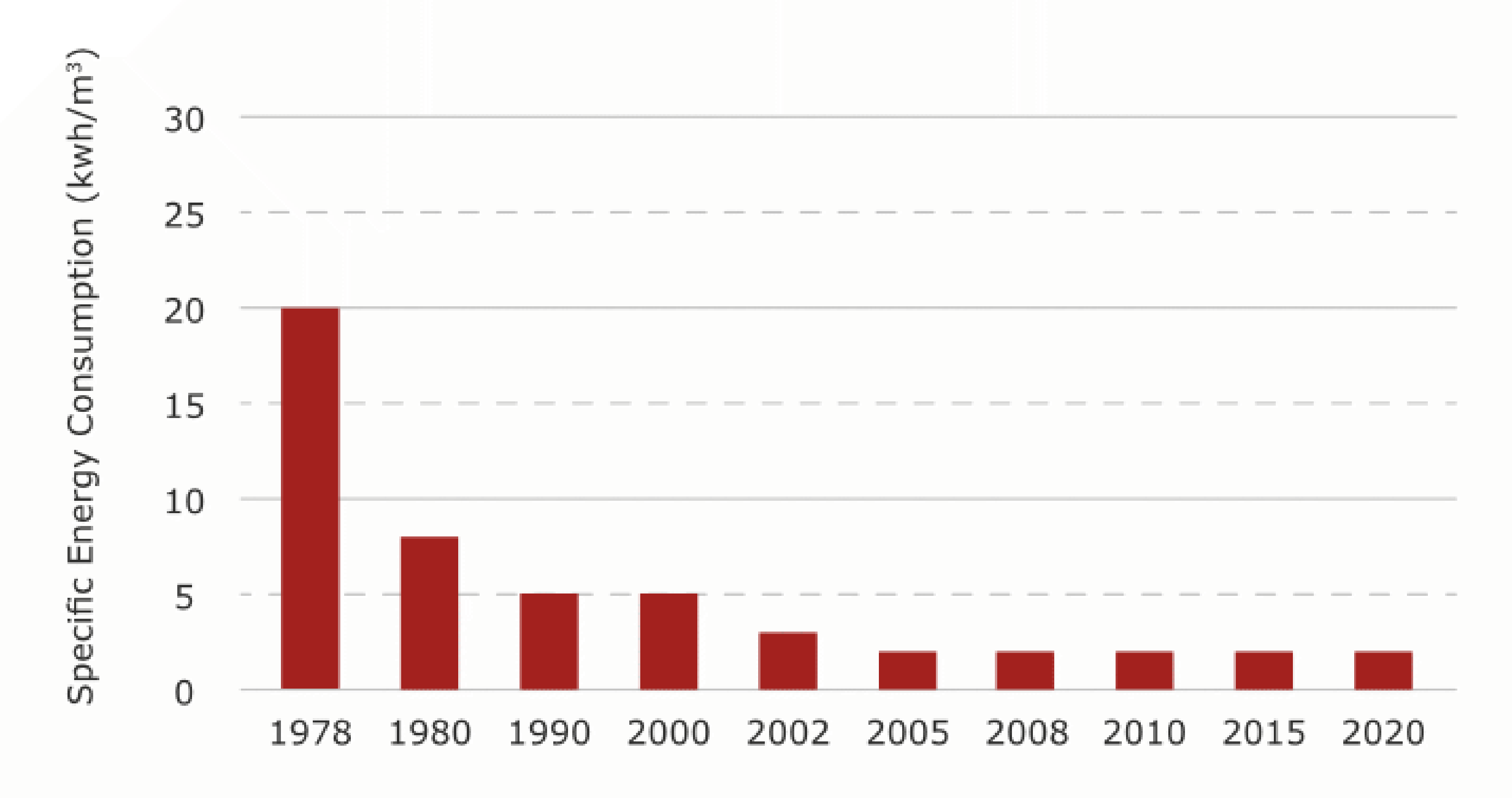
18k

Capacity

99.8 million m^3 day^{-1}

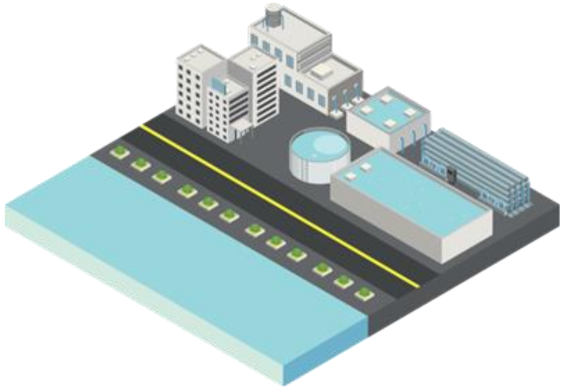
Jones E, Qadir M, van Vliet MTH, et al. Sci Total Environ 2019;657:1343-56.

Energy Consumption of Reverse Osmosis



Elimelech M, Phillip WA. Science (80) 2011

Salinity Gradient Energy (SGE)



SWRO
Desalination Plant

Brine

1.0-2.0 M

141.5
million m^3 day^{-1}

Seawater
~0.5 M

SG

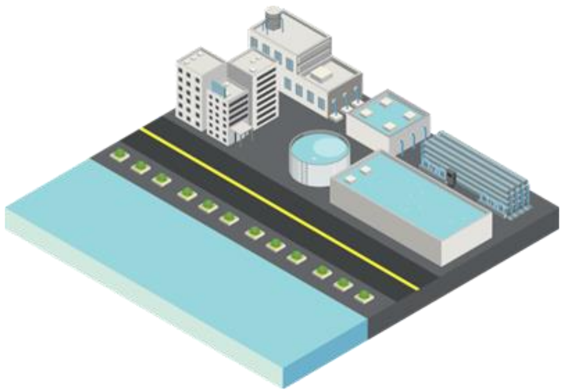
Salinity Gradient

Reclaimed
WW

20-40 mM

WWTP
Wastewater
treatment plant

Salinity Gradient Energy (SGE)

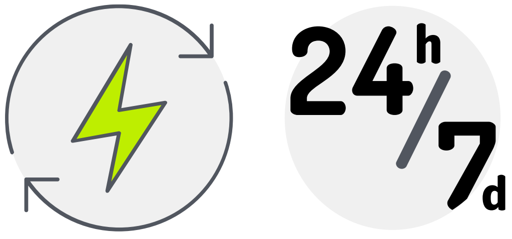


Brine

1.0-2.0 M

Reclaimed WW 20-40 mM

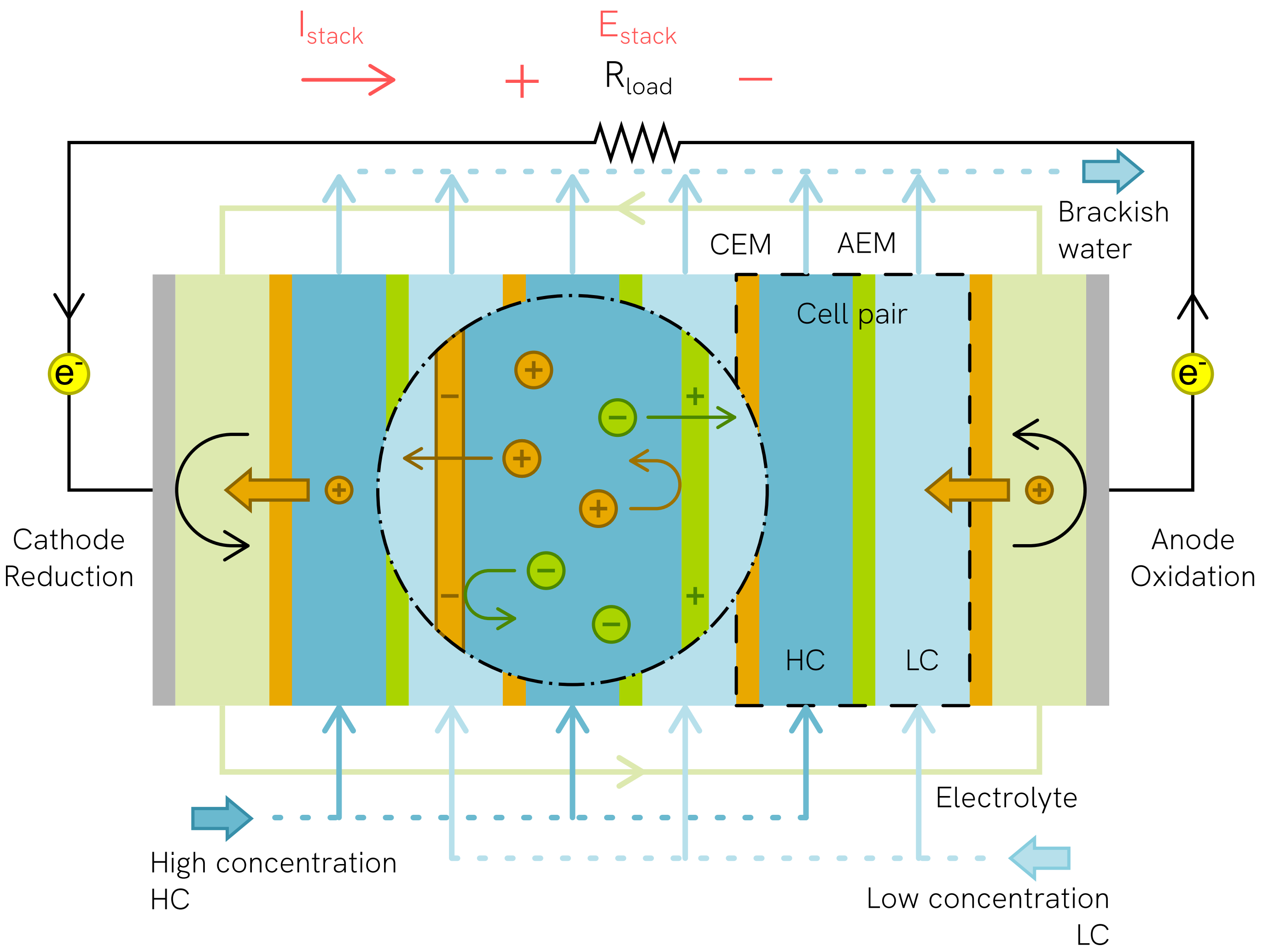
SG



SGE

0.85 kWh m^{-3}

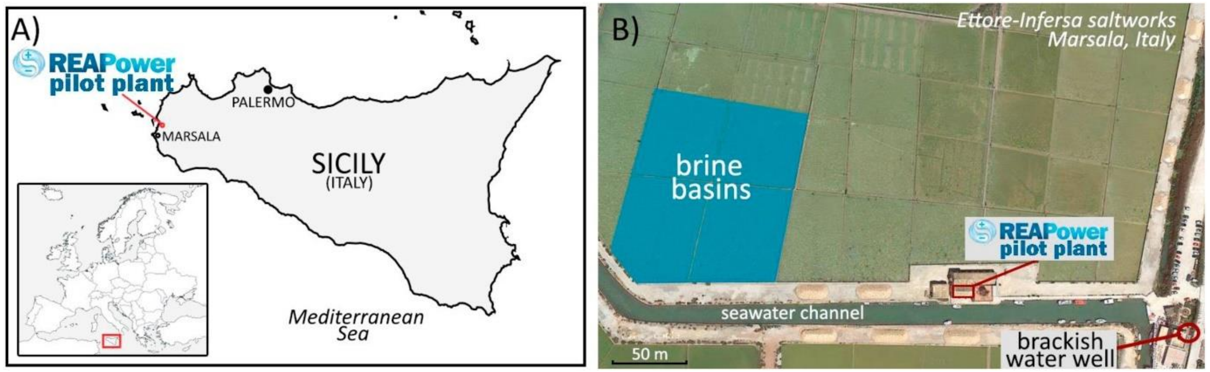
Reverse Electrodialysis (RED)



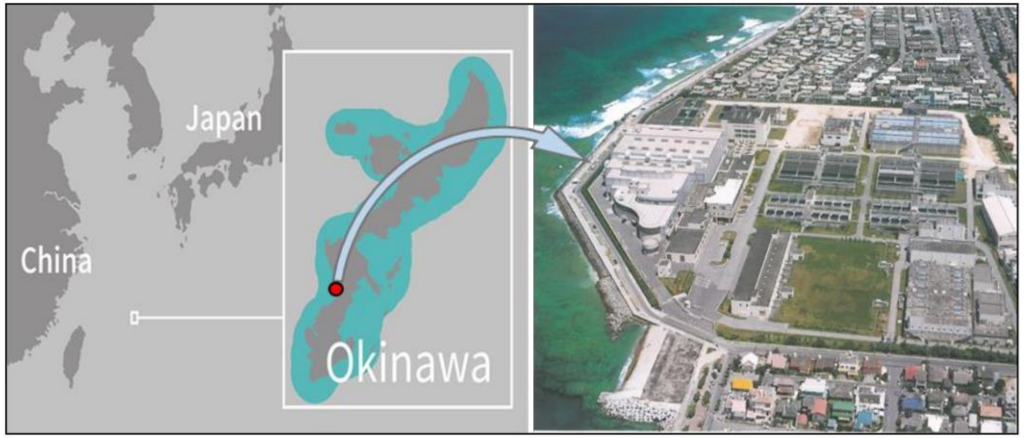
RED is Progressing but...

REDStack
Afsluitdijk, Netherlands

REAPower
Trapani, Italy



Okinawa, Japan



MAIN OBJECTIVES

Modelling framework to provide valuable support in **decision-making** for **full-scale RED implementation** in the **water sector**.

How can we assess RED **technical performance**?

Is RED technology **environmentally sound**?

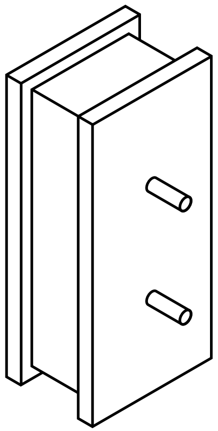
How can we define **powerful, efficient, sustainable**, and **cost-effective** designs for RED?

How can we assess RED technical performance?

02 | MODELLING RED PROCESS

Predicting RED System Performance

Stand-alone RED stack



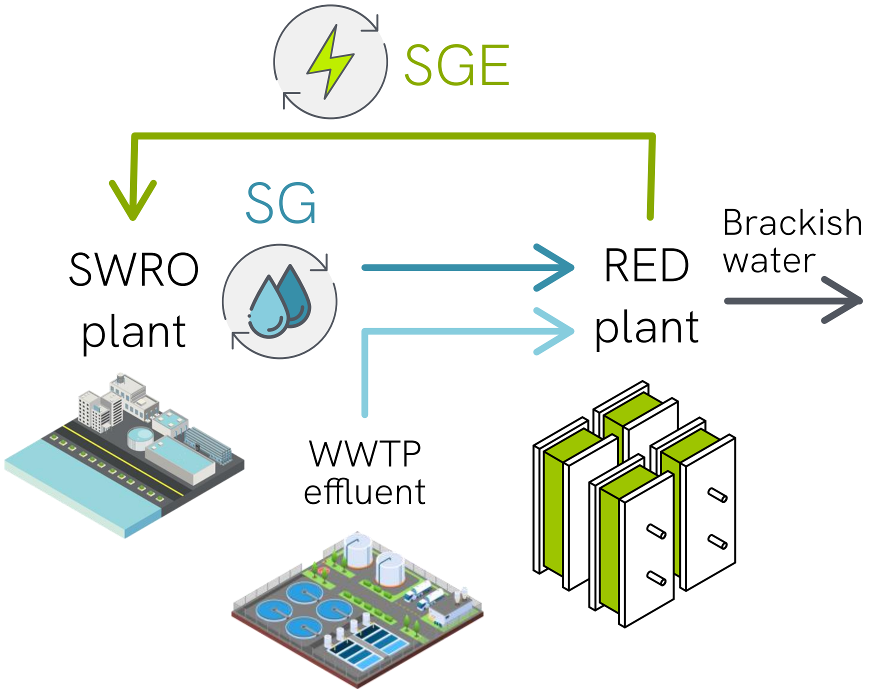
Operational conditions

Performance Metrics

Net Power

Energy Efficiency

RED plant

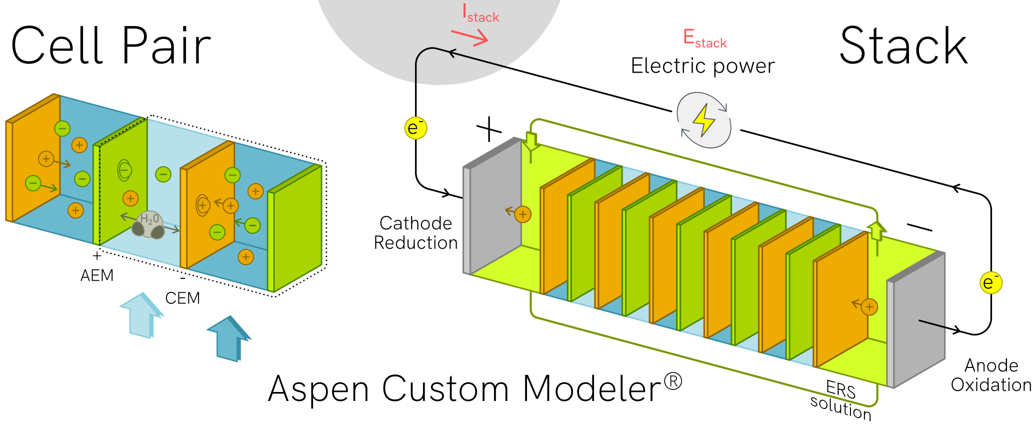


Multiscale Model

Model

Cell Pair

Stack



Aspen Custom Modeler®

R. Ortiz-Imedio, L. Gomez-Coma, M. Fallanza, et al. *Desalination*, 2019, 457, 8-21.

Updates

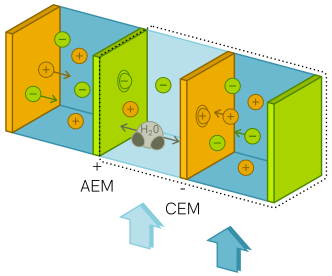
- ☑ Feed solution properties $f(x,p,x_i,T)$
- ☑ Membranes resistance $f(T)$
- ☑ Pressure drop $f(x, \text{spacer properties})$

Tristán, C.; Fallanza, M.; Ibáñez, R.; et al. *Desalination* 2020, 496, 114699

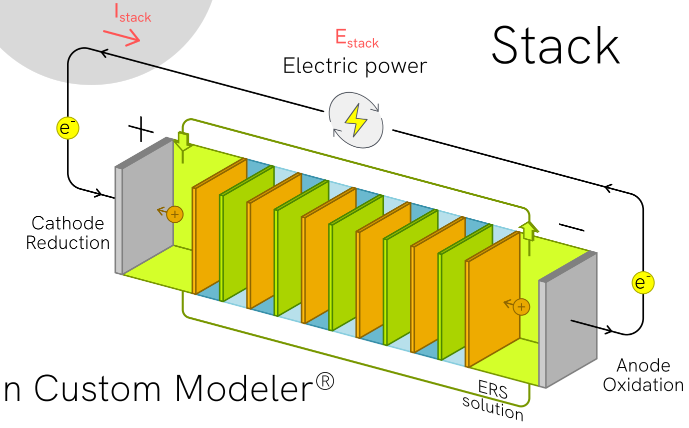
Multiscale Model

Model

Cell Pair

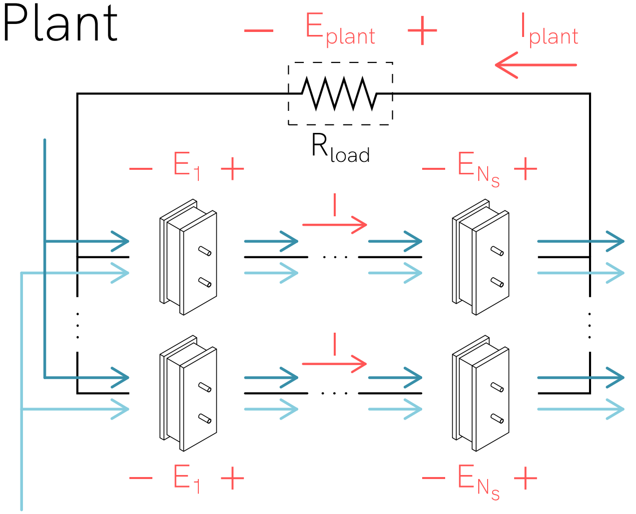


Stack



Aspen Custom Modeler®

Plant



Aspen Plus®

Updates

- Feed solution properties $f(x,p,x_i,T)$
- Membranes resistance $f(T)$
- Pressure drop $f(x, \text{spacer properties})$

Tristán, C.; Fallanza, M.; Ibáñez, R.; et al. *Desalination* 2020, 496, 114699

Multiscale Model

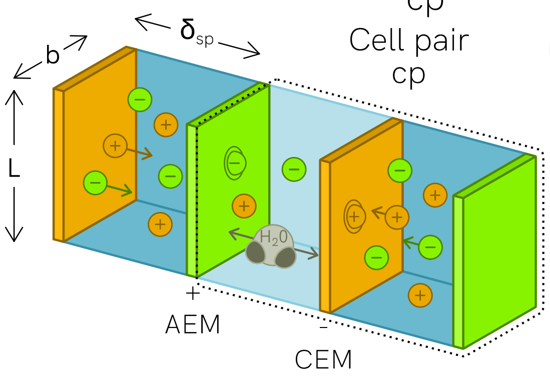
Tristán, C.; Fallanza, M.; Ibáñez, R.; et al.
Desalination 2020, 496, 114699

Input

Feed Sol.
C (0), T

Operational Conditions
Q (0), p (0)
External Load

RED stack



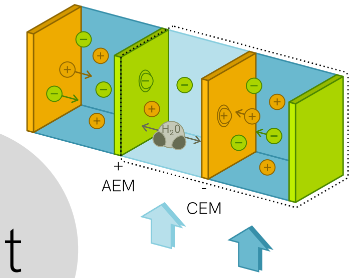
N_{cp}
Cell pair
cp

Spacers
Thickness
Porosity

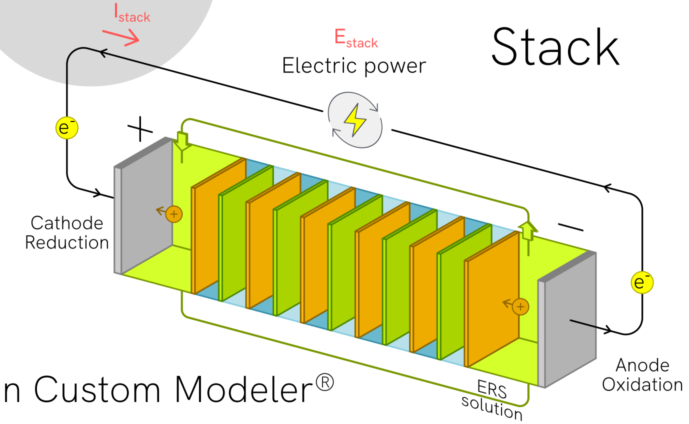
Membranes
Resistance @T_{ref}
Permselectivity
Diffusivity
Thickness

Model

Cell Pair

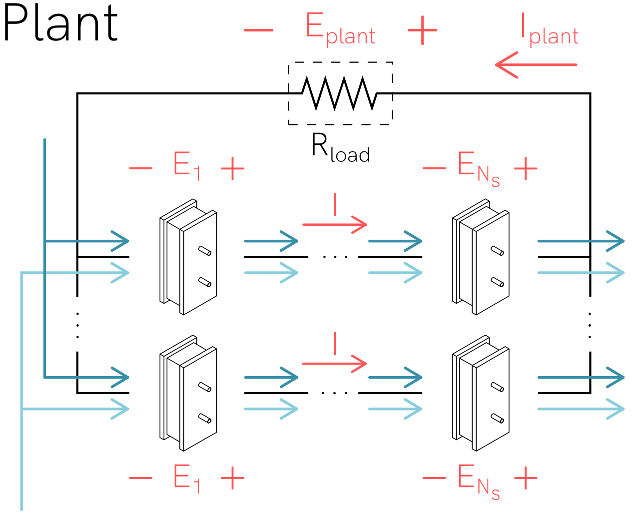


Stack



Aspen Custom Modeler®

Plant



Aspen Plus®

Output

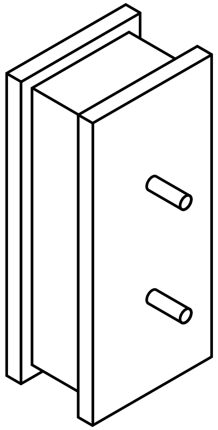
Gross Power
Net Power
Pumping Power

Power Density
$W\ m^{-2}$

Specific Energy
$kWh\ m^{-3}$

Model validation

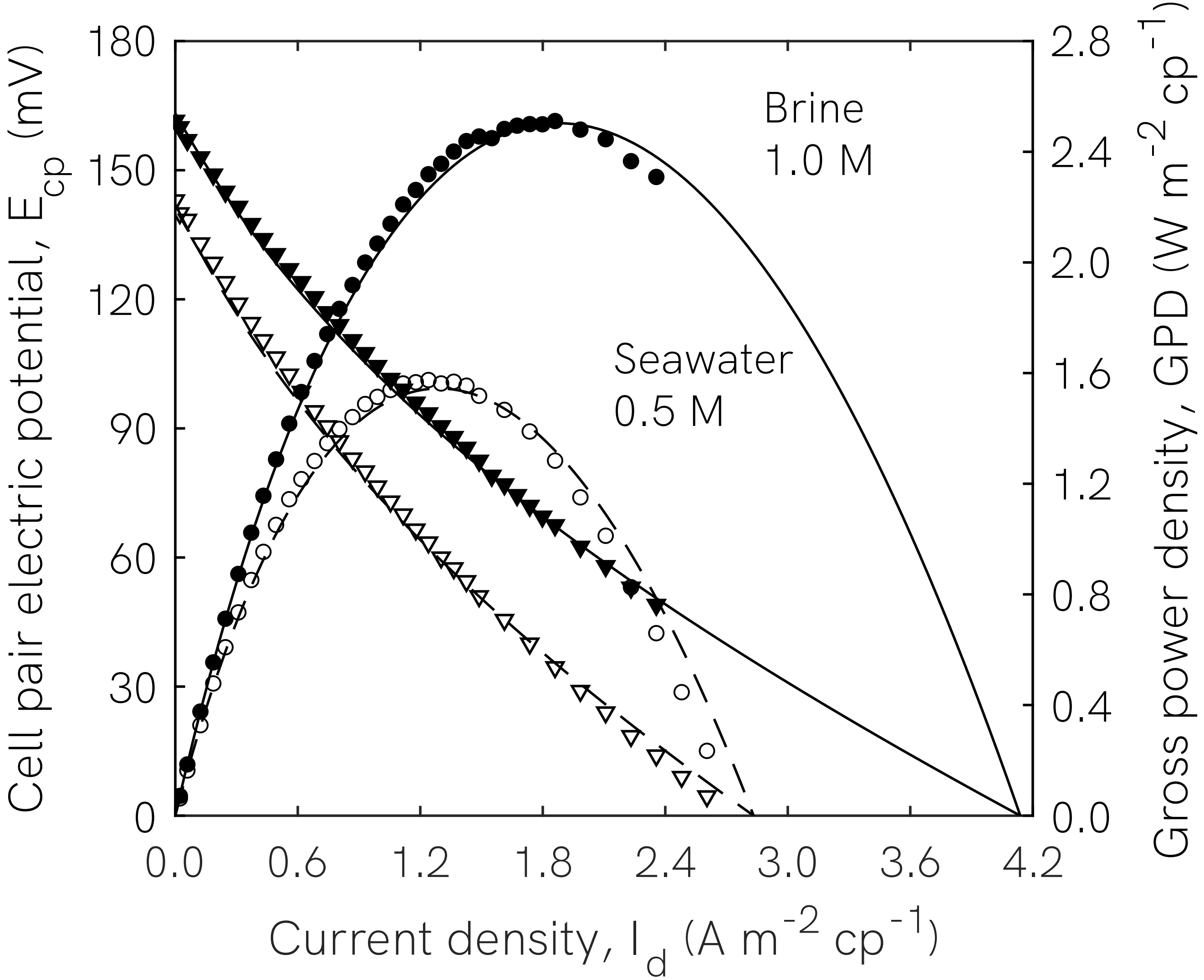
ED-200-2-20
fumatech®



20 cell pairs

Spacers
Thickness: 270 µm
Porosity: 82.5%

Membranes
Thickness: 50 µm
200 cm^2
FKS-50 / FAS-50
(fumasep®, fumatech®)



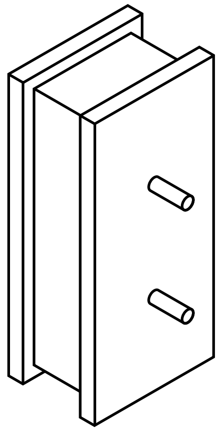
LC
Wastewater
20 mM

v ($cm\ s^{-1}$)
1.0

T (°C)
24

Model validation

ED-200-2-20
fumatech®



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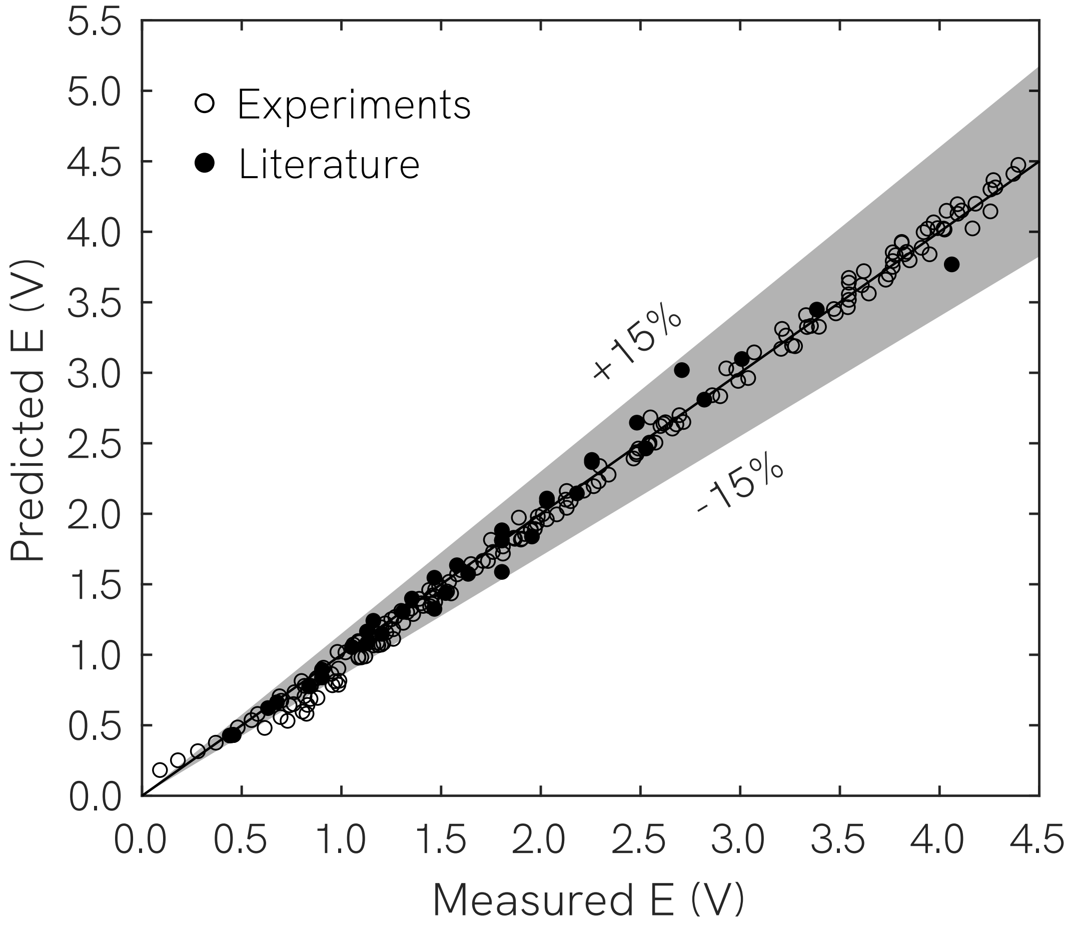


Tedesco, M.; Cipollina, A.; Tamburini, et al. *Chem. Eng. Res. Des.* 2015, 93, 441-456
Długołęcki, P.; Gambier, A.; Nijmeijer, K.; et al. *Sci. Technol.* 2009, 43 (17), 6888-6894

Concentration (M)	
HC	LC
0.5-5.0	0.02-0.5

v (cm s^{-1})

0.6-3.0

T (°C)

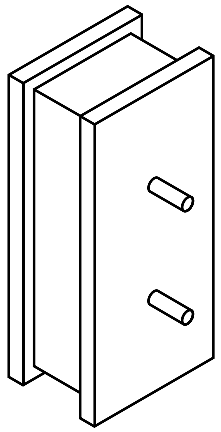
13-24

Stand-alone RED stack

Operational Conditions

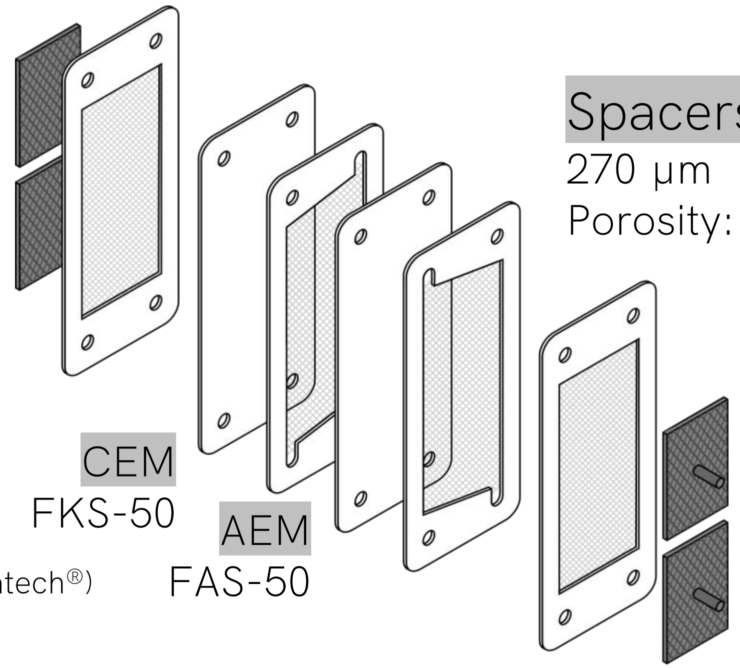
- [x] Concentration
- [x] Flow Rate
- [x] Temperature

RED stack Parameters



ED-1750
fumatech®

1000
cell pairs



Spacers
270 μm
Porosity: 82.5%

IEMs
0.175 m^2
(fumasep®, fumatech®)

CEM
FKS-50

AEM
FAS-50

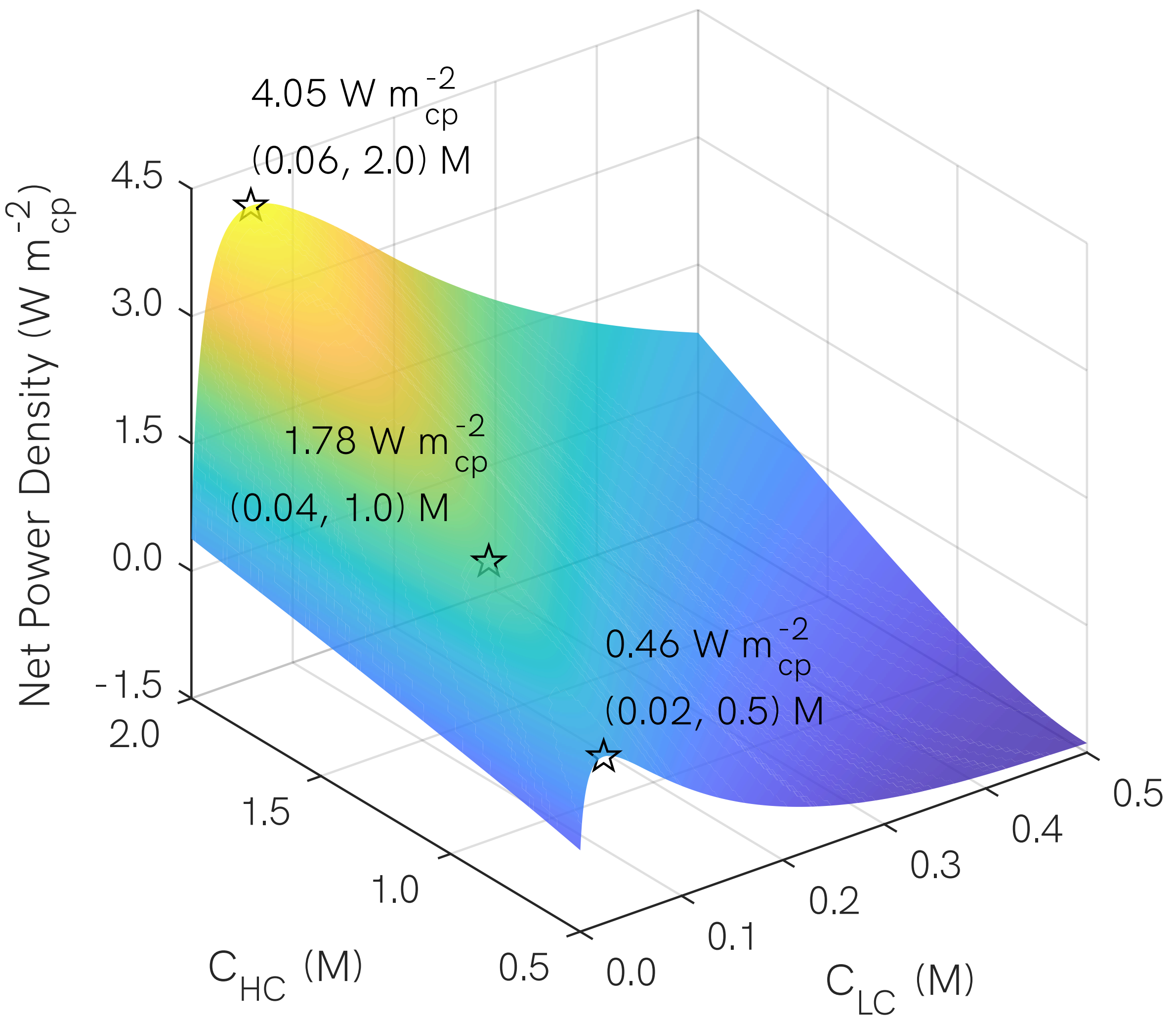
Tristán, C.; Fallanza, M.; Ibáñez, R.; et al. *Desalination* 2020, 496, 114699

Stand-alone RED stack

Operational Conditions

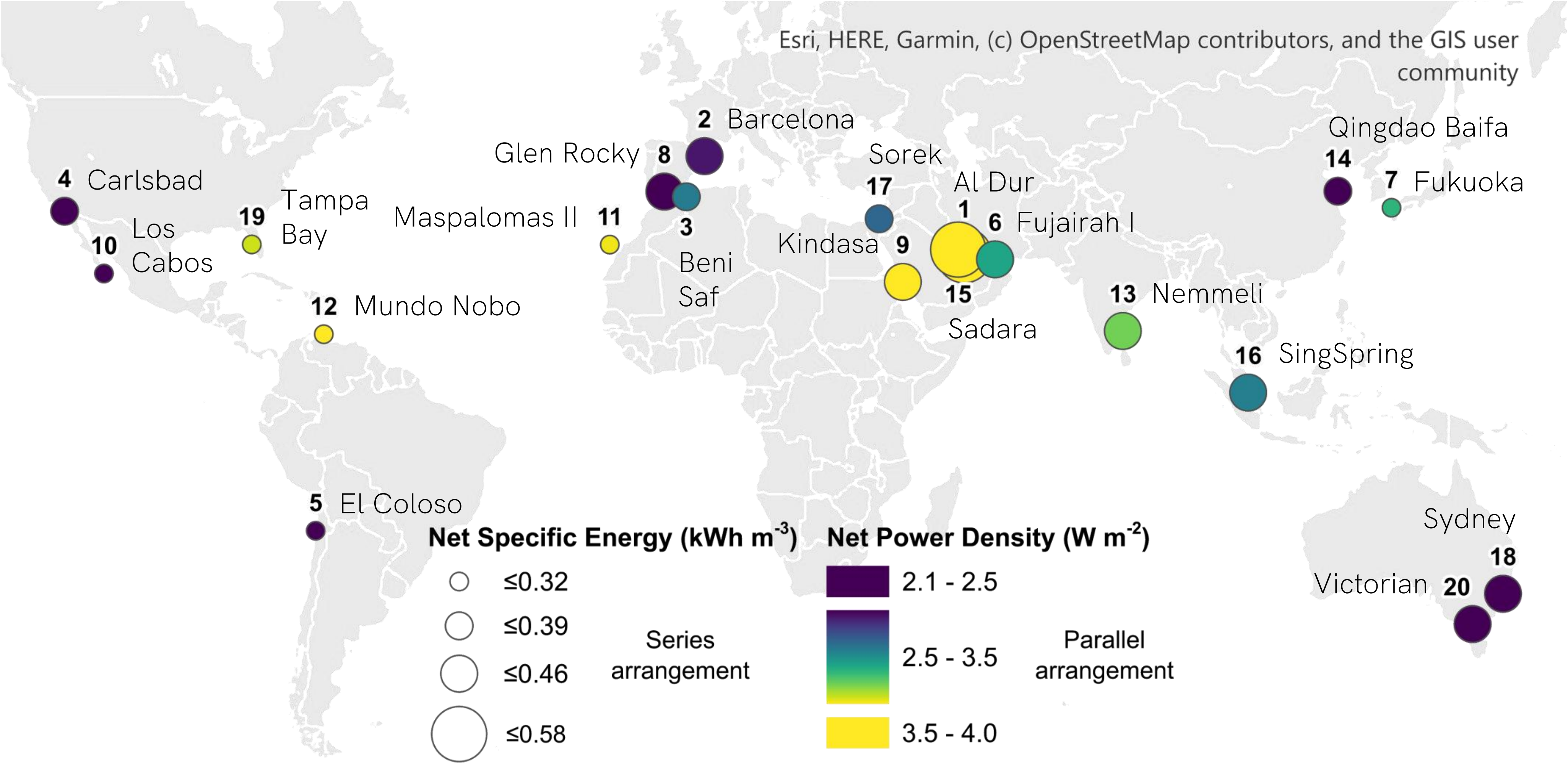
☑ Concentration

v (cm s^{-1})	T (°C)
3.0	24



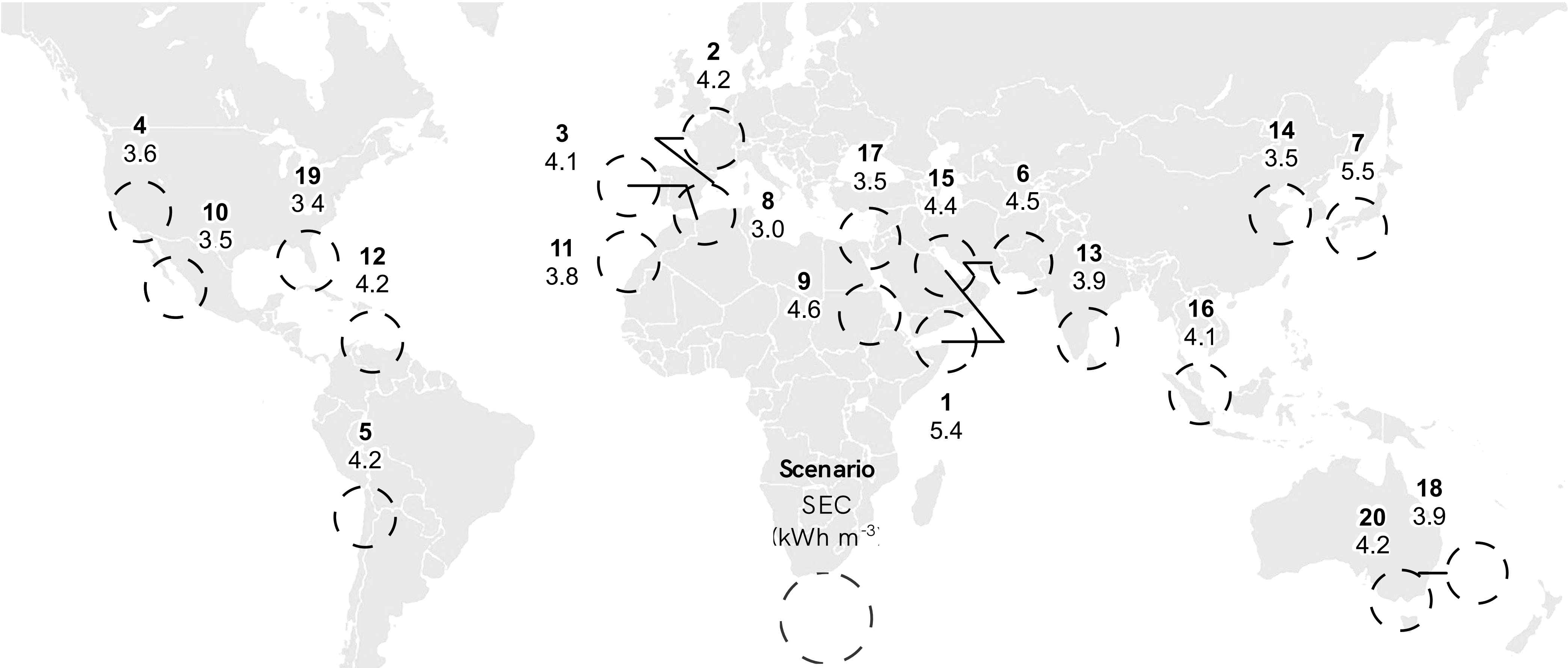
Tristán, C.; Fallanza, M.; Ibáñez, R.; et al. *Desalination* 2020, 496, 114699

RED Deployment in Desalination Plants



Tristán, C.; Fallanza, M.; Ibáñez, R.; et al. *Appl. Sci.* 2020, **10**, 7317

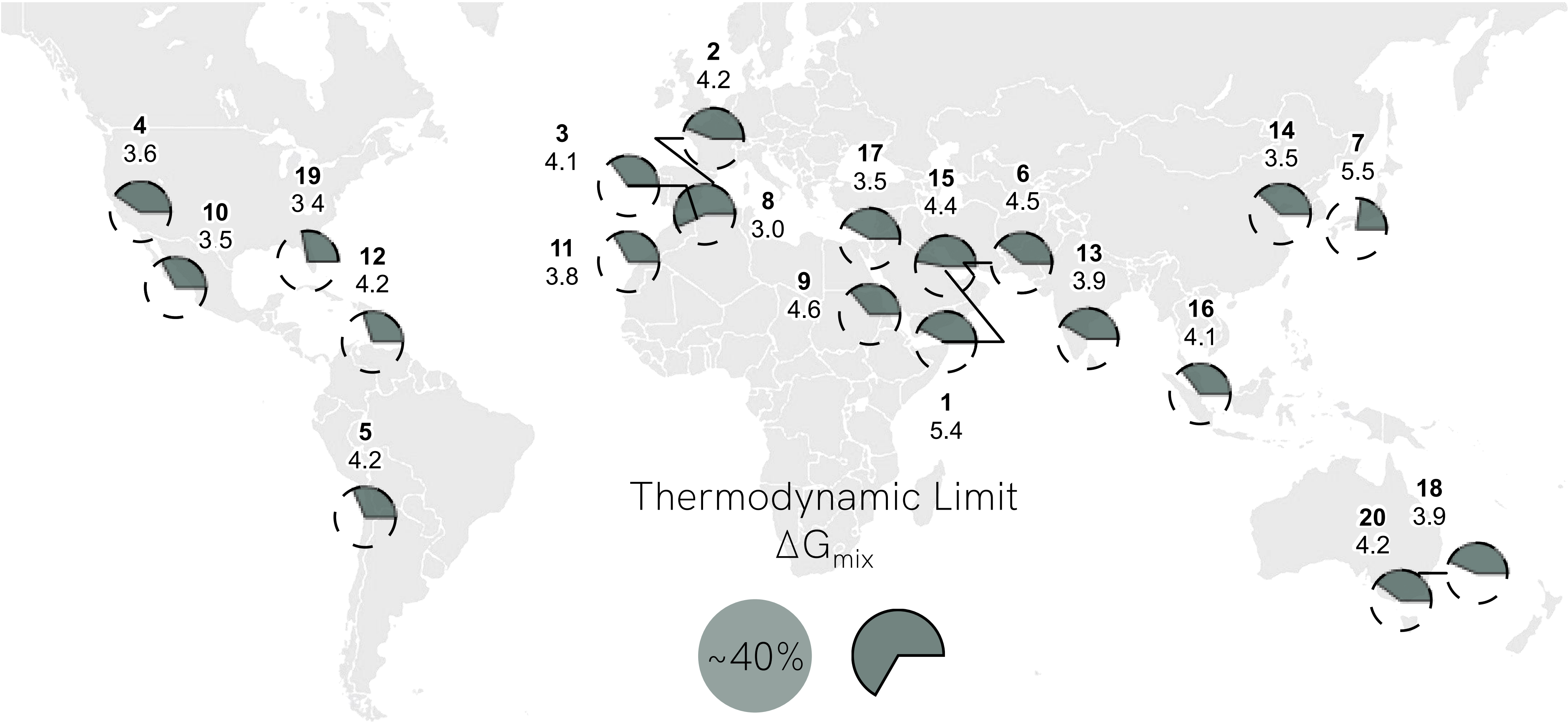
RED Deployment in Desalination Plants



100%
Grid mix

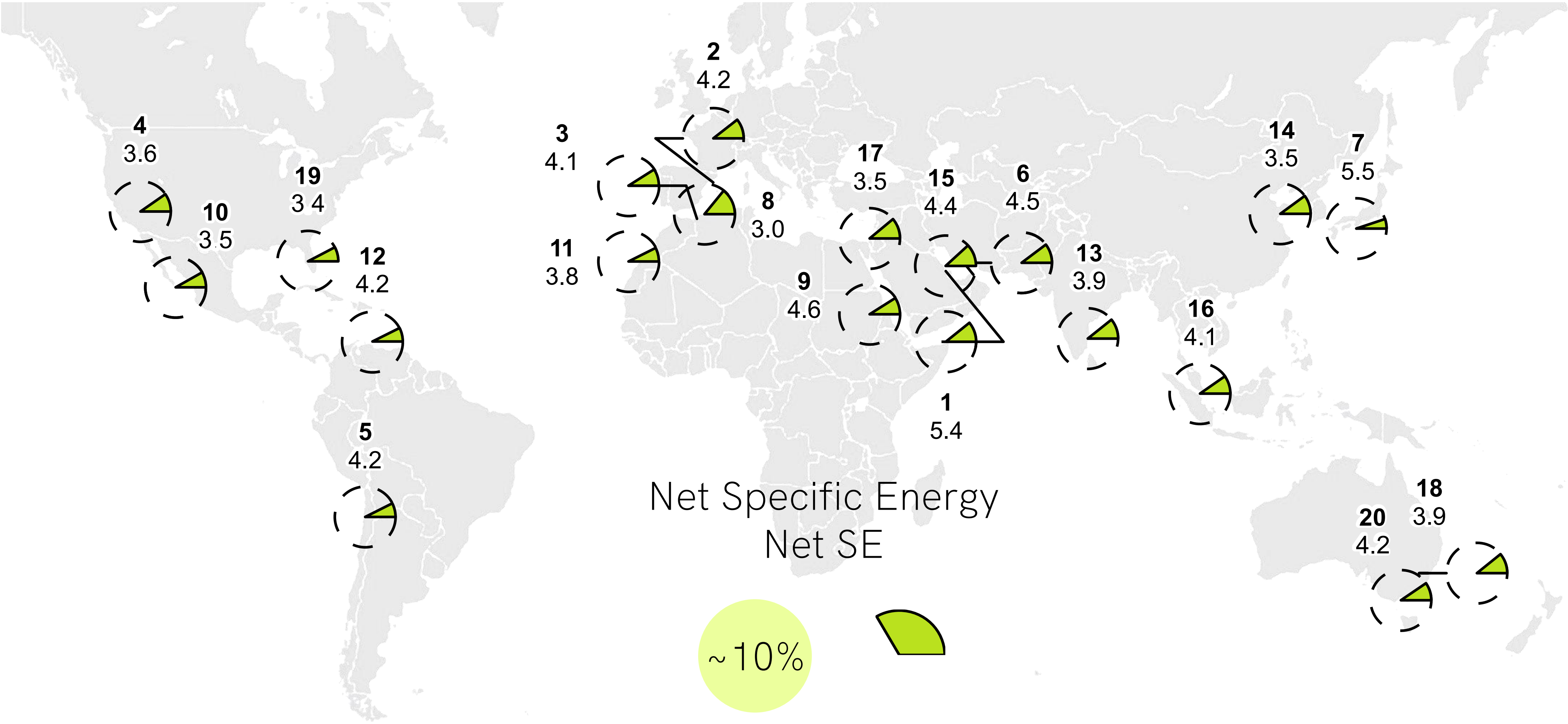
Tristán, C.; Fallanza, M.; Ibáñez, R.; et al. *Appl. Sci.* 2020, 10, 7317

RED Deployment in Desalination Plants



Tristán, C.; Fallanza, M.; Ibáñez, R.; et al. *Appl. Sci.* 2020, 10, 7317

RED Deployment in Desalination Plants



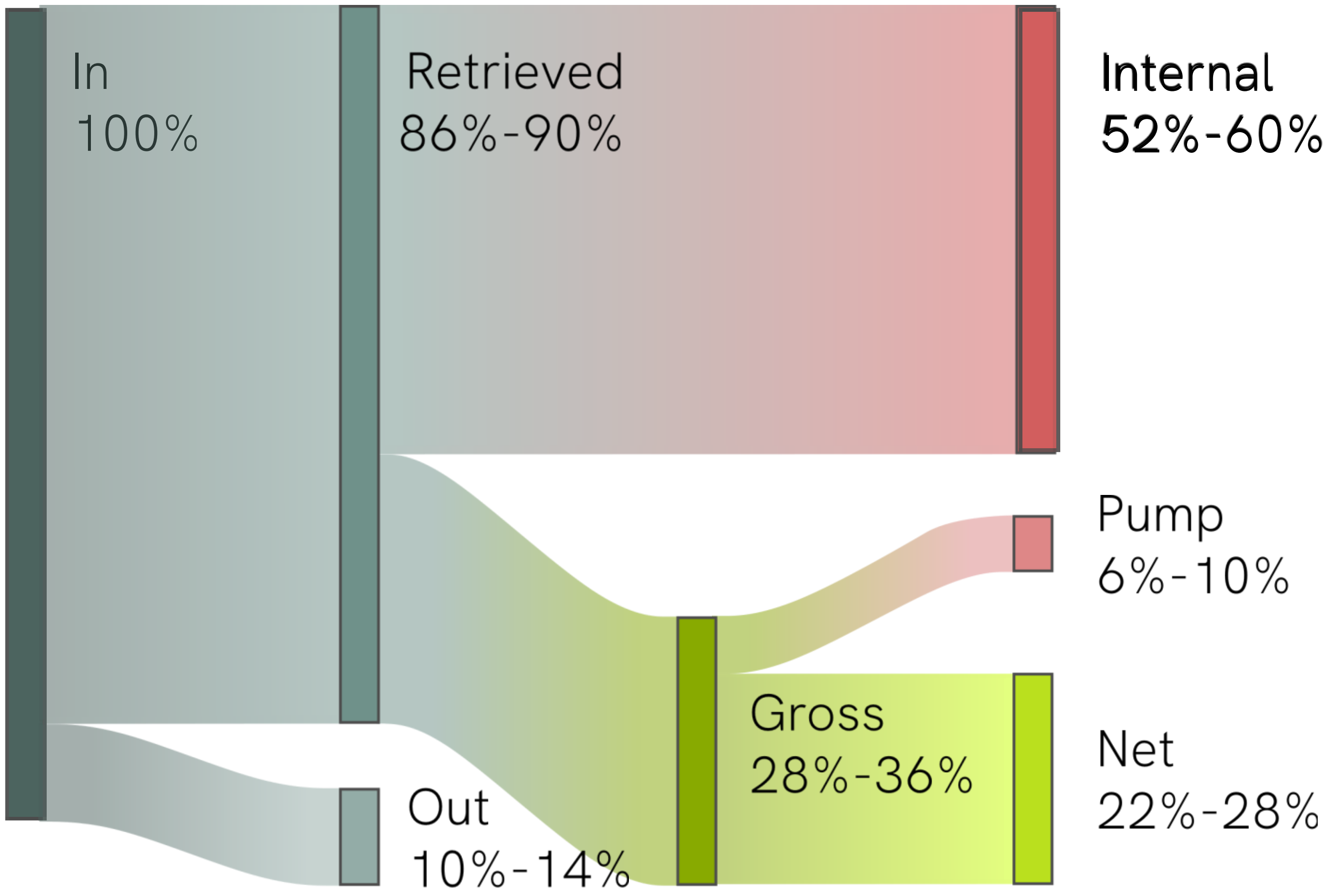
Tristán, C.; Fallanza, M.; Ibáñez, R.; et al. *Appl. Sci.* 2020, 10, 7317

RED Deployment in Desalination Plants

~40% SEC

1.0–2.3 kWh m^{-3}

Thermodynamic limit ΔG_{mix}



SEC

~10%

Tristán, C.; Fallanza, M.; Ibáñez, R.; Ortiz, I. *Appl. Sci.* **2020**, *10*, 7317

How can we assess RED technical performance?

Rigorous mathematical model of the RED process with a good agreement between experimental and simulated results to quantify the technical potential of RED recovering energy from desalination concentrates.

RED could supply 10% of the total desalination plant energy demand in its current state of development.

Is RED technology environmentally sound?

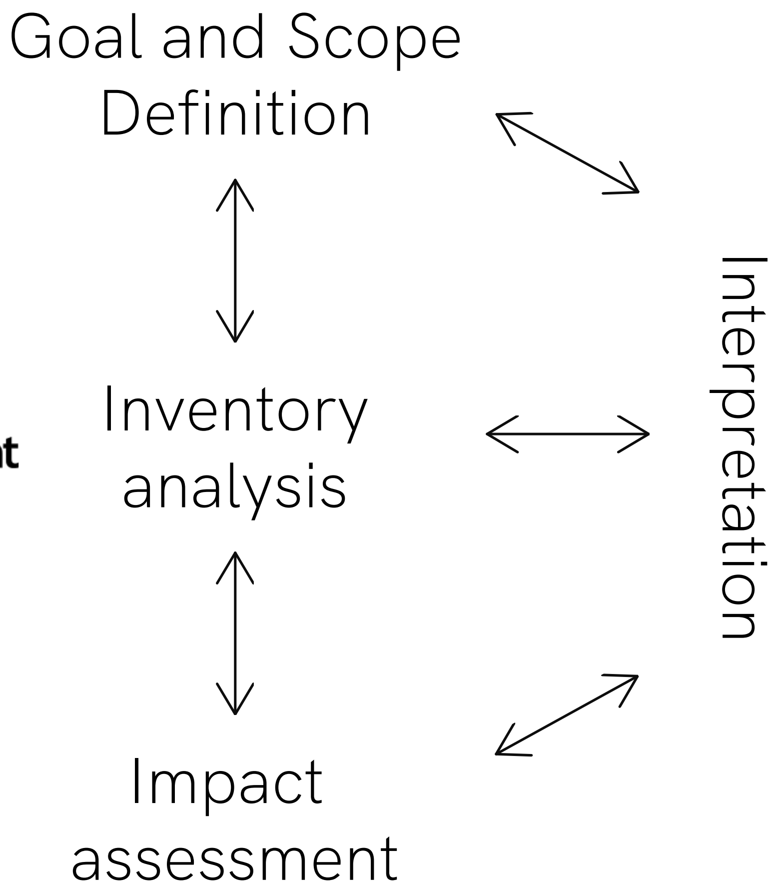
03 | LCA OF THE RED PROCESS

Sosprocan
DePRO
Desarrollo de Procesos Químicos y Control de Contaminantes

UC UNIVERSIDAD DE CANTABRIA

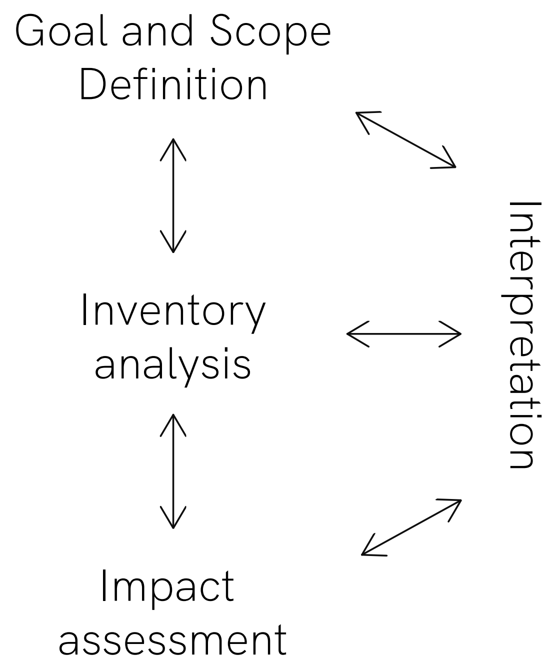
Life Cycle Assessment Framework

ISO 14040:2006 | ISO 14044:2006

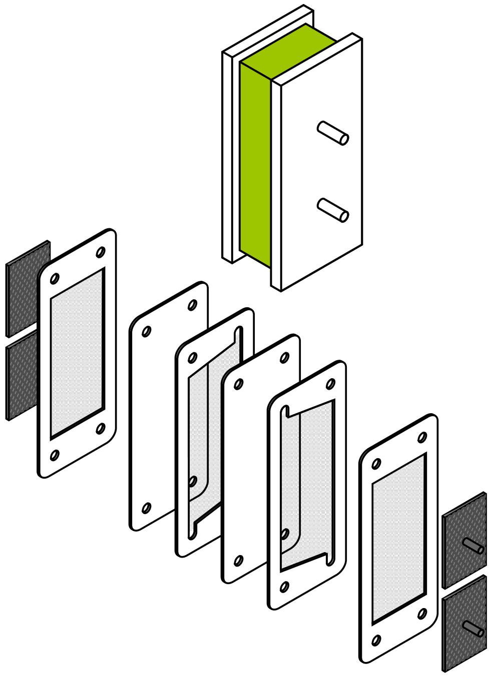


Life Cycle Assessment Framework

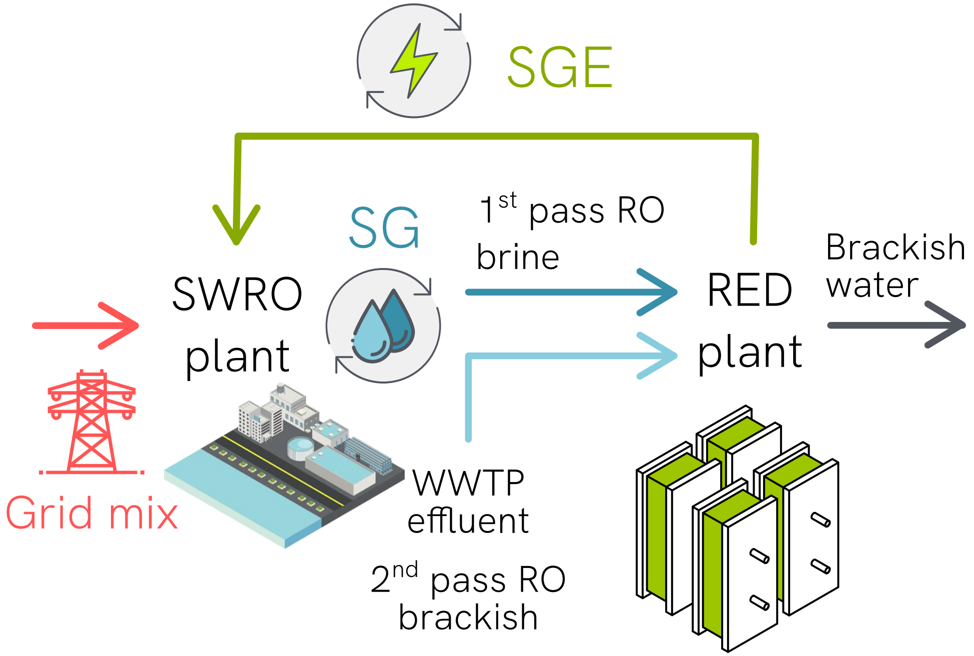
ISO 14040:2006 | ISO 14044:2006



Stand-alone RED stack

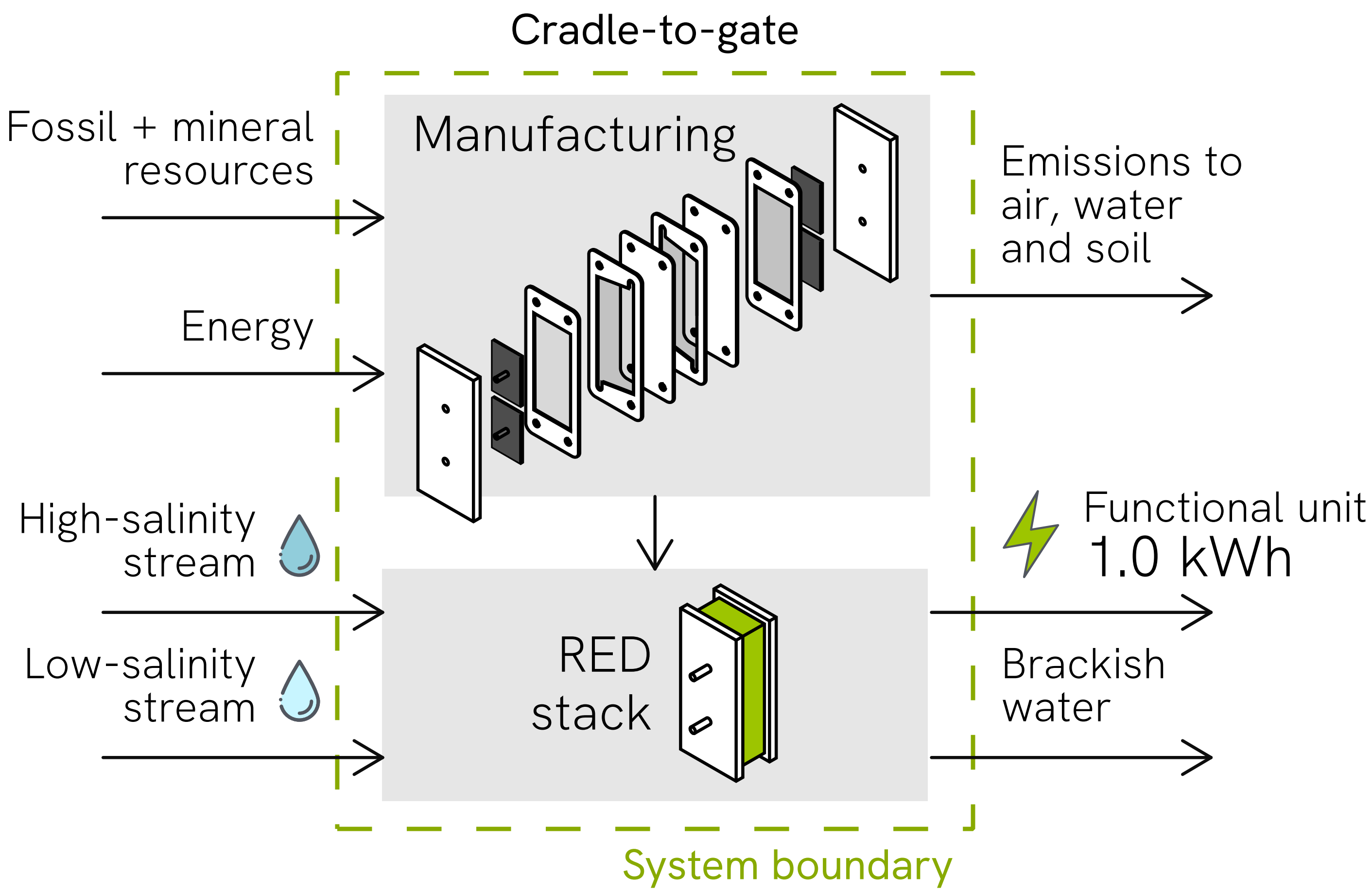


RED system into a desalination plant



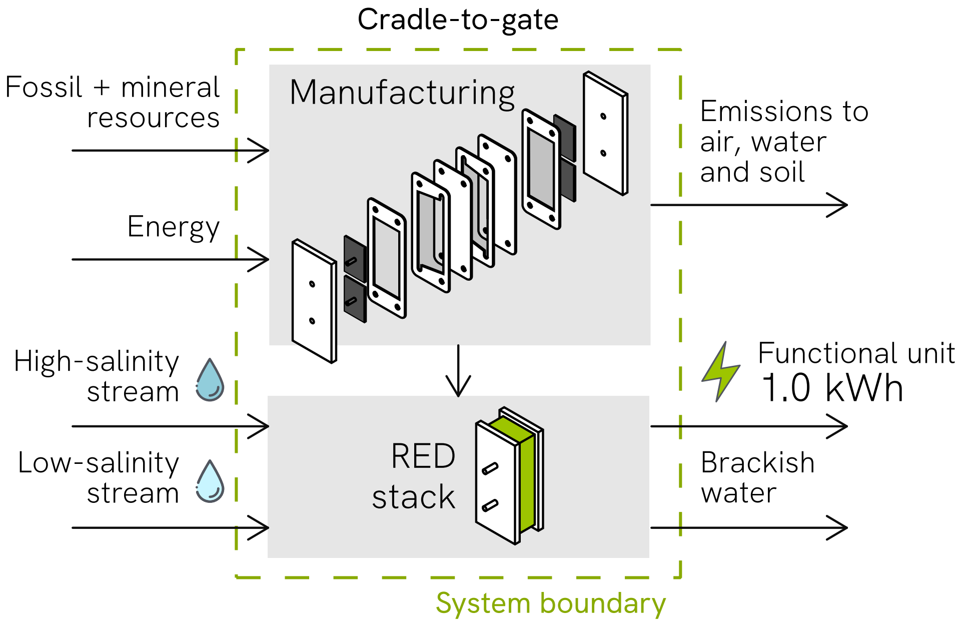
Stand-alone RED stack

Goal & Scope



Stand-alone RED stack

Goal & Scope



Midpoint Impact Indicators

CML 2001 April 2016

Impact assessment

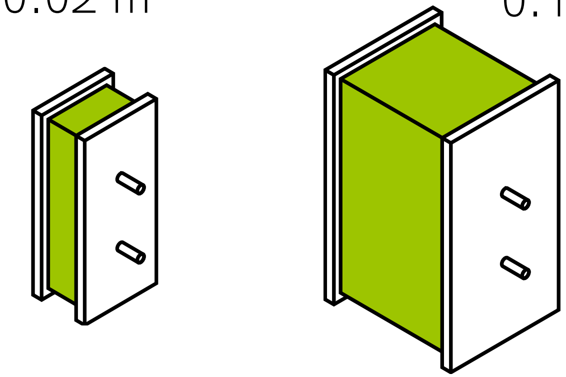
Global Warming Potential GWP_{100}

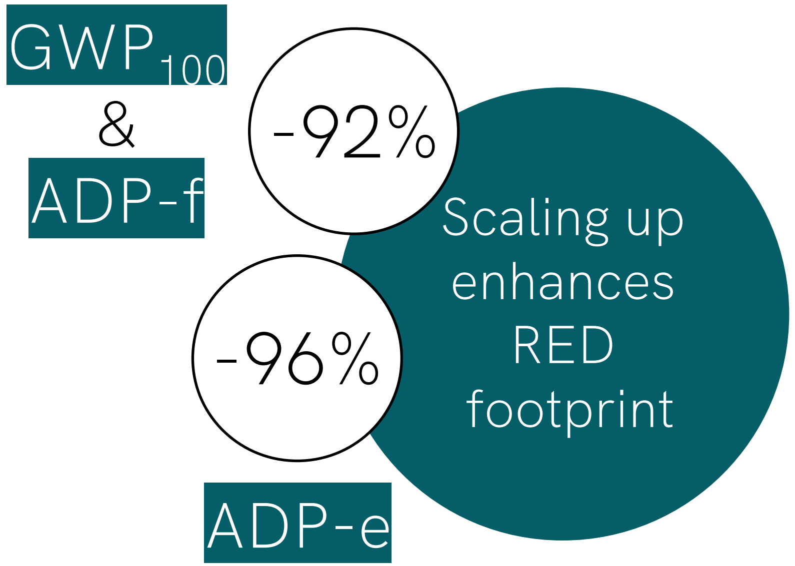
Abiotic Depletion Potential fossil ADP-f

Abiotic Depletion Potential elements ADP-e

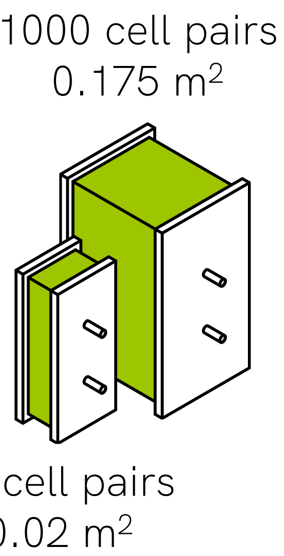
Stand-alone RED stack

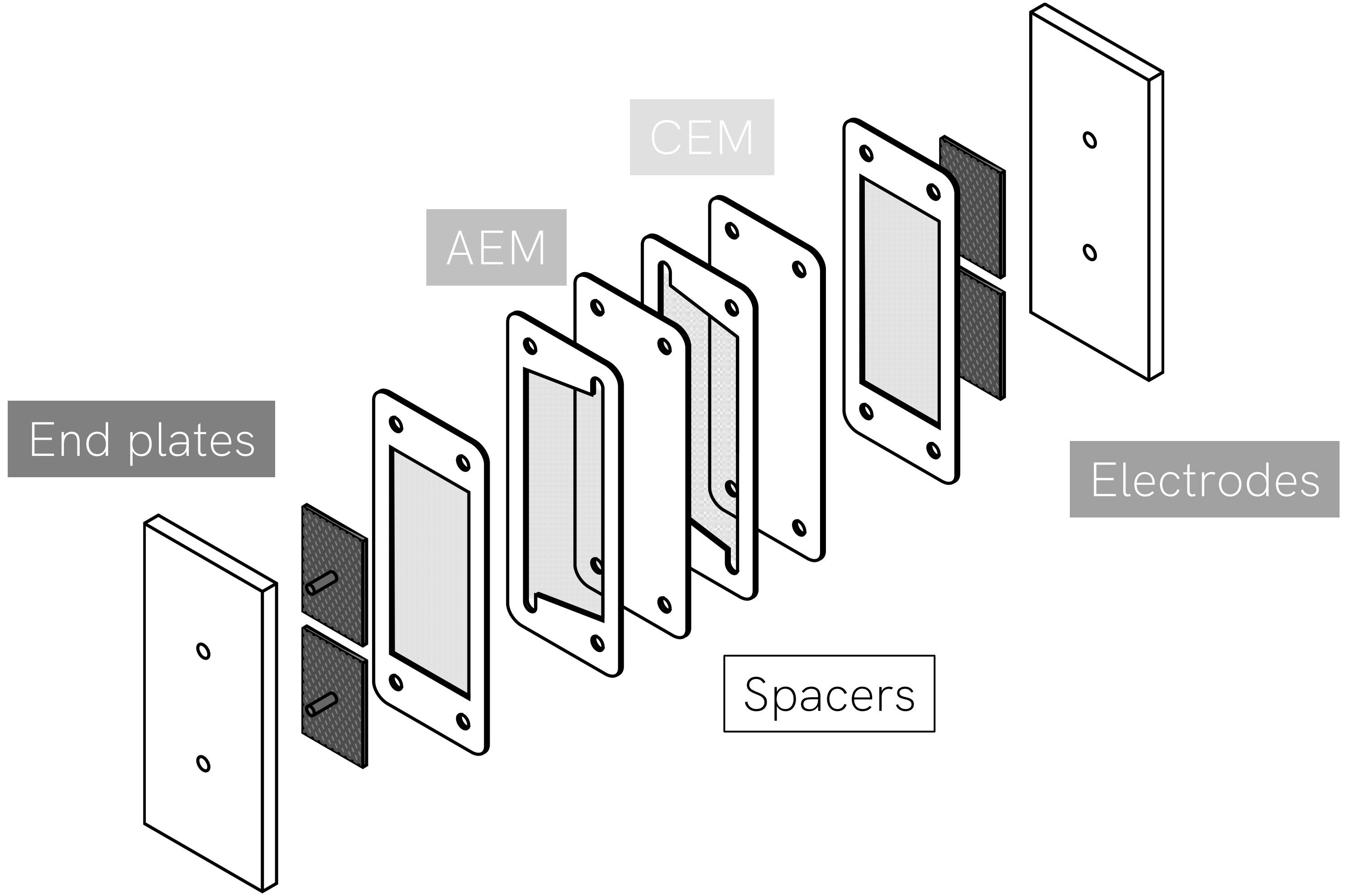
	20 cell pairs 0.02 m^2	1000 cell pairs 0.175 m^2	
Energy yield	11	4640	kWh $year^{-1}$
GWP_{100}	245	18	g CO_2-eq kWh^{-1}
ADP-f	4.22	0.32	MJ kWh^{-1}
ADP-e	1.86	0.08	mg Sb-eq kWh^{-1}





Stand-alone RED stack

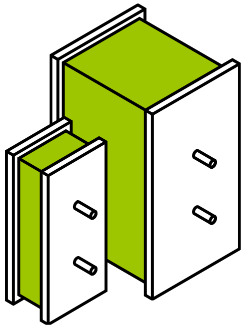




Stand-alone RED stack

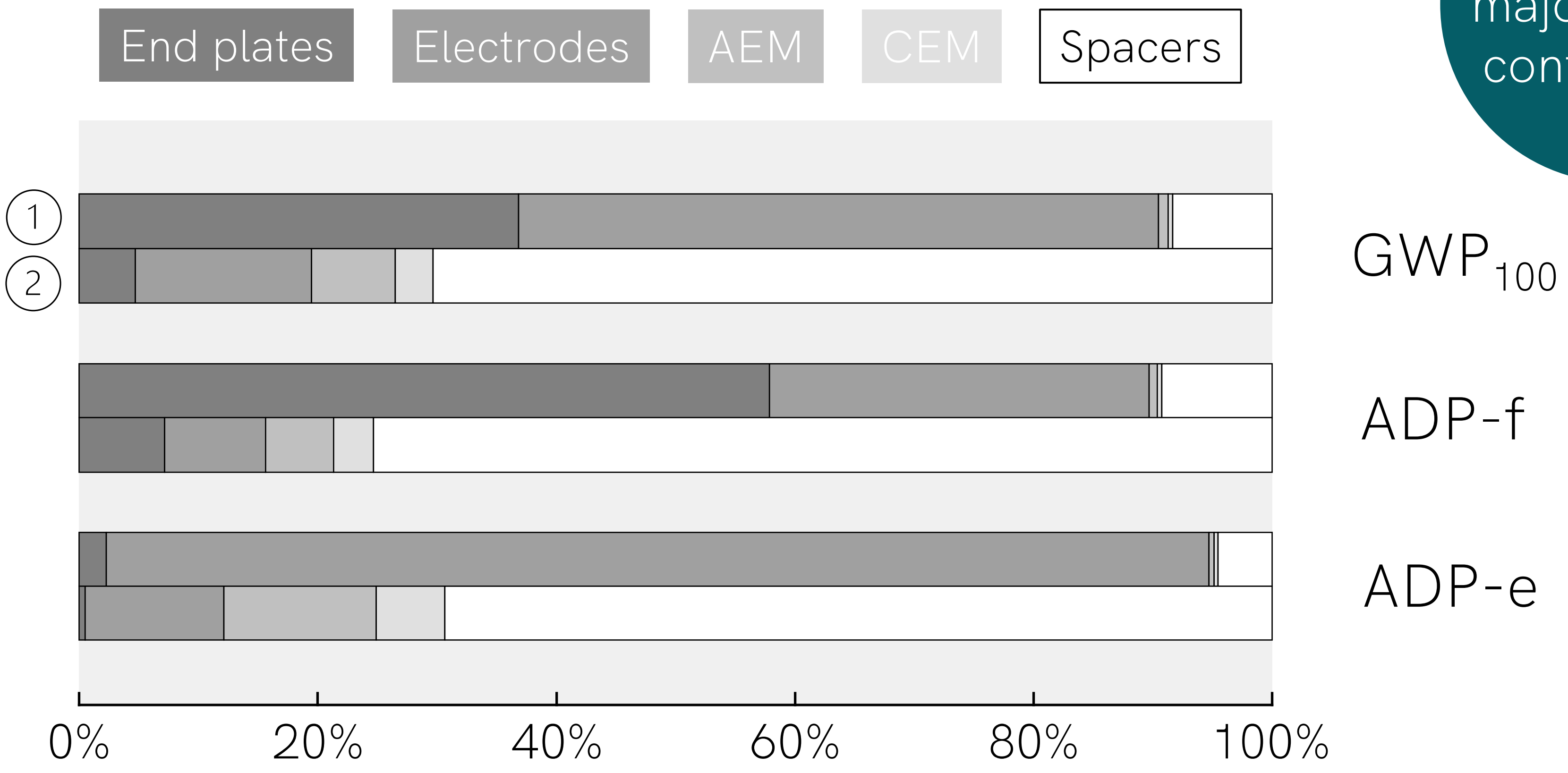
2

1000 cell pairs
0.175 m²



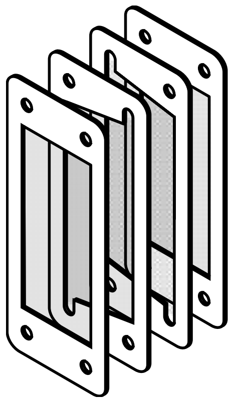
20 cell pairs
0.02 m²

1



Spacers major impact contribution

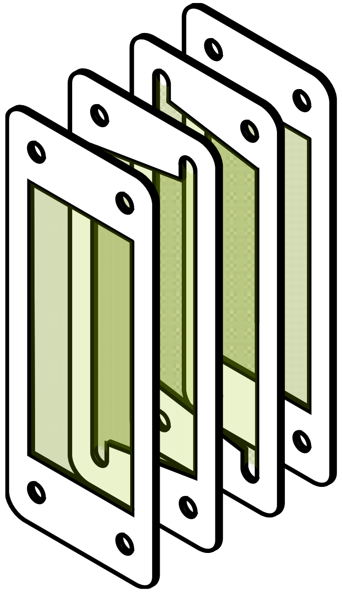
~70%



Stand-alone RED stack

Spacers
major impact
contribution

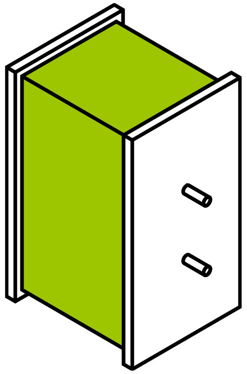
~70%



PES
Polyether sulfone

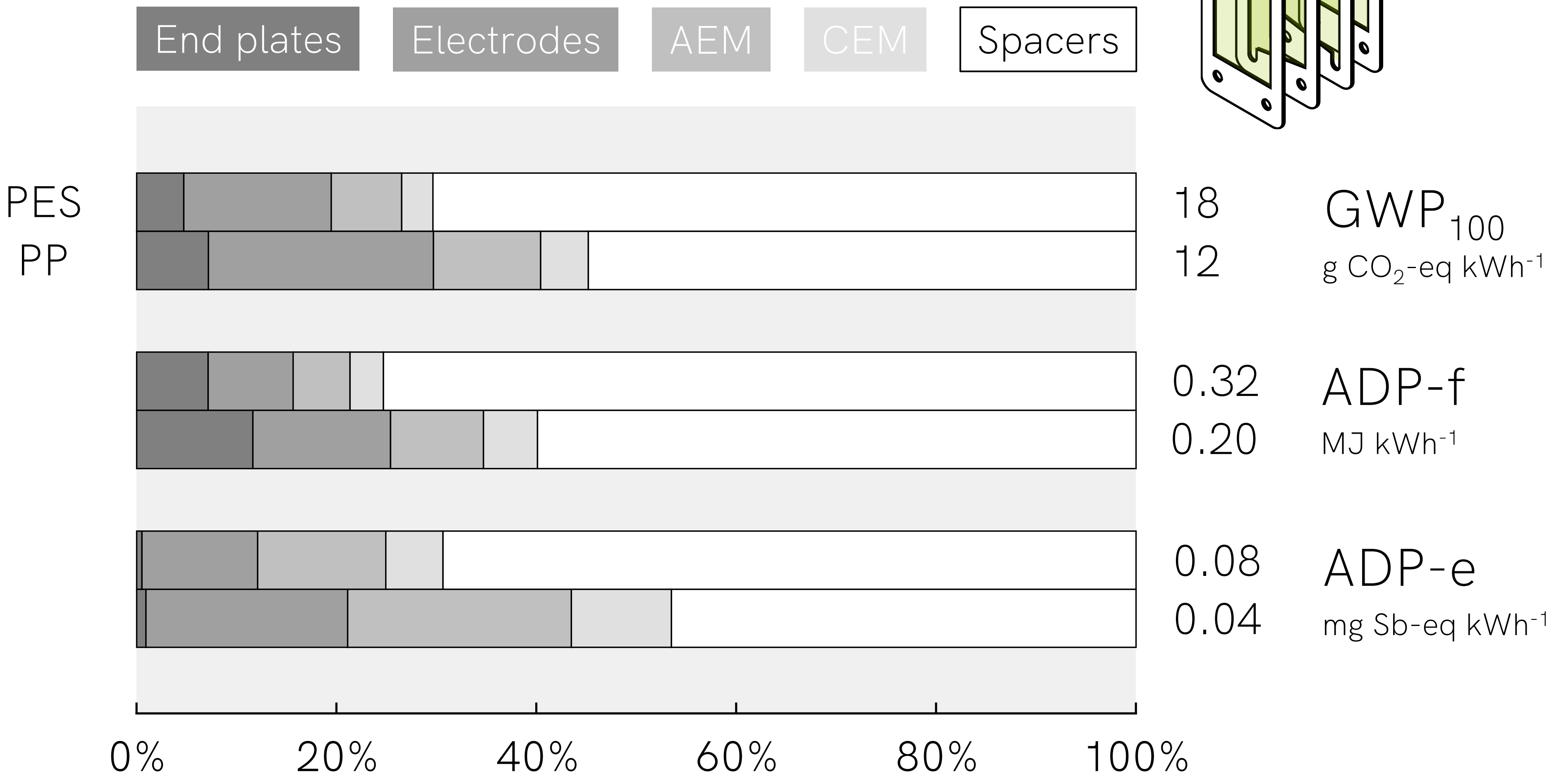
by

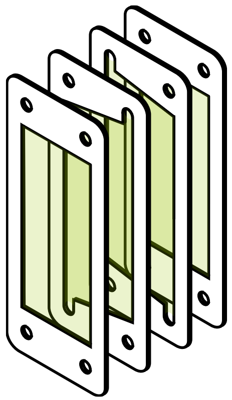
PP
Polypropylene



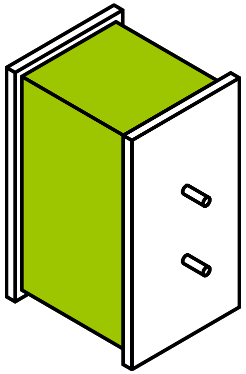
1000 cell pairs
0.175 m^2

Stand-alone RED stack



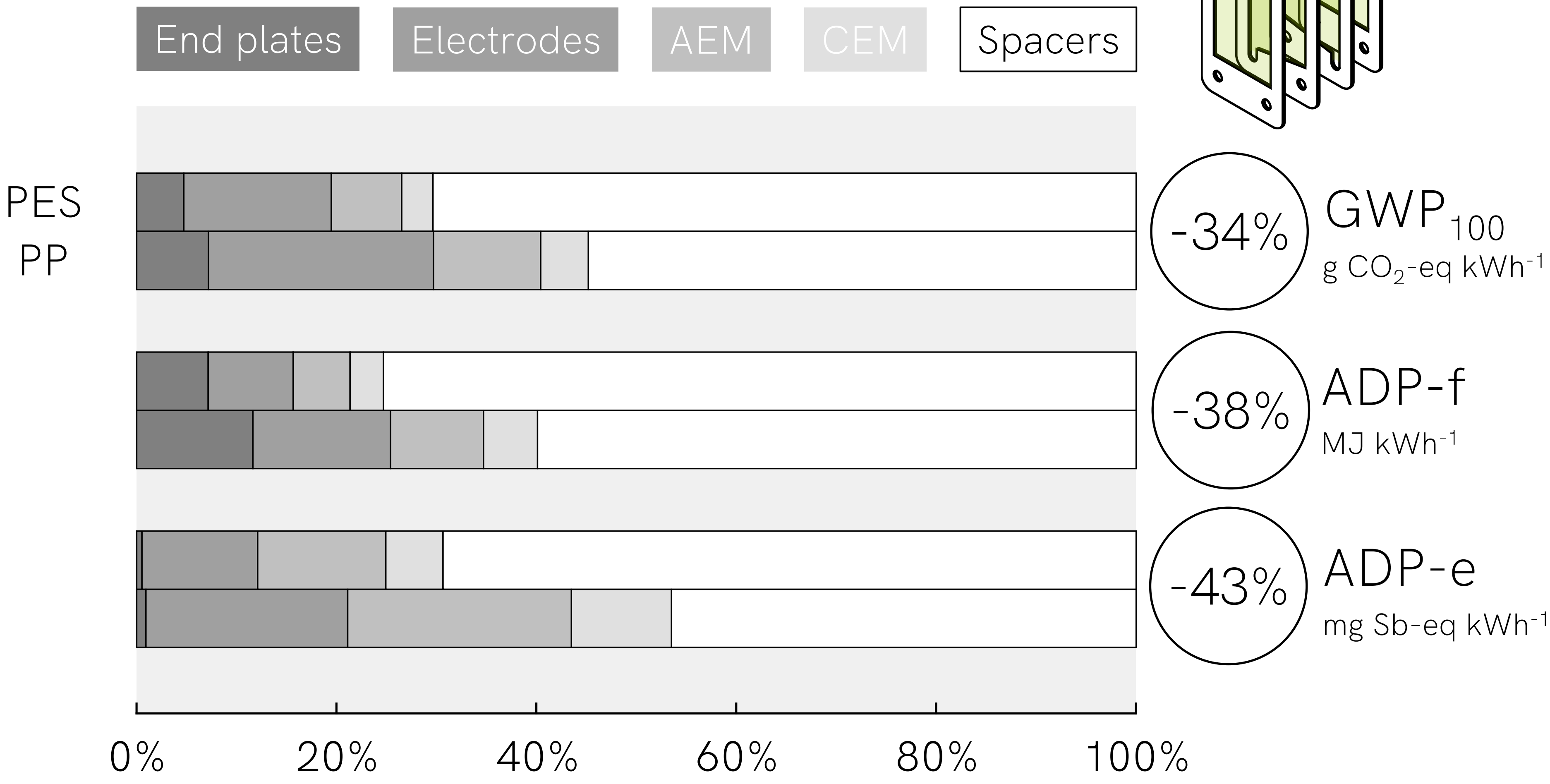


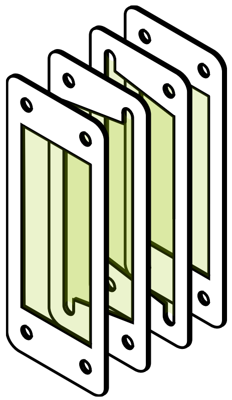
Spacers of PP reduce impact burden



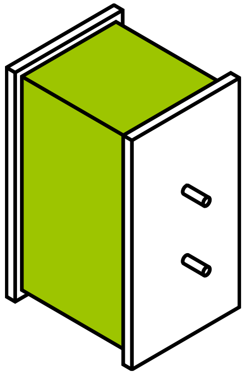
1000 cell pairs
0.175 m^2

Stand-alone RED stack



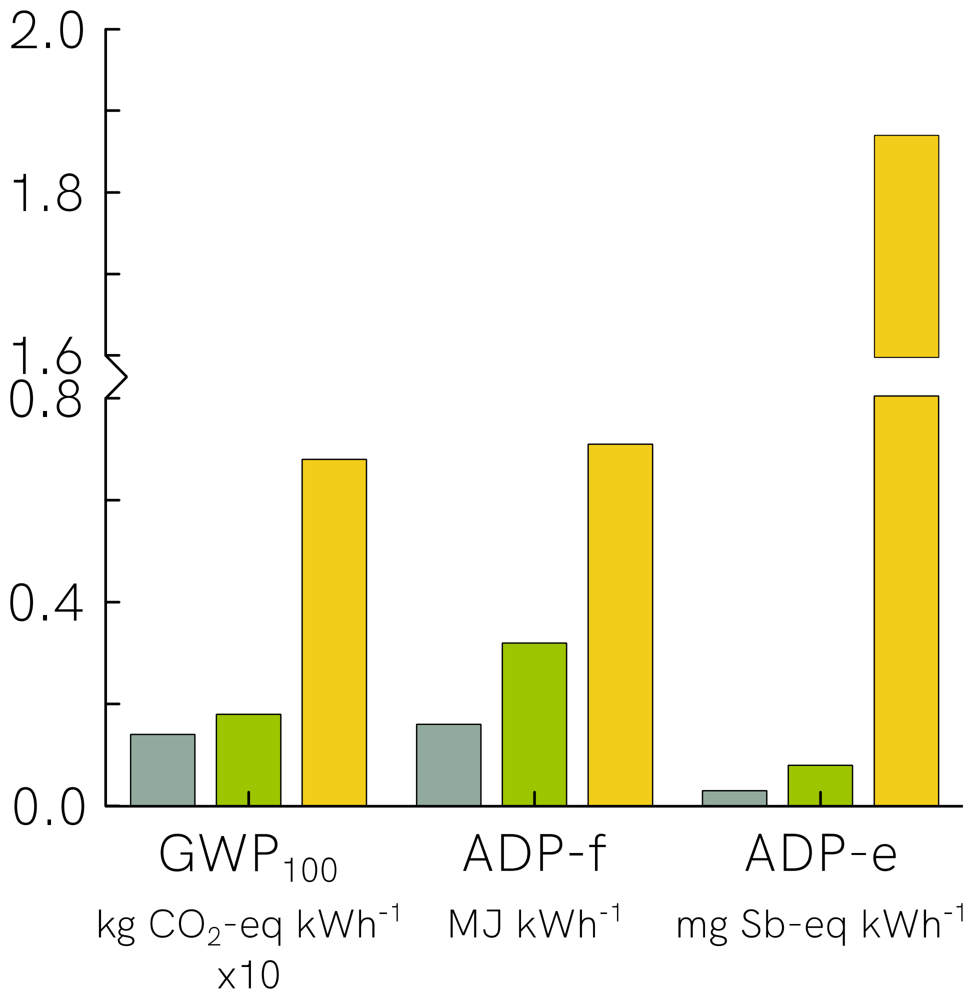


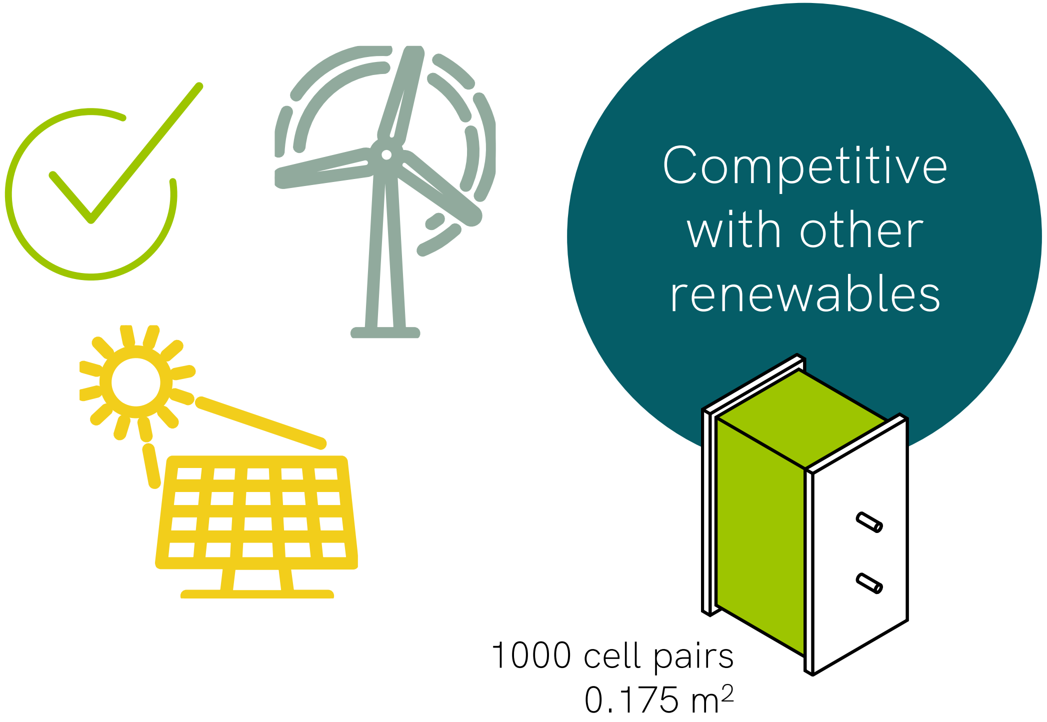
Spacers of PP reduce impact burden



1000 cell pairs
0.175 m²

Stand-alone RED stack

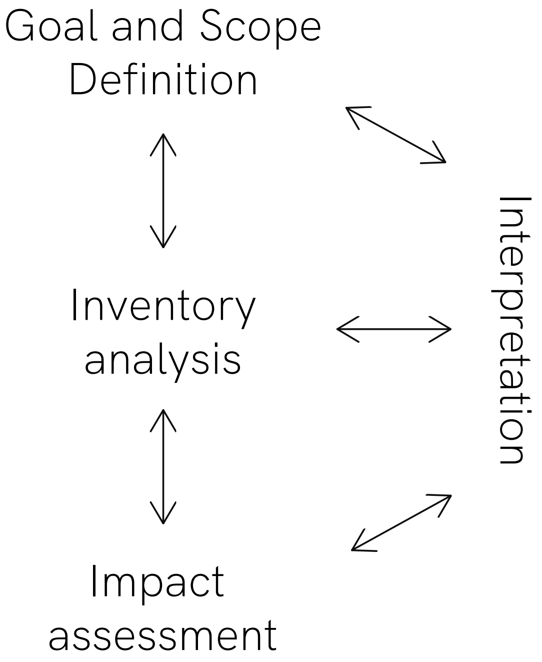




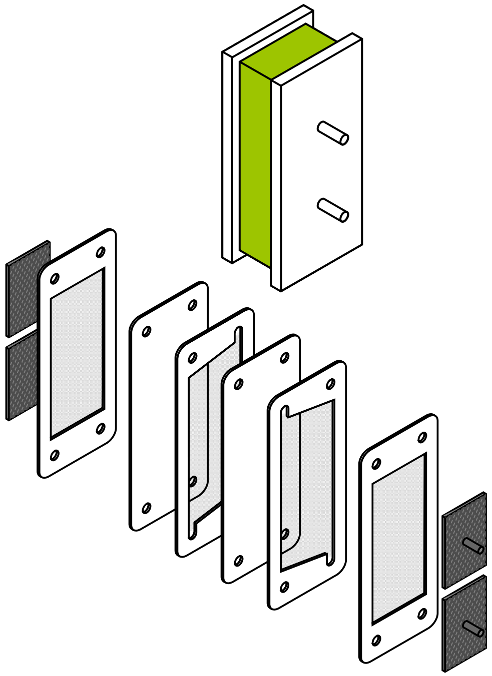
Electricity production ES; reference year: 2014 (ecoinvent v3.5)
*PV, 570 kWp open ground installation, multi-Si
**Wind, 1-3MW turbine, onshore

Life Cycle Assessment Framework

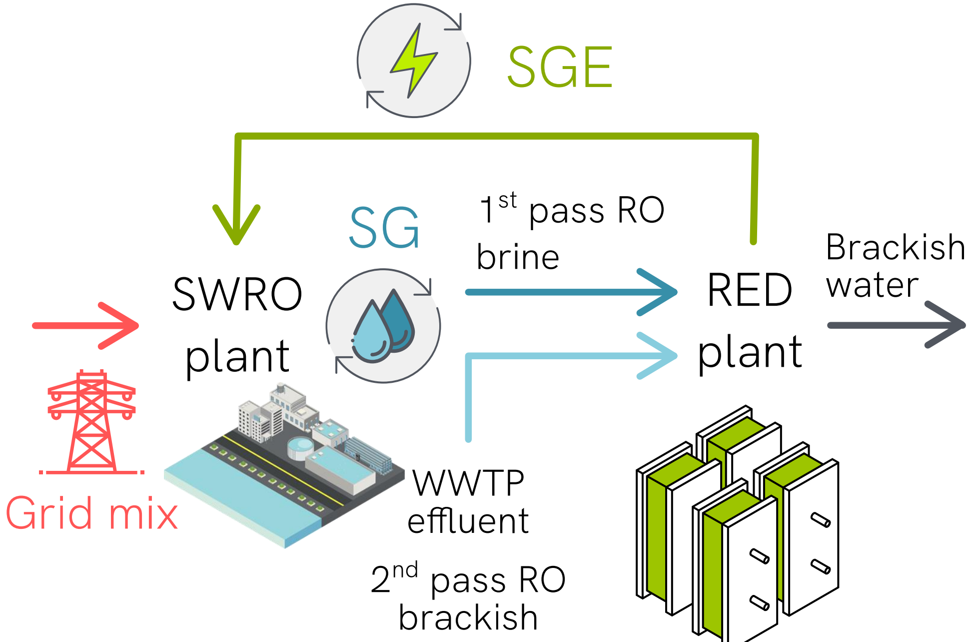
ISO 14040:2006 | ISO 14044:2006



Stand-alone RED stack

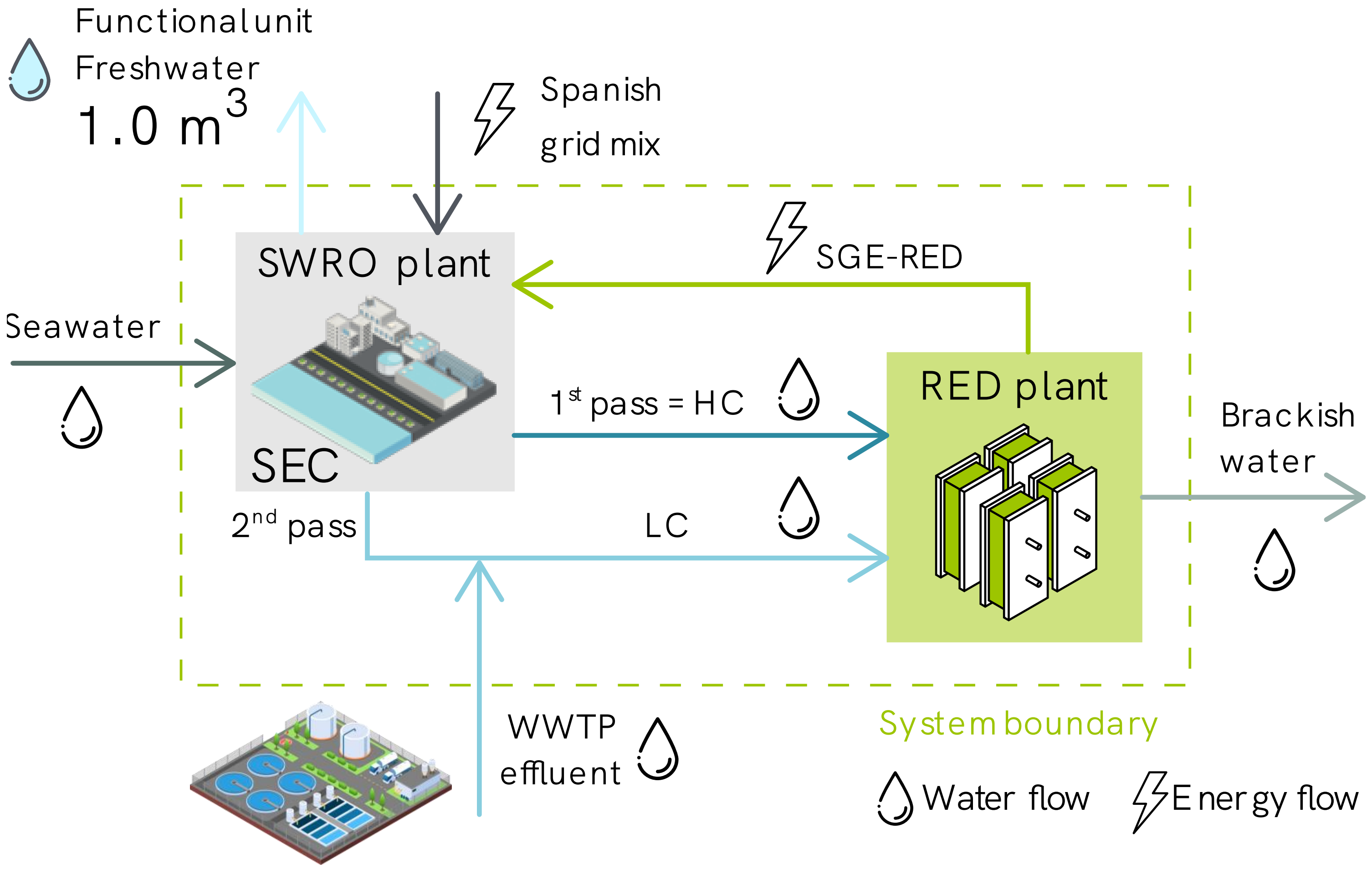


RED system into a desalination plant

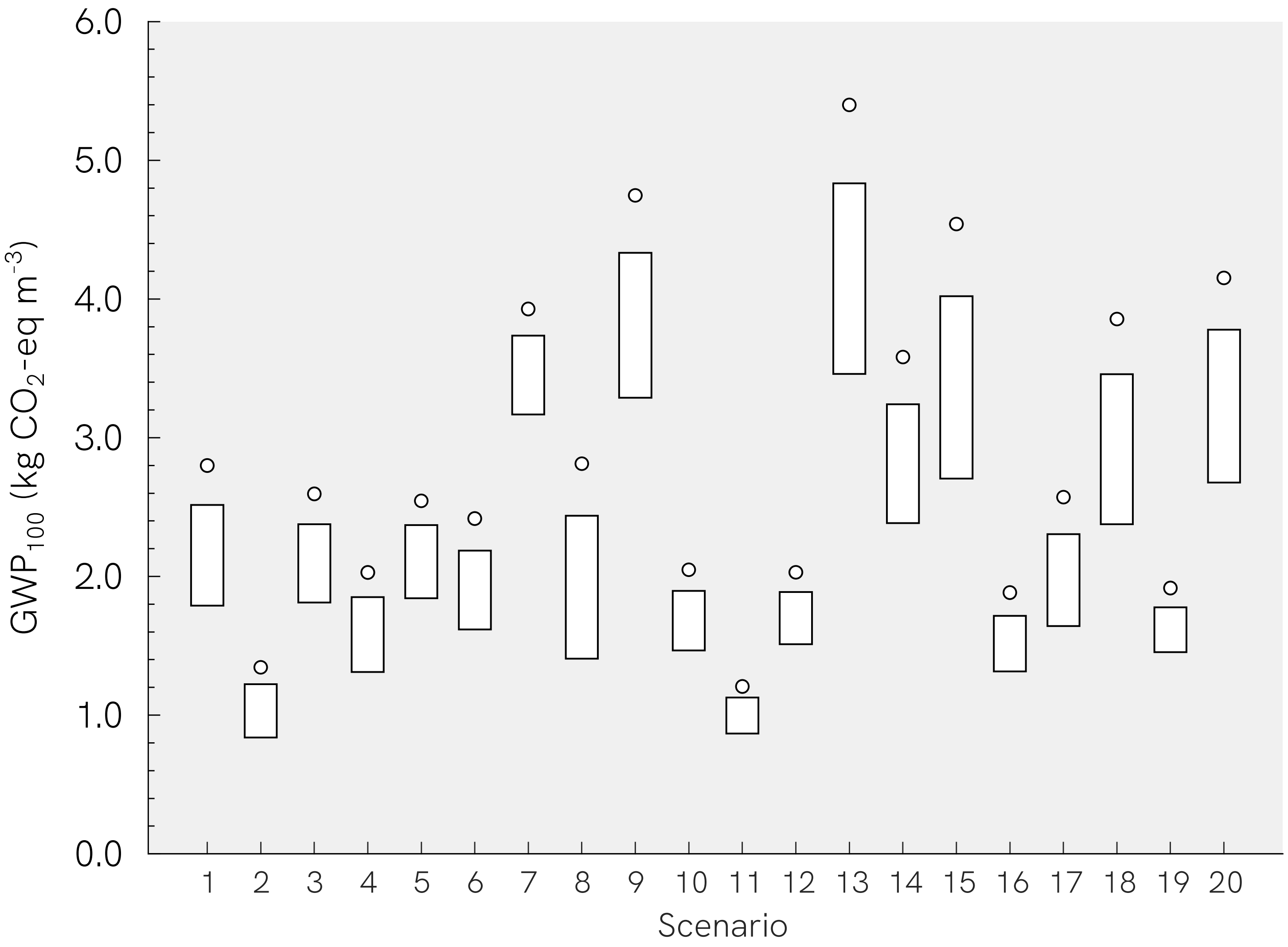


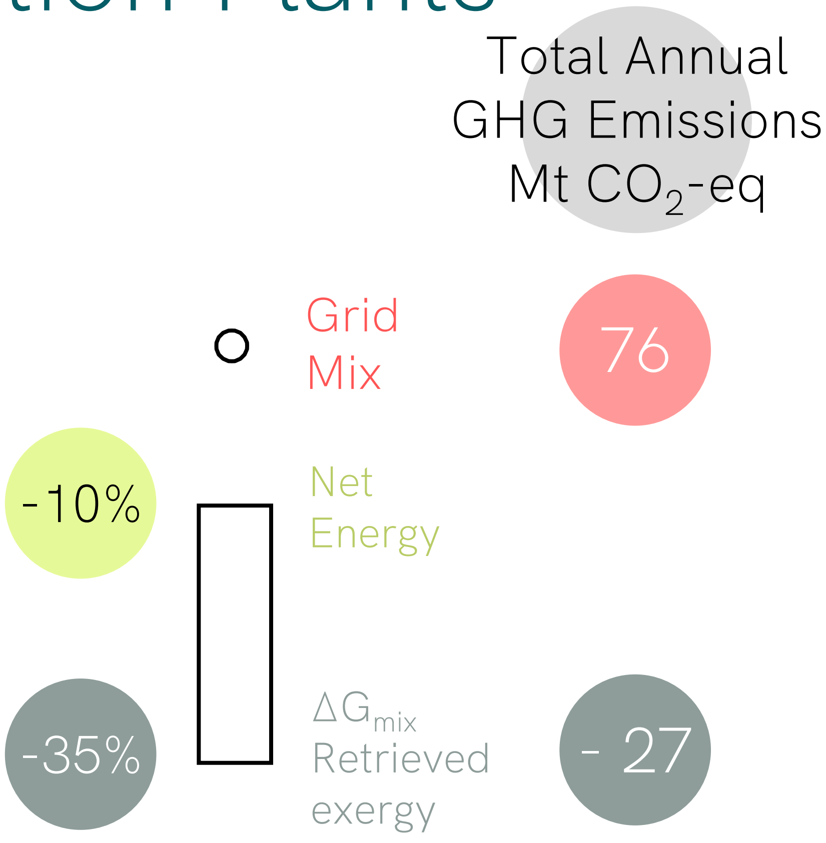
RED Deployment in Desalination Plants

Goal & Scope



RED Deployment in Desalination Plants





Global Clean Water Desalination Alliance "H_20 minus CO_2" Concept paper; Global Clean Water Desalination Alliance: Abu Dhabi, UAE, 2015.

Global Desalination (2015)

Tristán, C.; Fallanza, M.; Ibáñez, R.; Ortiz, I. *Appl. Sci.* 2020, **10**, 7317

Is RED technology environmentally sound?

1st ever LCA of RED.
Competitive with other RES.
Spacers major contribution in all impact categories.
PES by PP spacers → -35% GWP, -40%.ADP-f and ADP-e.

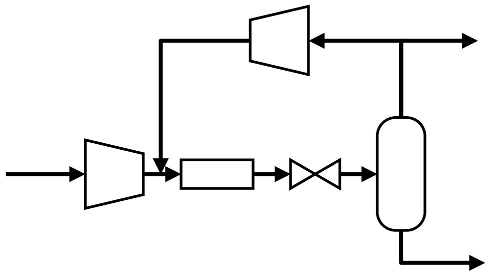
RED improves desalination environmental performance.
Up to -35% of desalination GHG emissions (~30 Mt CO_2-eq year^{-1}).

How can we define powerful, efficient, sustainable, and cost-effective designs for RED?

04 | OPTIMIZATION RED PROCESS

Prof. Ignacio E. Grossmann

Mathematical Programming



Superstructure Representation

↓

Optimization Model

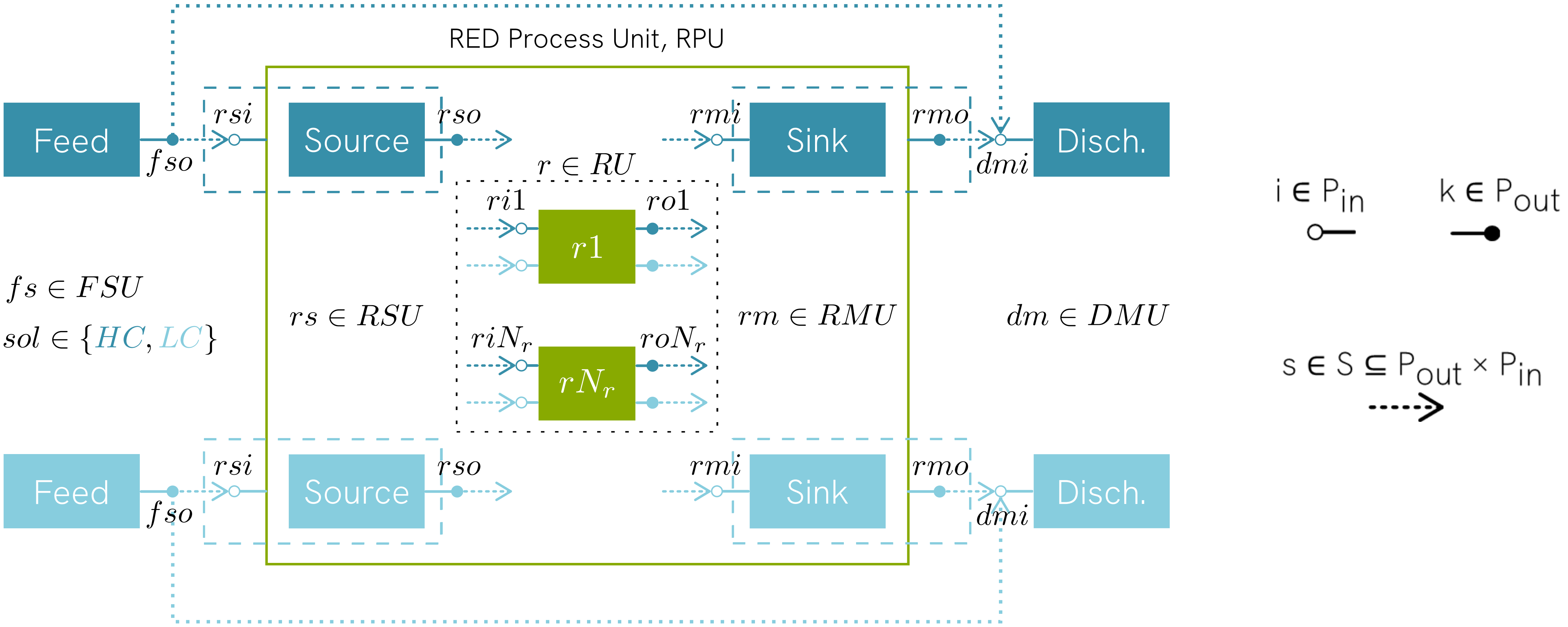
$$
\begin{aligned}
\max obj = \; & f(x) \\
s.t. \; & g(x) \leq 0 \\
& \begin{bmatrix} Y_r \\ r_r(x) \leq 0 \end{bmatrix} \veebar \begin{bmatrix} \neg Y_r \\ B^r \; x = 0 \end{bmatrix} \quad \forall \; r \in RU \\
& \Omega(Y_r) = True \\
& x \in X \subseteq R^n \\
& Y_r = \{True, \; False\} \quad \forall \; r \in RU
\end{aligned}
$$

Optimization algorithm

↓

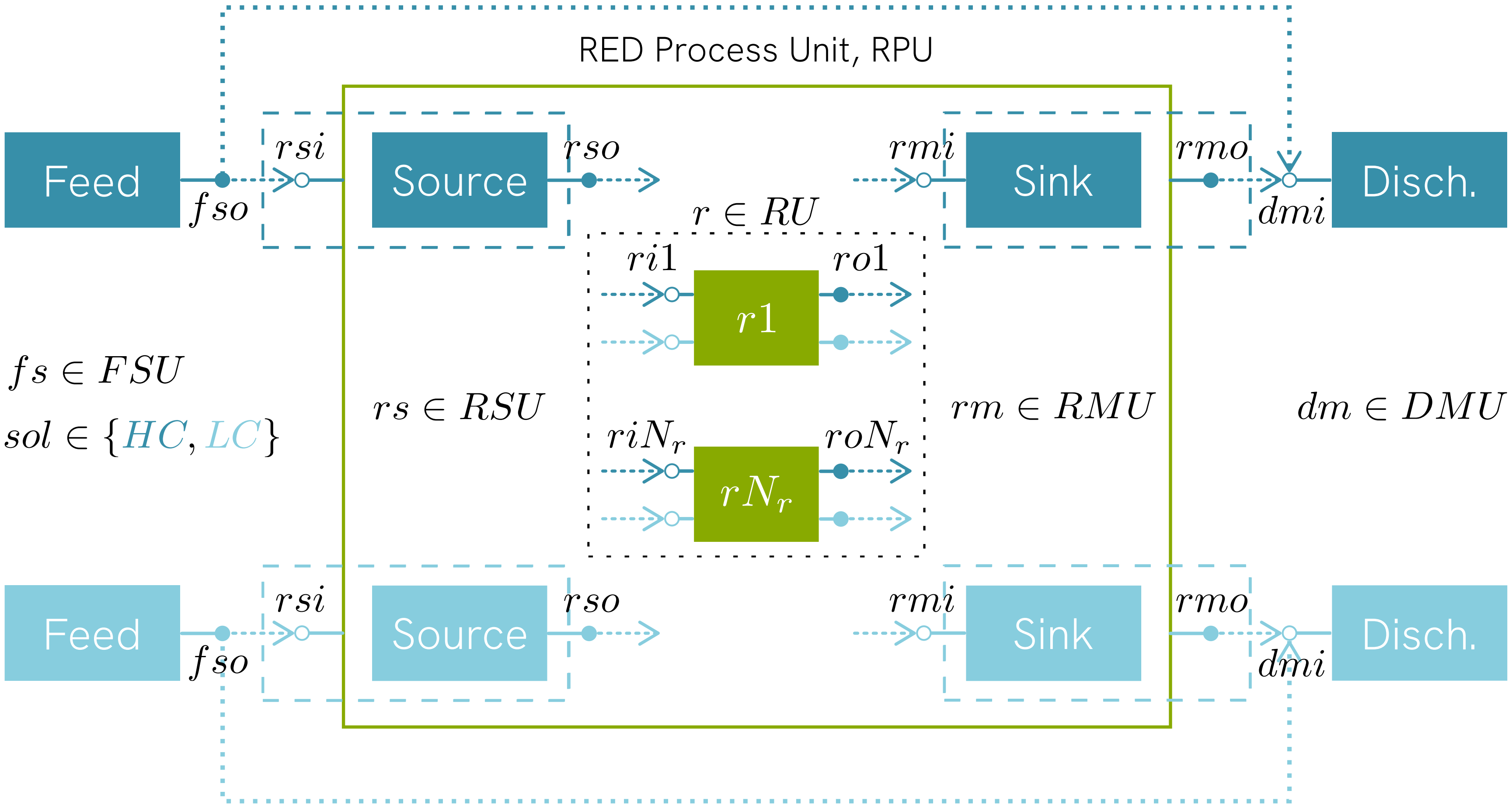
Optimal Solution

Superstructure Representation



Q. Chen, Y. Liu, G. Seastream, J.D. Siirola, I.E. Grossmann, Comput. Chem. Eng. (2021) 107414.

Superstructure Representation



Flow Representation

Total flow

Species Composition

Quesada I, Grossmann IE. Comput Chem Eng 1995;19:1219-42.

Non-Convex GDP Optimization Model

Net Present Value

Objective max obj = f(x) max NPV

s.t. $g(x) \leq 0$

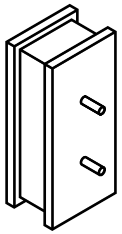
$$\begin{bmatrix} Y_r \\ r_r(x) \leq 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y_r \\ B^r x = 0 \end{bmatrix} \quad \forall\, r \in RU$$

$$\Omega(Y_r) = True$$

$$x \in X \subseteq \mathbb{R}^n$$

$$Y_r = \{True, False\}$$

RED Stack



ED-1750
fumatech®

Feed Streams

Molar Concentration
Flow rate
Temperature

Financial Parameters

e.g., project lifetime,
discount rate

Non-Convex GDP Optimization Model

Semi-rigorous RED Stack Model

Net Present Value

Objective $\quad \max obj = f(x)$ max NPV

s.t. $g(x) \leq 0$ Global Constraints

Mass Balances

Feed Splitter | RED Process Splitter/Mixer | Discharge Mixer

RED Stack Model — RED Stack Equations Constraints

$$\begin{bmatrix} Y_r \\ r_r(x) \leq 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y_r \\ B^r x = 0 \end{bmatrix} \quad \forall\, r \in RU$$

Disjunction

RED unit exist
XOR
RED unit absent

$\Omega(Y_r) = True$ Logic Propositions

$x \in X \subseteq \mathbb{R}^n$ Continuous Variables

$Y_r = \{True, False\}$ Boolean Variables

Objective Function: Net Present Value

$$\max NPV = \frac{TNP\ LF\ 8760\ (ep + cp\ ef) - TAC}{CRF}$$

Total Annual Cost

$$TAC = CRF\ CAPEX + OPEX$$

CAPEX = Stack + Pumps + Infrastructure

OPEX = Electricity cost pumps + IEMs replacement + O&M

Capital Recovery Factor

$$CRF = \frac{r}{1 - (1 + r)^{-LT}}$$

Objective Function: Net Present Value

$$\max NPV = \frac{TNP\ LF\ 8760\ (ep + cp\ ef) - TAC}{CRF}$$

Revenue

Annual Energy yield (EY) = TNP LF 8760

Electricity sales = EY ep

Emission allowances = EY cp ef

Capital Recovery Factor

$$CRF = \frac{r}{1 - (1 + r)^{-LT}}$$

Techno-Economic Metrics

Technical

Net Power Density

Net Efficiency

Economic

NPV

LCOE

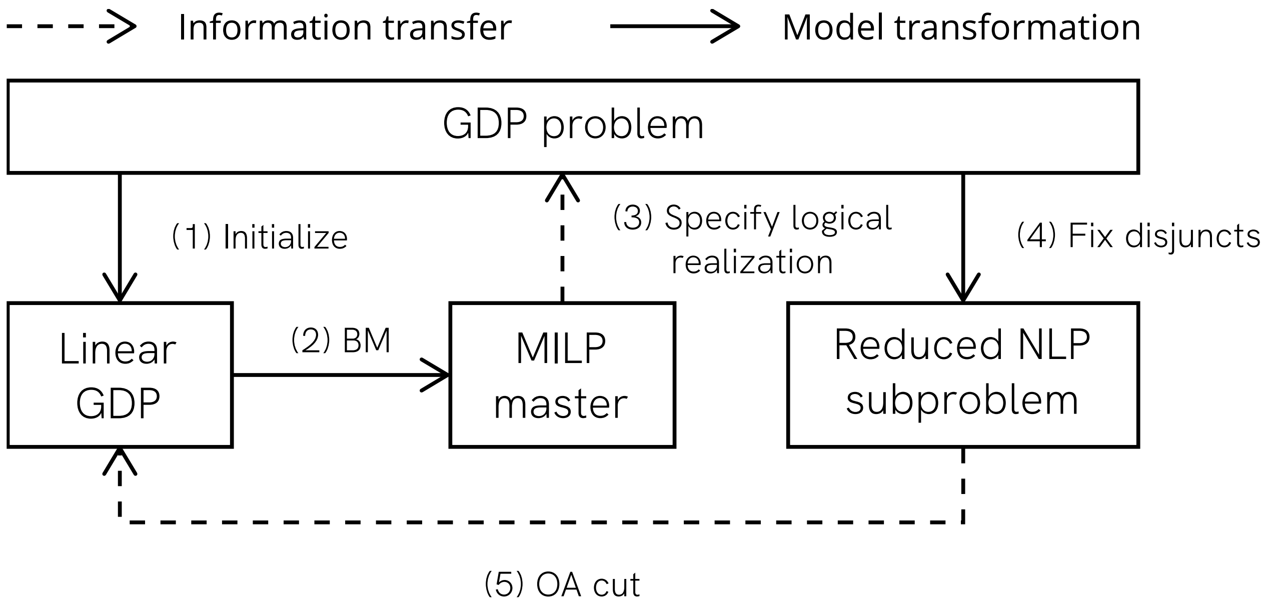
Solution Strategy

Solver
GDPopt 20.2.28

Strategy
Global Logic Outer Approximation (GLOA)

Sub-solvers GAMS 34.1.0
NLP: MSNLP (IPOPTH)
MILP: CPLEX

Intel® Core™ i7-8700 CPU @3.2 GHz, RAM 16 GB
Windows 10 (x64)



Illustrative Example

Problem Statement

RED stack Parameters

ED-1750
fumatech®

Feed Solutions

	C (M)	Q ($m^3\ h^{-1}$)	T (°C)
HC	1.23	10	19
LC	4×10^{-3}		

Financial Parameters

Plant lifetime (years)	20
IEMs lifetime (years)	2
Load factor	90%
Discount rate	7.5%
Electricity price (€ kWh-1)	0.11

Optimal Solution

Net Present Value

max NPV

Hydraulic Topology

Active RED units

Arrangement

Operational Conditions

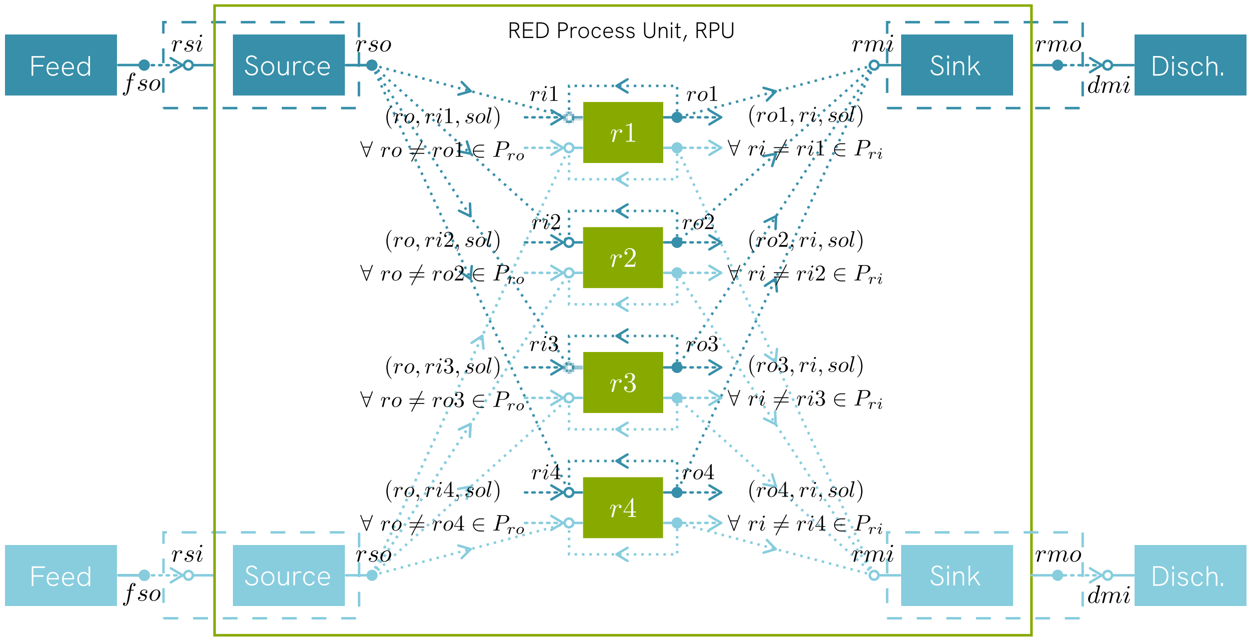
Inlet C,Q

Electric current

Illustrative Example

Model Size

# Continuous Var.	#Boolean Var.	# Constraints	#Disjunctions
1218	8	1298 Non-linear 278	4



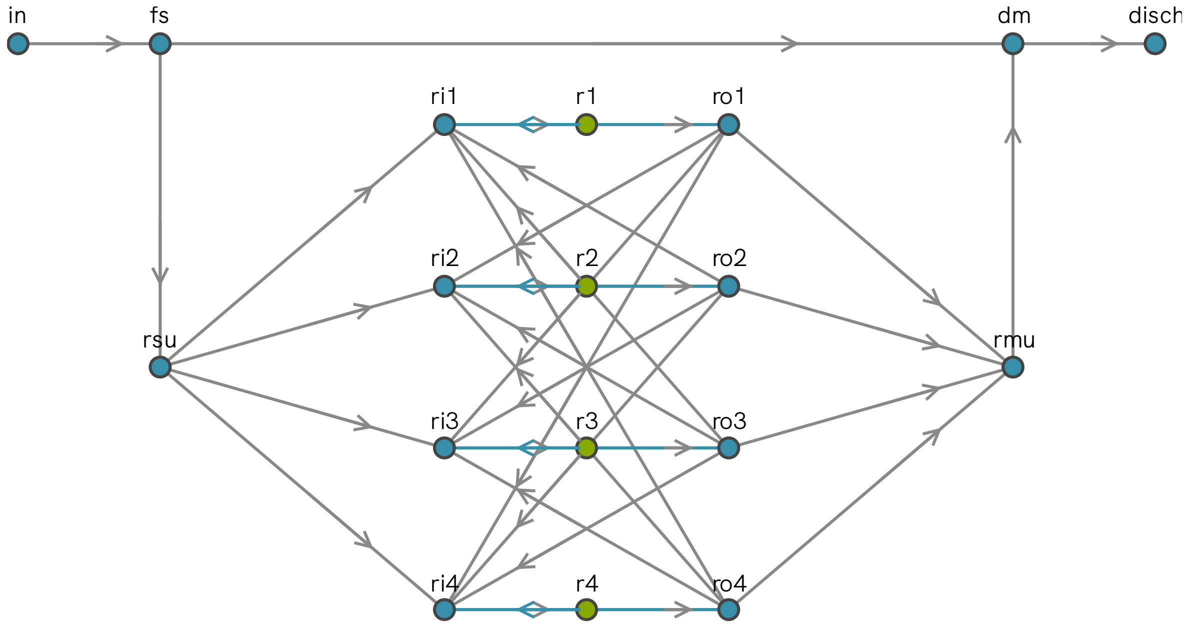
$sol \in \{HC, LC\}$

Superstructure Representation

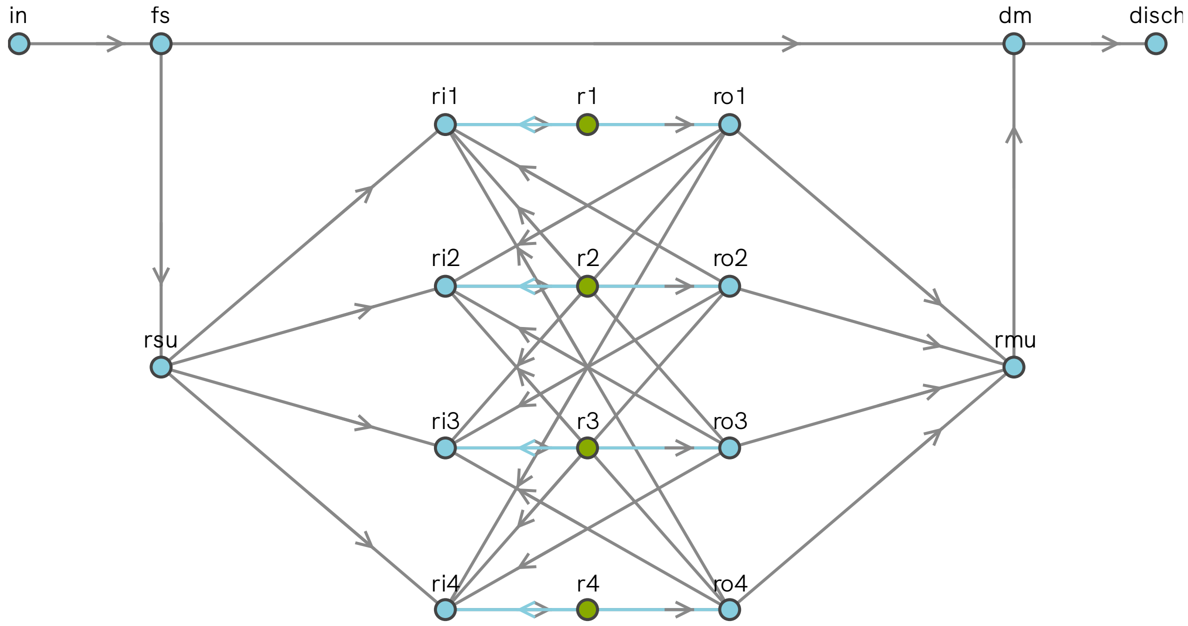
Illustrative Example

Port Representation

High Salinity



Low Salinity

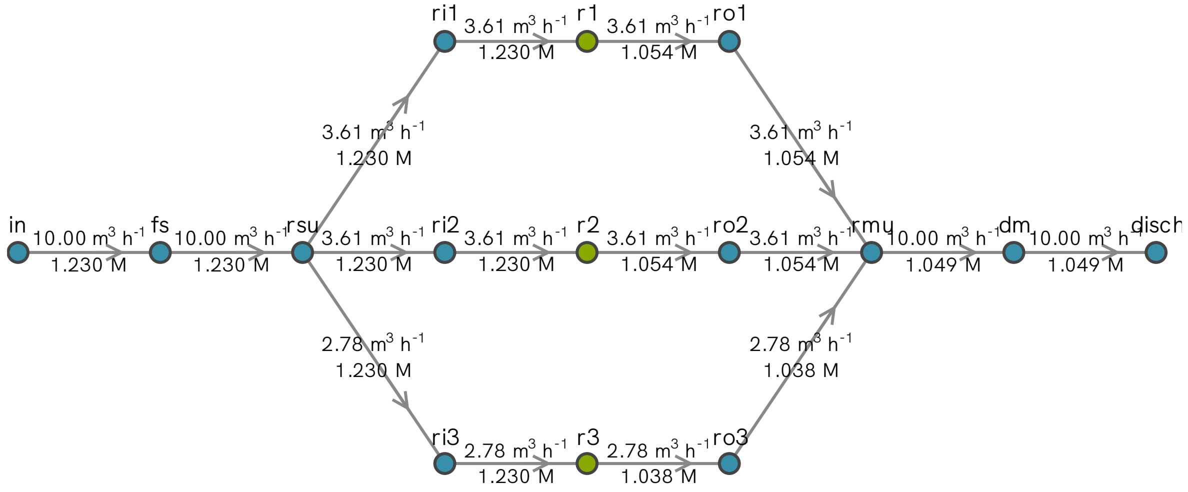


Hydraulic Topology

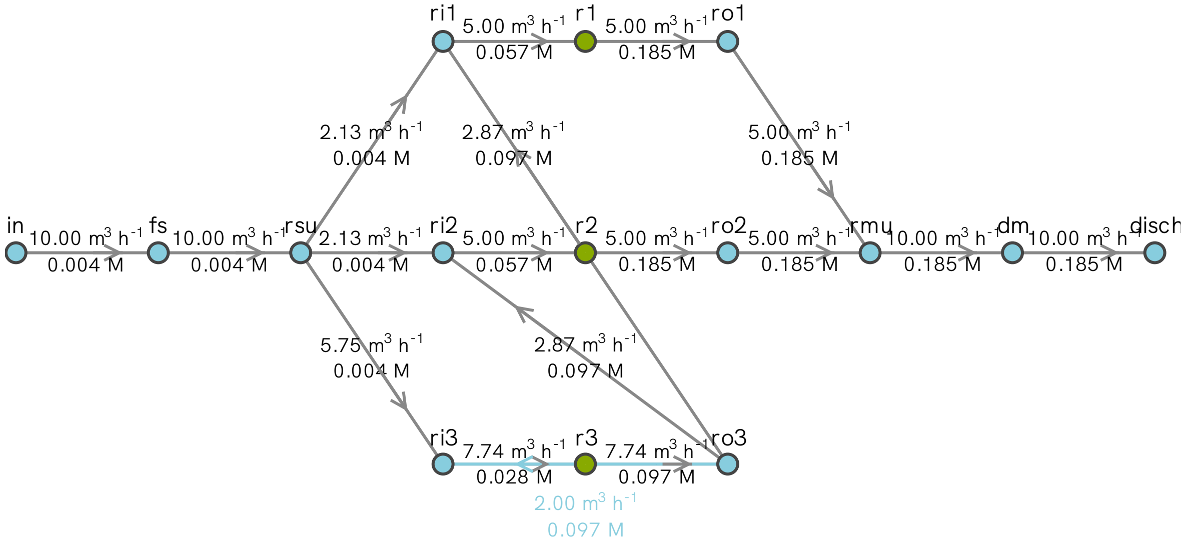
Illustrative Example

Optimal Solution

High Salinity



Low Salinity

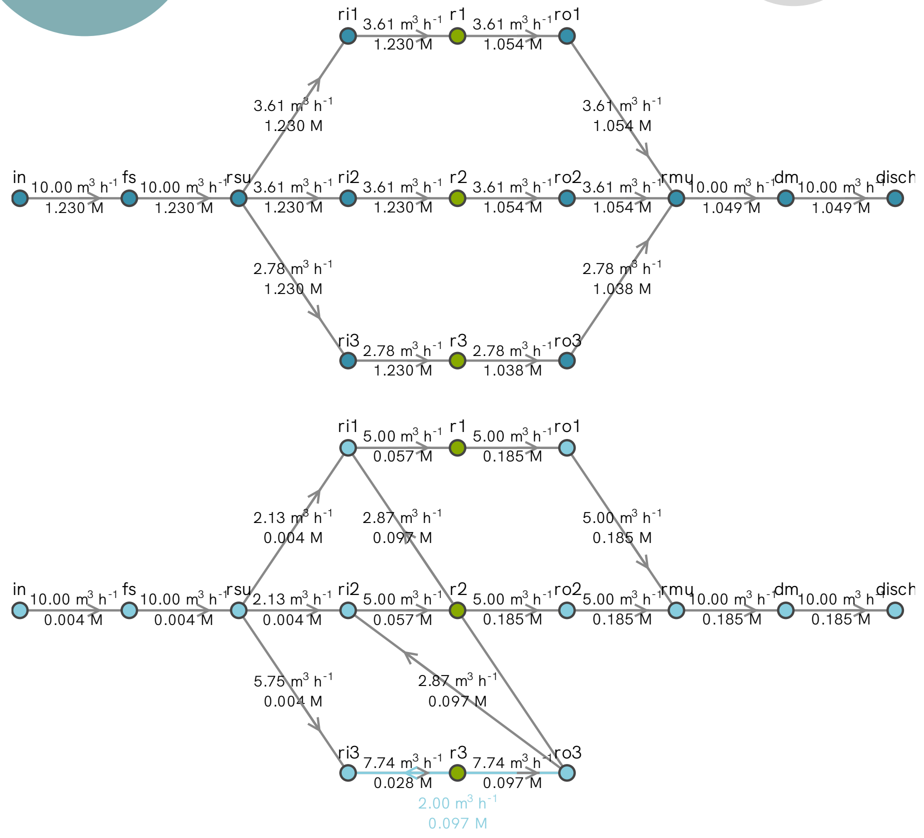


Hydraulic Topology

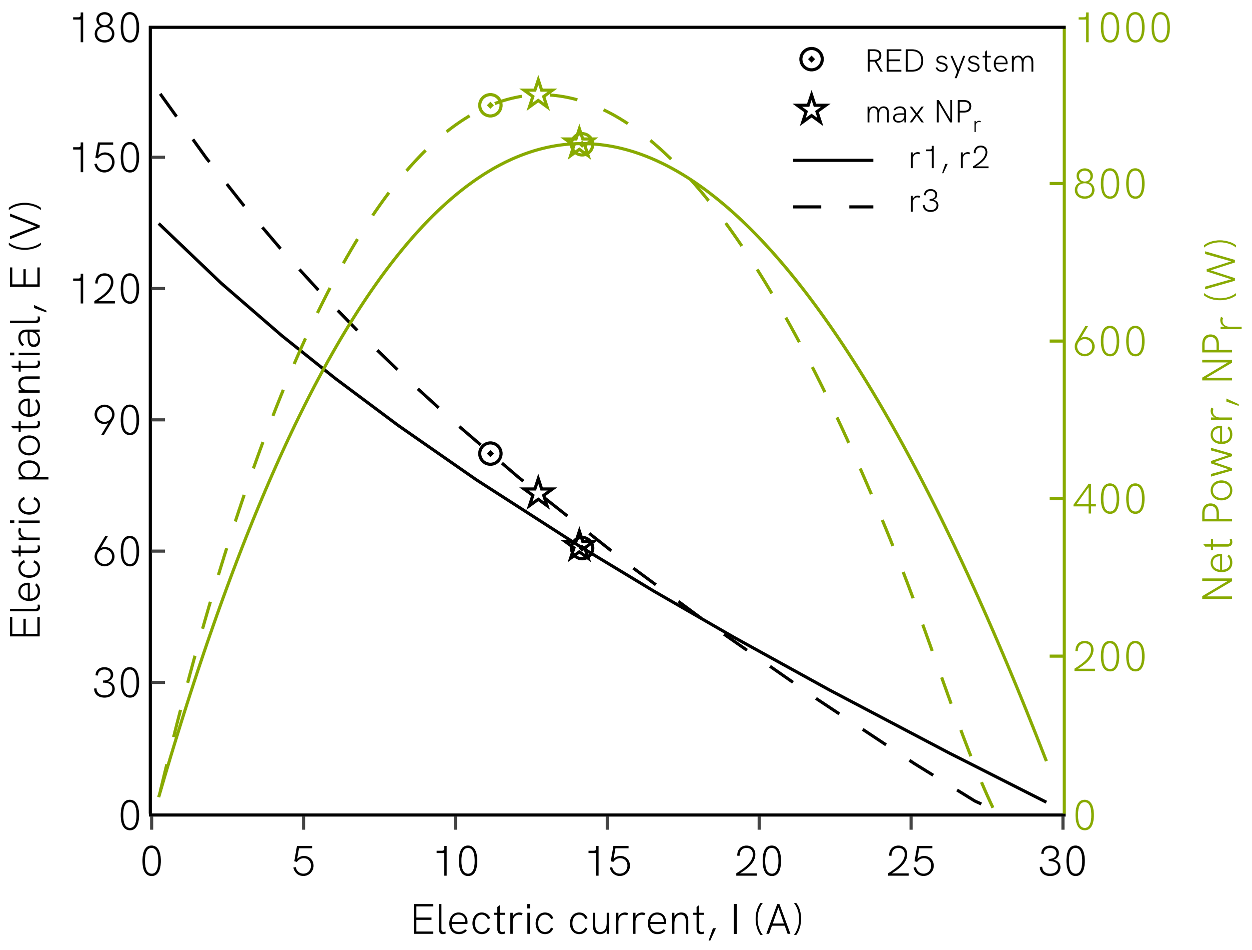
Illustrative Example

Optimal Solution

Hydraulic Topology



Operational Conditions

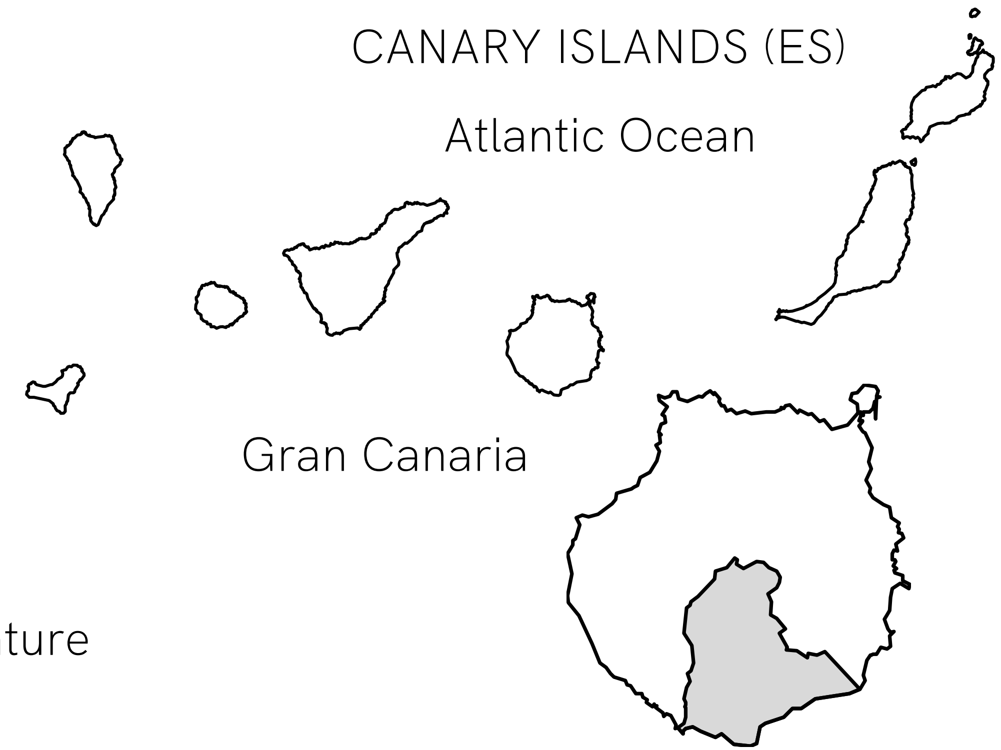


Case Study: Maspalomas II SWRO plant

SEC (kWh m^{-3})	Capacity (m^3 day^{-1})
3.8	26,184

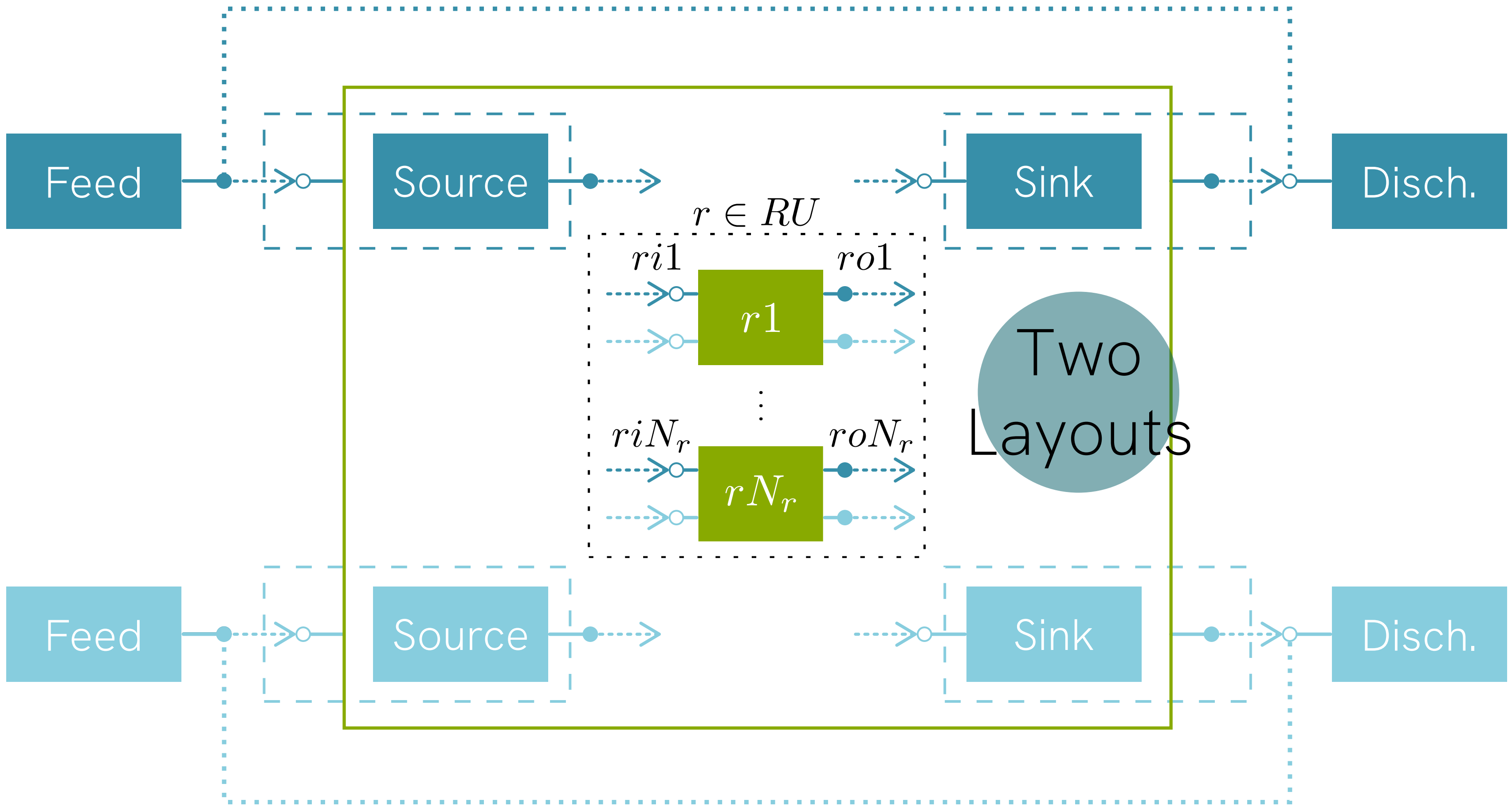
SWRO Concentrate

Concentration (M)	Volume (m^3 m^{-3})	Temperature (°C)
1.67	0.7	20



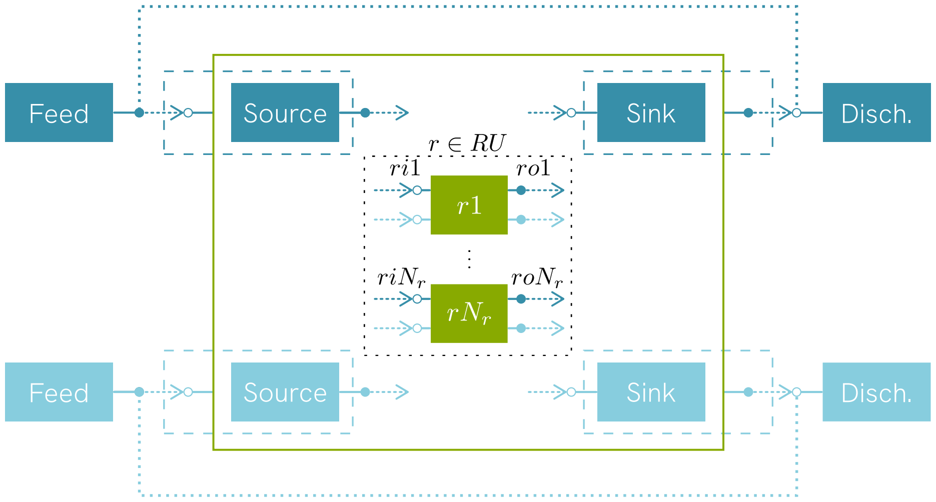
Portillo, E.; de la Rosa, M. R.; Louzara, G.; et al. *Desalin. Water Treat.* 2014, 52 (1-3), 164-177
Sadhwani Alonso, J. J.; Melián-Martel, N. Environmental Regulations—Inland and Coastal Desalination Case Studies. In Sustainable Desalination Handbook: Plant Selection, Design and Implementation; Gude, V. G., Ed.; Butterworth-Heinemann, 2018; pp 403-435

Case Study: Maspalomas II SWRO plant

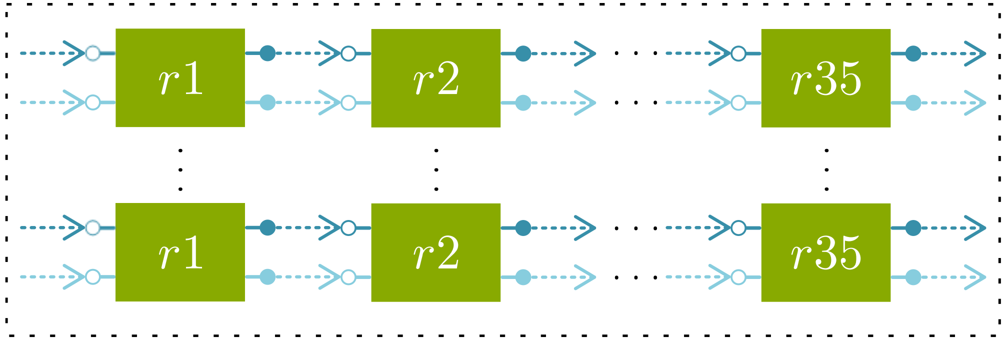


Case Study: Maspalomas II SWRO plant

Two Layouts

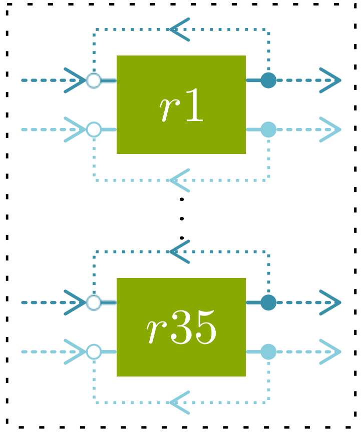


Series Parallel



max TNP

GDP

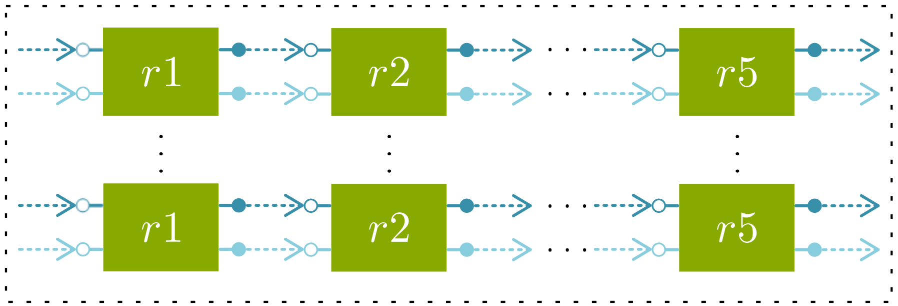


max NPV

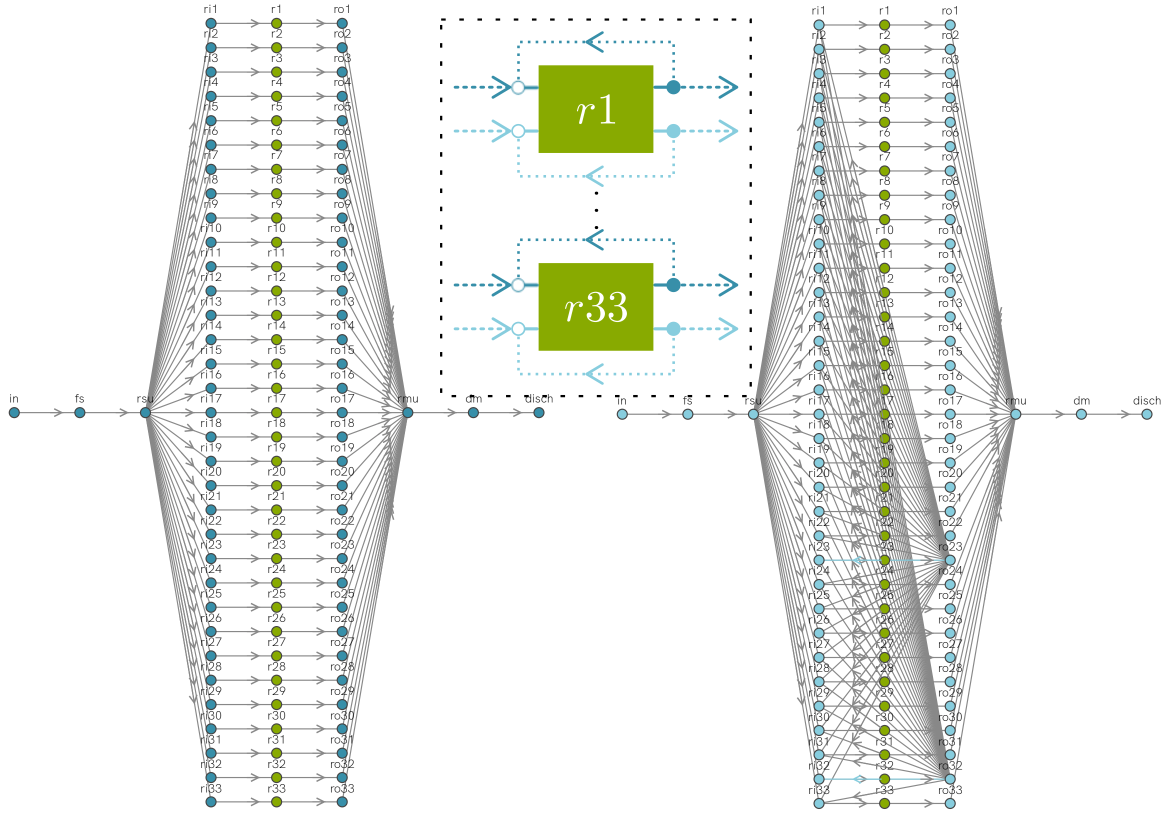
Case Study: Maspalomas II SWRO plant

Optimal Solution

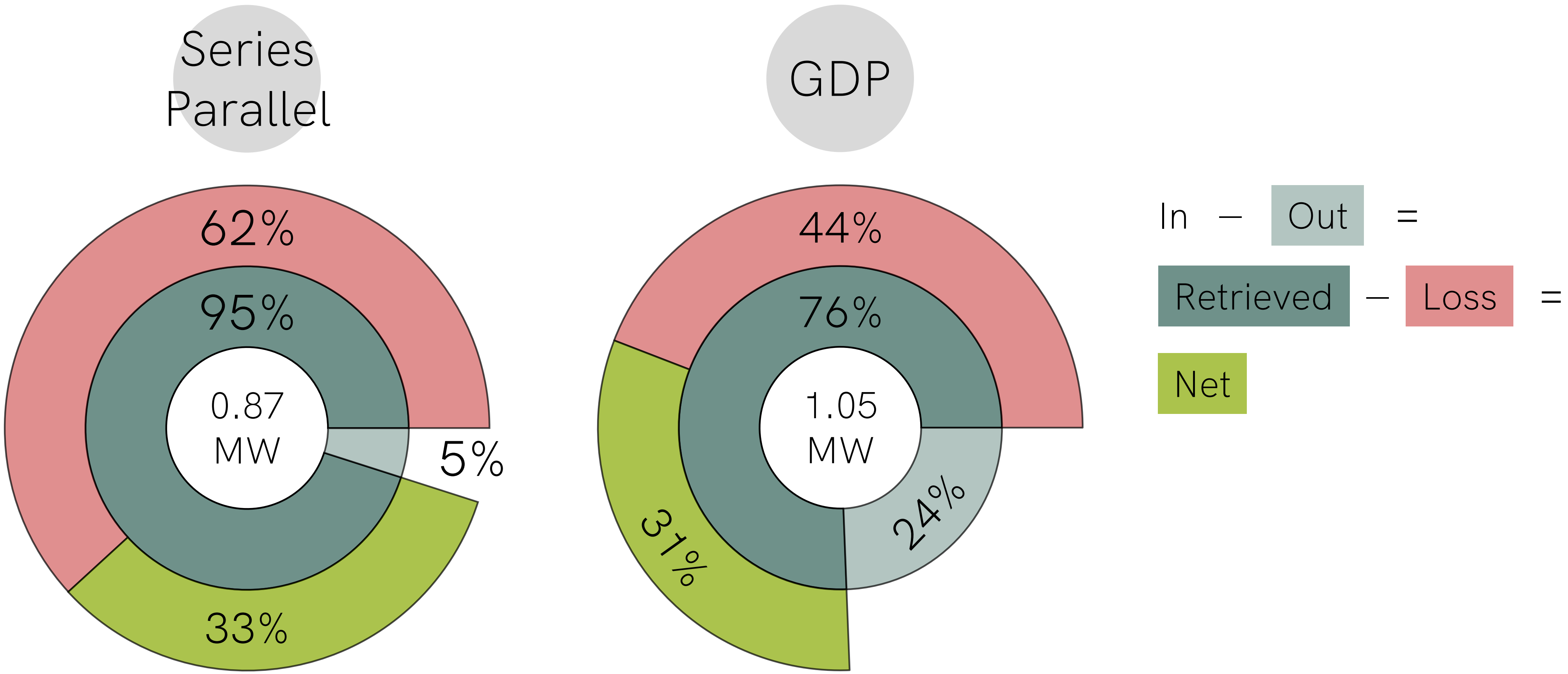
Series Parallel | 55 | #RU | 33 | GDP



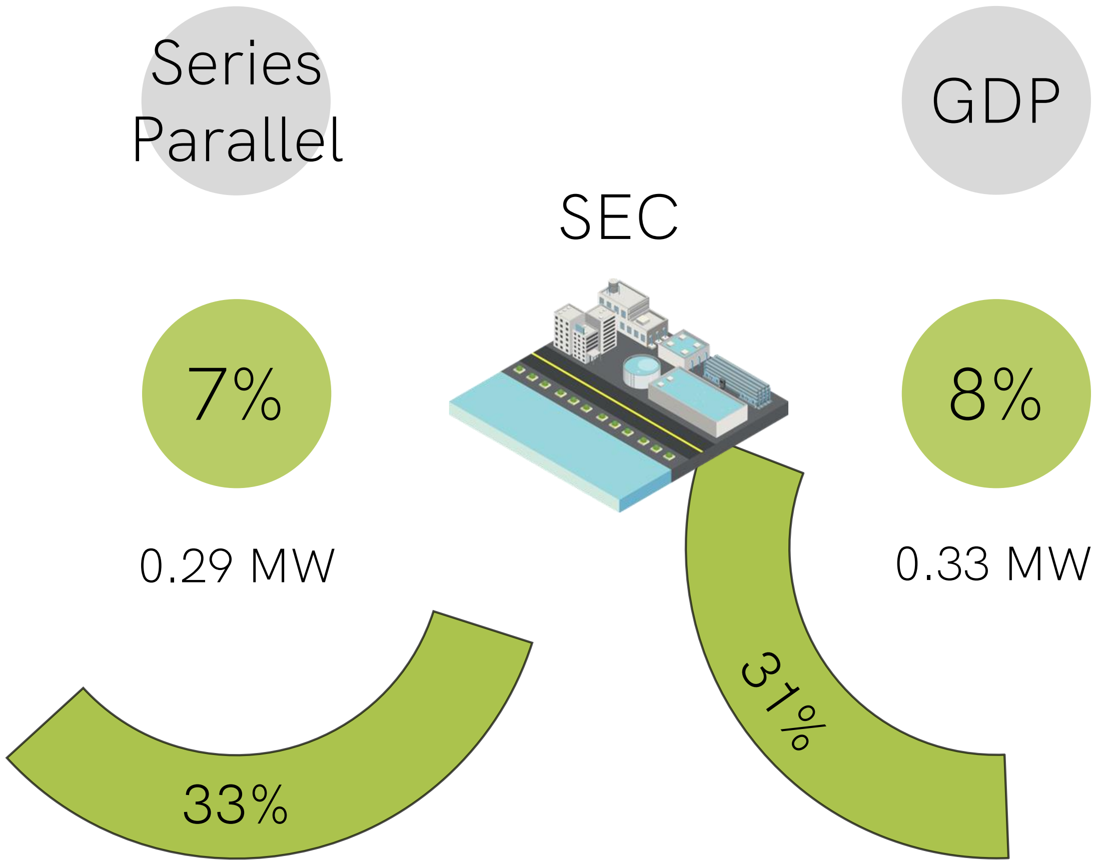
5 units × 11 parallel branches



Case Study: Maspalomas II SWRO plant

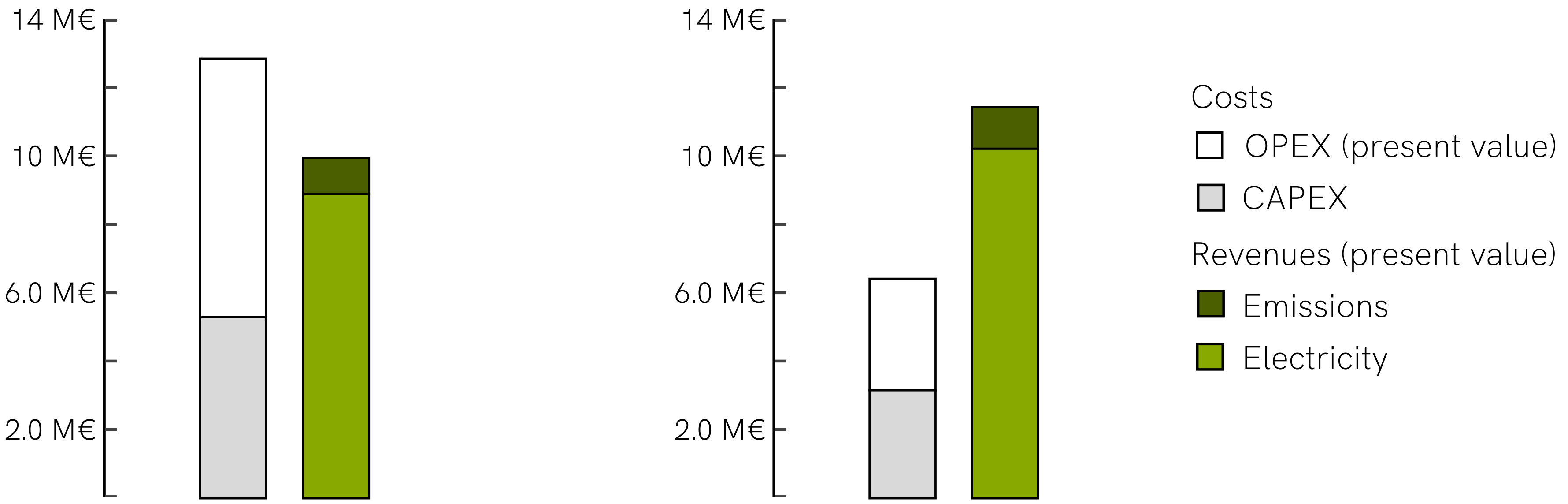


Case Study: Maspalomas II SWRO plant

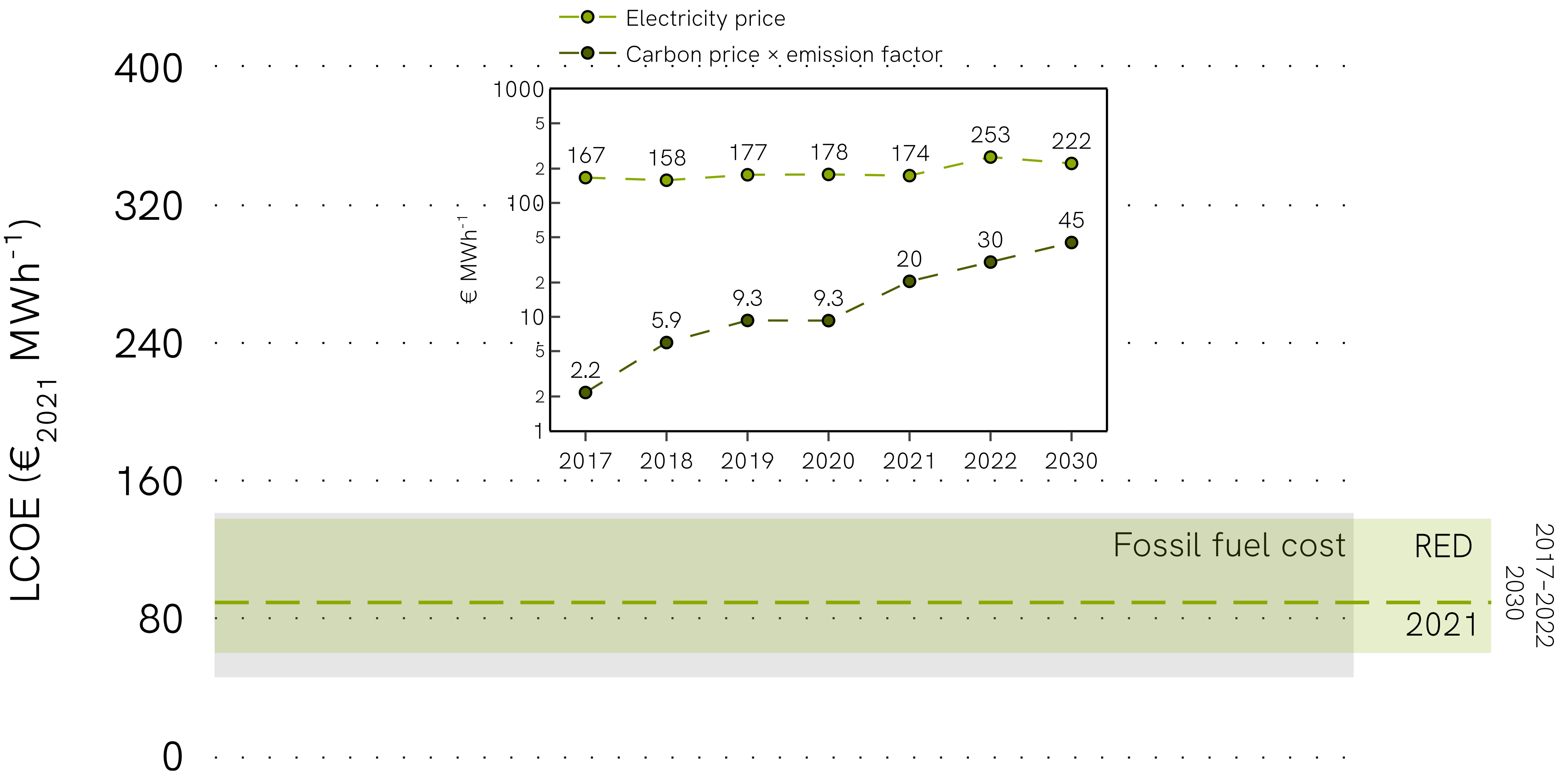


Case Study: Maspalomas II SWRO plant

Series Parallel		GDP
-2.9 M€	NPV	5.9 M€

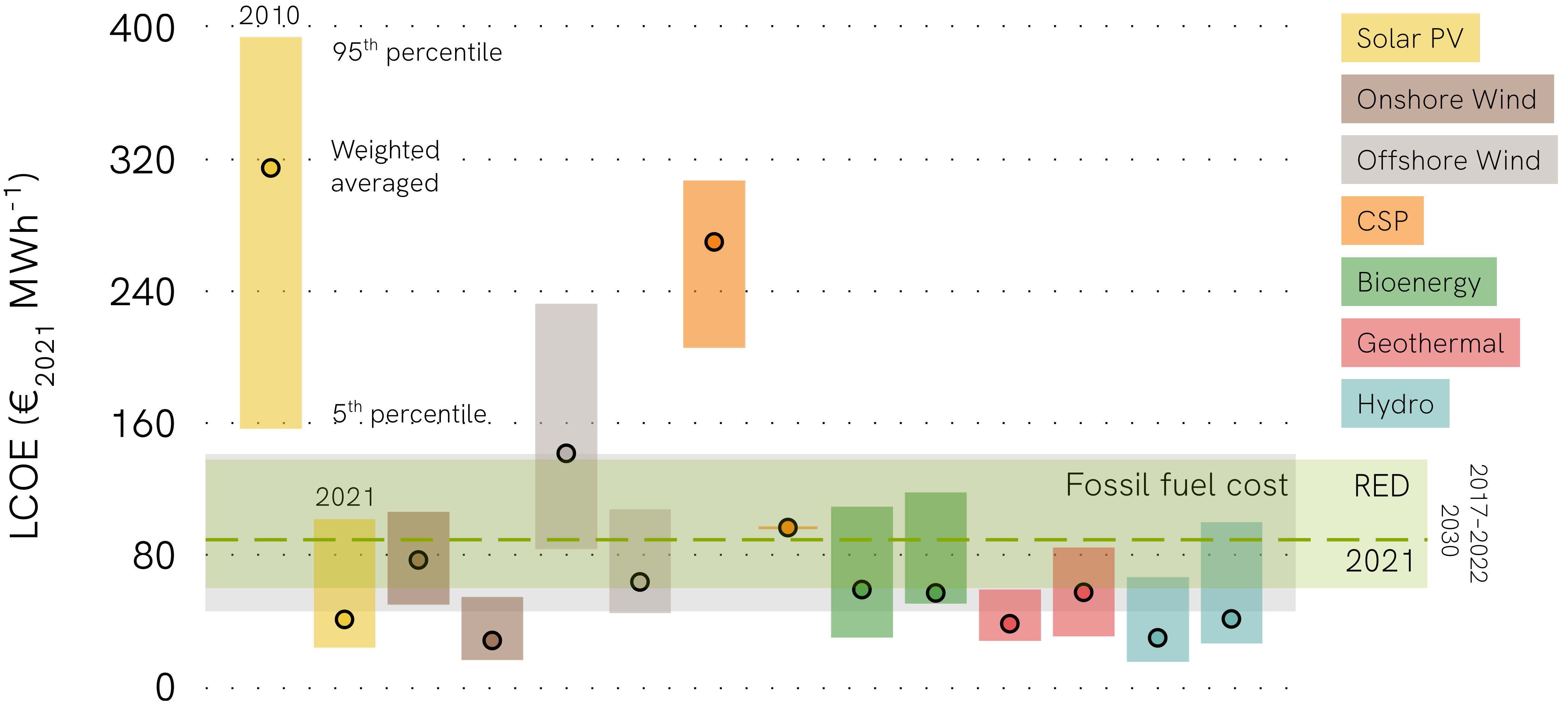


Case Study: Maspalomas II SWRO plant



IRENA. Renewable Power Generation Costs in 2021; Abu Dhabi, 2021.

Case Study: Maspalomas II SWRO plant

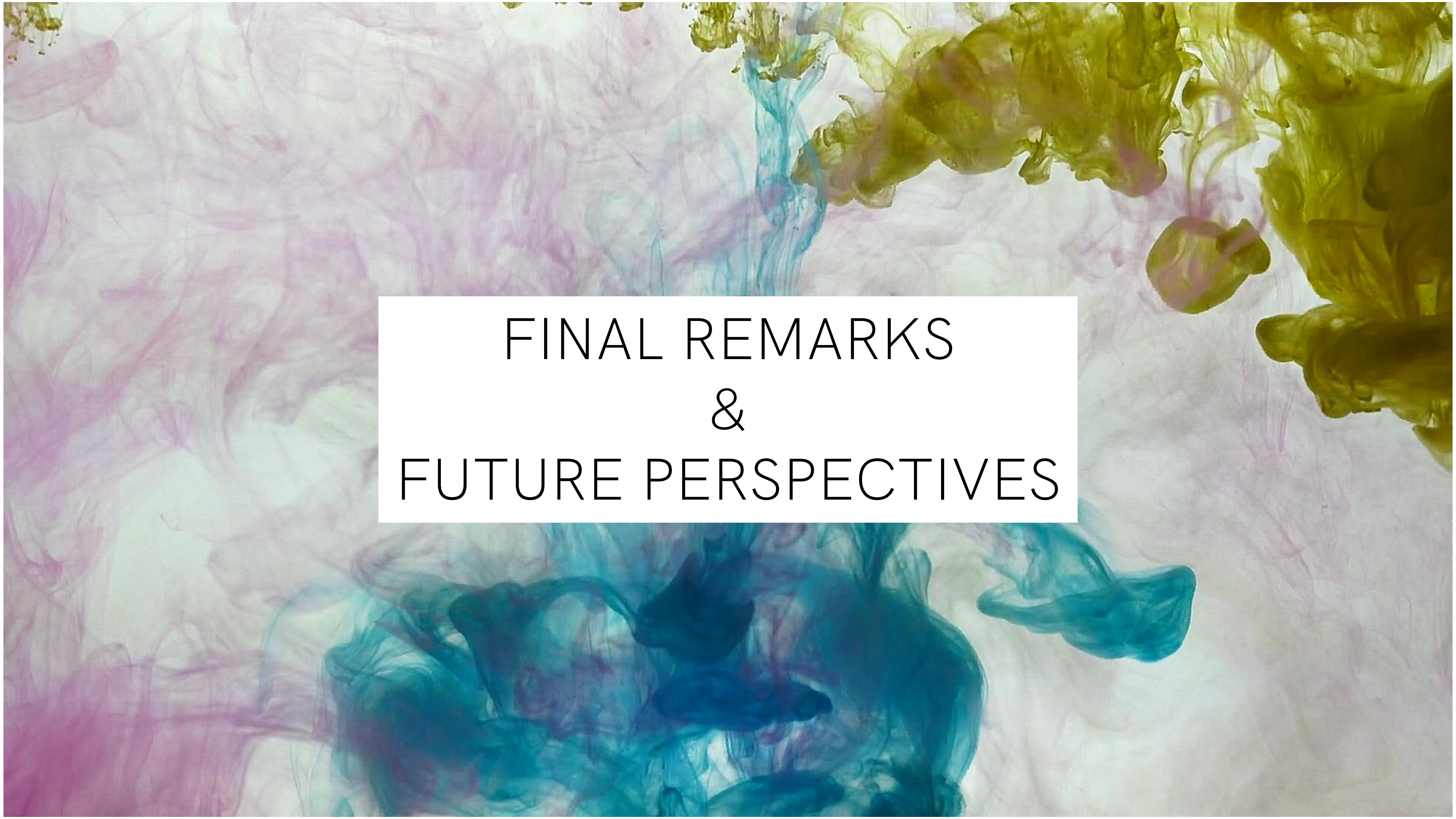


IRENA. Renewable Power Generation Costs in 2021; Abu Dhabi, 2021.

How can we define powerful, efficient, sustainable, and cost-effective designs for RED?

Optimization model for defining cost-effective and sustainable flowsheet designs of the RED process with LCOE of 66–126 € MWh^{-1} in the range of fossil-fired and renewables.

GDP vs. Series Parallel: Profit gain of 9 M€, twice power density, with equal thermodynamic efficiency and energy supply to Maspalomas II plant.



FINAL REMARKS & FUTURE PERSPECTIVES

FINAL REMARKS

Desalination is a drought and resilient proof but energy-intensive source of water that question their sustainability.

RED technology offer an integrated approach to the water-energy nexus (SDG 6, 7, 13) by providing clean, base-load electricity supply to desalination from the embed energy of an otherwise wasted stream.

1st ever LCA that quantifies the environmental loads of RED showing that RED is environmentally competitive with other RES.

RED optimization model is a valuable tool for gaining insight into future RED components design, screening RED implementation scenarios, and guiding prospective decisions to fully exploit the synergies of RED deployment in the energy-intensive desalination sector in the most cost-effective way.

FUTURE PERSPECTIVES

Development of **high-conductive, high-permselective affordable membranes** to advance RED progress.

Multi-objective optimization to consider environmental concerns.
Stochastic optimization to consider uncertainty in electricity and carbon price and membranes technological advances and price.
Reformulate GDP models into Quadratic GDP (QGDP) models for improved solving capabilities

Uncertainty estimation with sensitivity analysis and stochastic methods, e.g., applying Monte Carlo simulation, would help quantify the **soundness of the interpretation** of the results of the **LCA**.

Thank you!

PURDUE UNIVERSITY
College of Engineering

CAPD CENTER
Carnegie Mellon University

Supervisors

Prof. Raquel Ibáñez
Dr. Marcos Fallanza

Prof. Ignacio E. Grossmann

Dr. David Bernal
SECQUOIA

Departamento de Ingenierías Química y Biomolecular

Research Groups

SEP Sustainable Engineering Processes

ASP Advanced Separation Processes

DePRO Development of Chemical Processes and Pollution Control

Finanacial Support

Projects:
CTM2017-87850-R
PDC2021-120786-I00
RTI2018-093310-B-I00

FPI Grant
PRE2018-086454

MCIN/AEI/ 10.13039/501100011033

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PROCESS SYSTEMS ENGINEERING SEMINAR

West Lafayette, Feb 2nd, 2024

Optimizing Reverse Electrodialysis for Salinity-Driven Energy Recovery: A Sustainable Fix for the Water-Energy Nexus.

Dr. Carolina Tristán

Postdoctoral Researcher
Davidson School of Chemical Engineering
Purdue University, West Lafayette, IN, USA
ctristan@purdue.edu

PURDUE UNIVERSITY | College of Engineering