www.pecsys-horizon2020.eu

PECSYS Virtual Workshop
5th November 2020

WP 6: Simulation of hydrogen production based on weather data and its relation to socio-economic analysis in the PECSYS device design

M. Edoff , I. Bayrak Pehlivan, T. Edvinsson **(Uppsala Universitet,** SE**)**
S. Calnan (Helmholtz Zentrum Berlin, DE)
S. A. Lombardo, S. Privitera (Consiglio Nazionale delle Ricerche, IT)

Disclaimer

Marika.Edoff@angstrom.uu.se

Workpackage objectives and main tasks

Objective: Understanding of the system in terms of technology development and cost-potential. Technology potential will be screened based on band gap and band energies calculations, which will be determined from photosensitivity measurements.

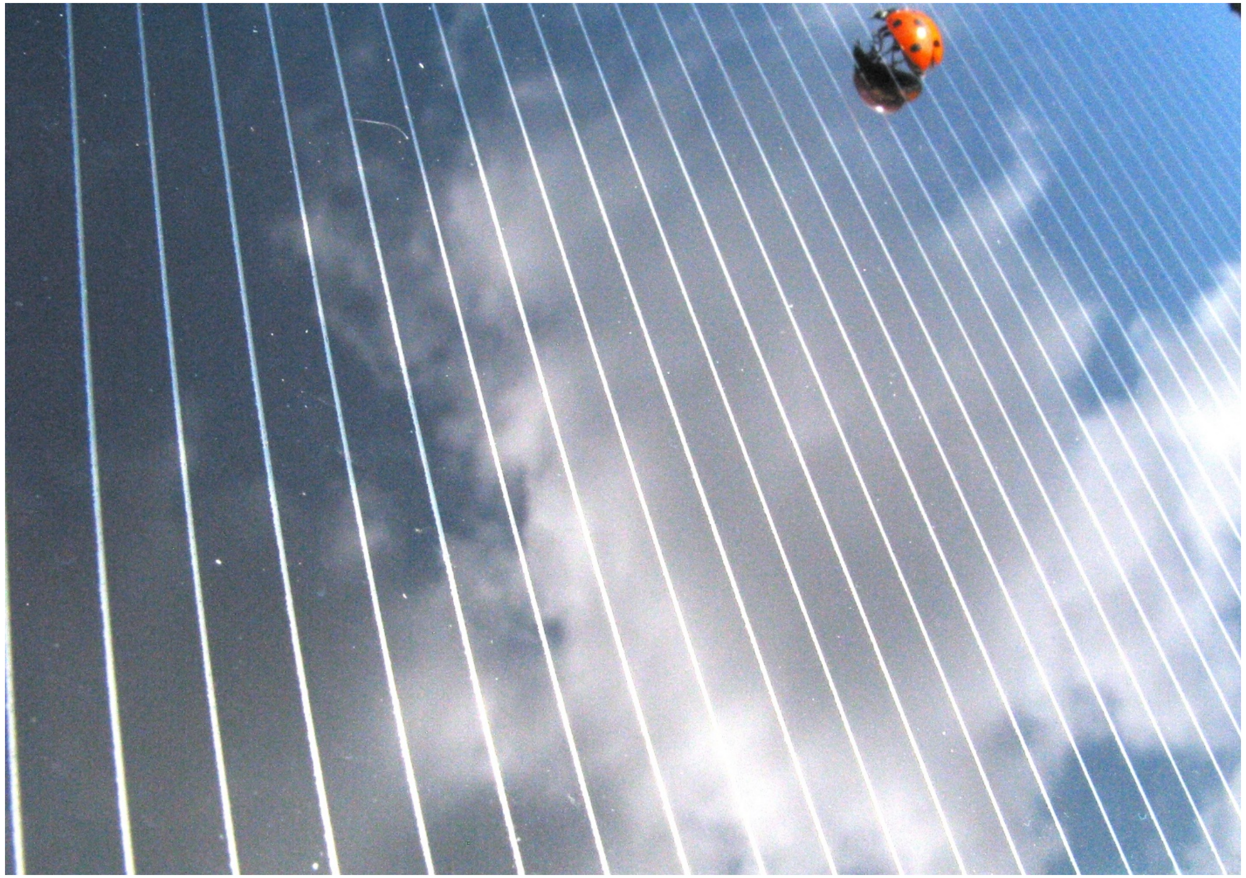
A complete socio-techno-economic model based on cost and performance of each essential component will be developed including BoP.

Task description
T 6.1 (UU) PV device simulation
T 6.2 (FZJ) EC device simulation
T 6.3 (HZB) Socio-Techno-Economic and life cycle analysis

Marika.Edoff@angstrom.uu.se

Explanation of the concept: modeling

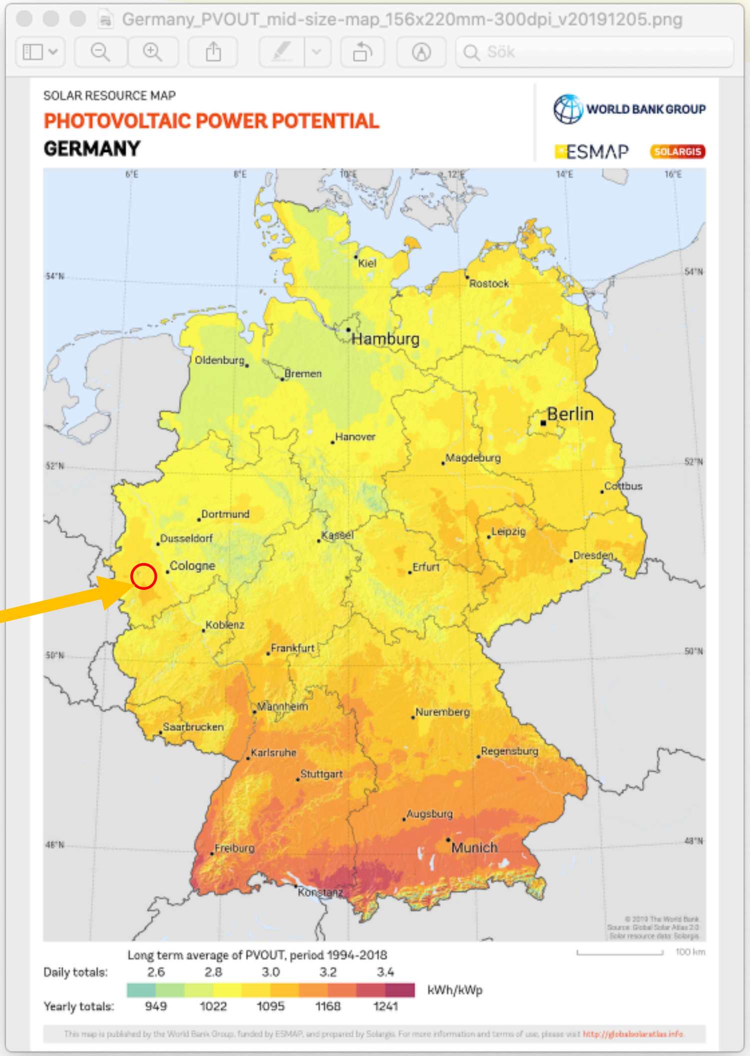
- The main goal of the modeling is:
  - Prediction of yearly hydrogen yield
  - Distribution of hydrogen production based on climate data
  - Design rules for optimum match between PV and EC part of the device



Marika.Edoff@angstrom.uu.se

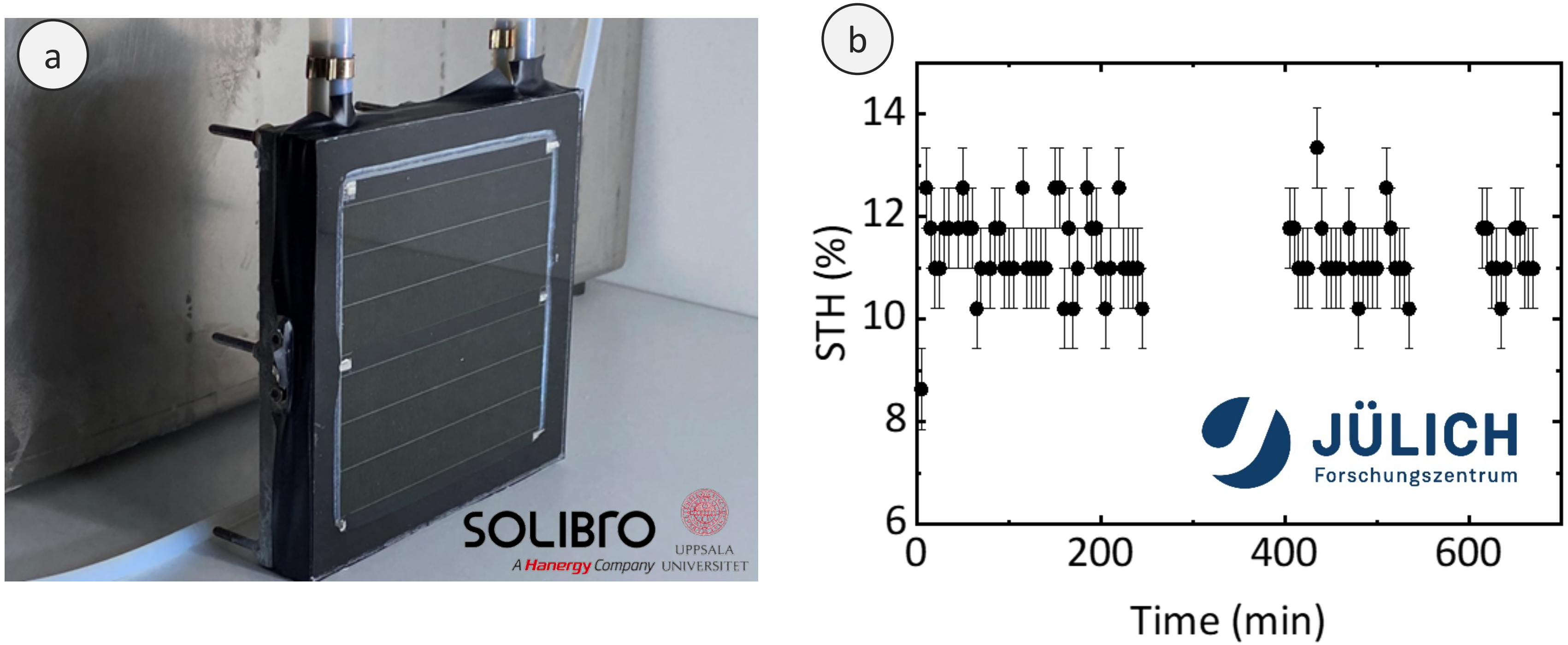
Explanation of the concept: weather data

- Climate model
    - Hourly data for Jülich
        - Temperature, hourly average
        - Solar irradiation [W/m^2], hourly average



Jülich data
Year 2016

Marika.Edoff@angstrom.uu.se

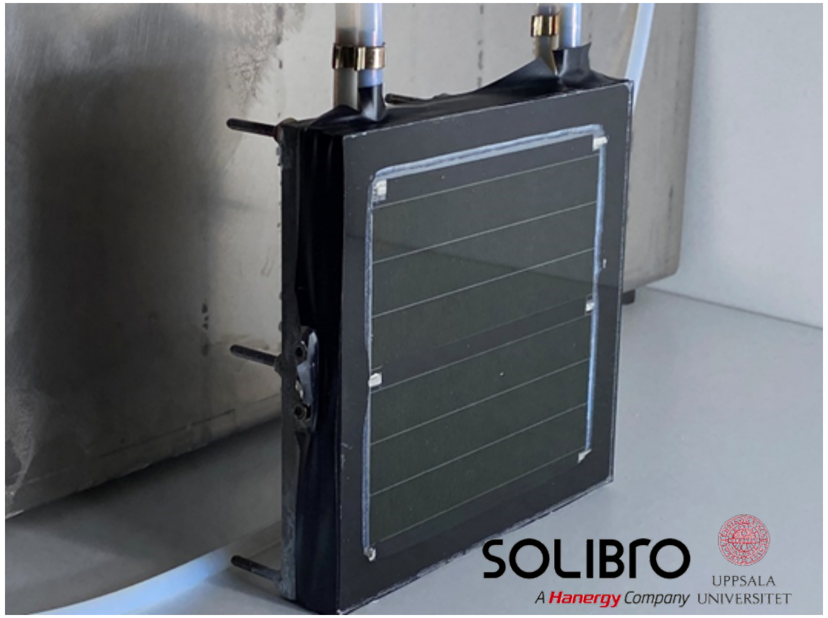


A thermally integrated device made up of a 2×3-cell CuInGaSe photovoltaic module (active area ~ 82.3 cm^2) and a FeNiOH (cathode)-FeNiOH (anode)-based alkaline electrolyser with an electrode area of 100 cm^2 (a). The solar to hydrogen conversion efficiency (STH) remains above 10 % for more than 1 hour at 1000 W/cm^2 without active temperature control (b), resulting in an average hydrogen production rate of 5.74 mL/min.

Marika.Edoff@angstrom.uu.se

Explanation of the concept: PV part

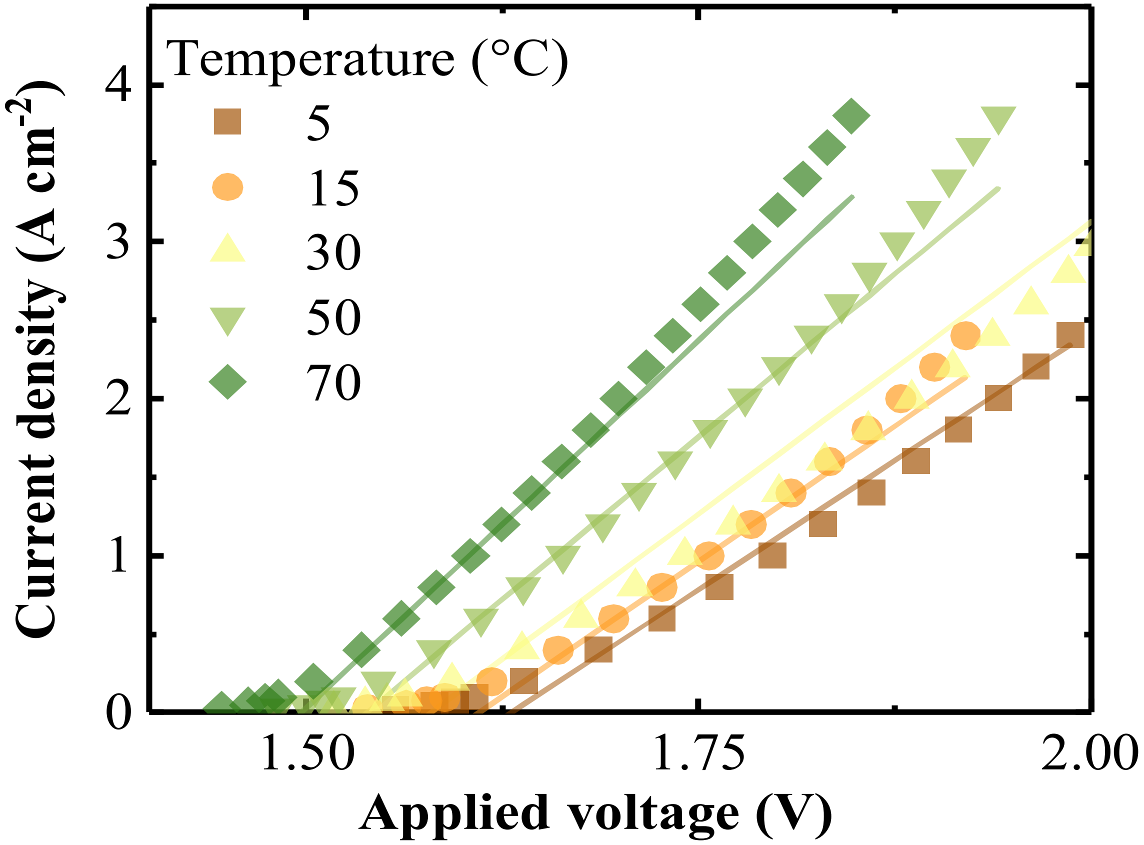
- Solar cell module, 3 interconnected cells
- Four different technologies
  - CIGS (Solibro)
  - Silicon heterojunction (HZB)
  - Amorphous silicon tandem (Jülich)
  - Silicon PERT (ENEL green power)
- Parameter fit as function of irradiation and temperature to make a model



Marika.Edoff@angstrom.uu.se

Explanation of the concept: EC part

- Technologies
  - EC Jülich, PEM Pt-IrO_2 catalyst
  - EC alkaline Fe-Ni-based, UU
  - EC CNR, alkaline Pt-IrO_2 catalyst
- Parameter set: JV-data as a function of temperature



Example: EC part FZJ

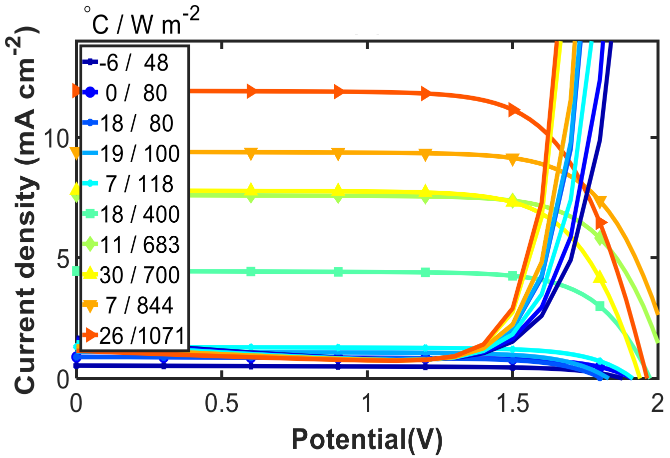
Marika.Edoff@angstrom.uu.se

Simulation: Combining PV to alkaline EC (UU) Varying temperature and irradiation

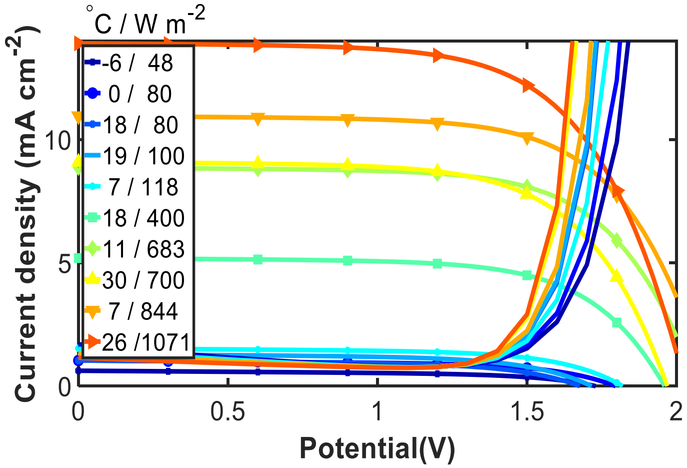
EC-UU

area of PV=
area of EC

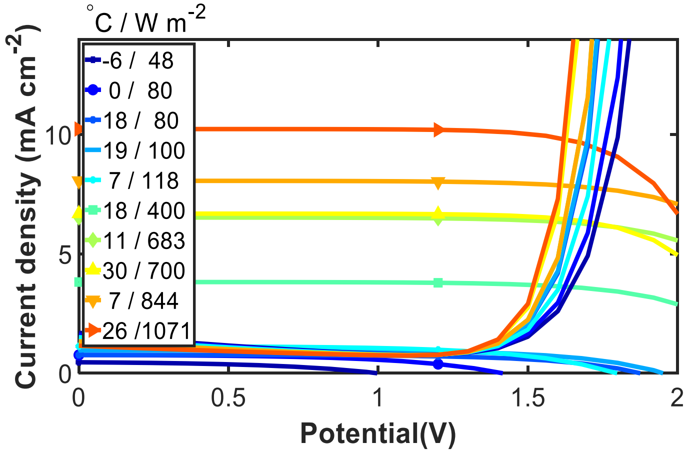
PV-SRAB



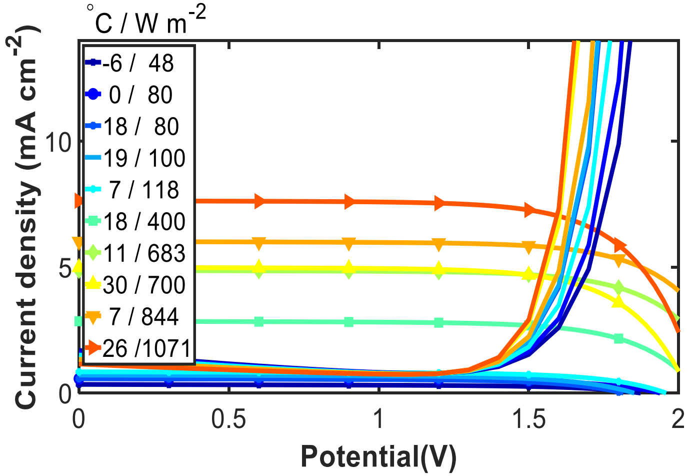
PV-HZB



PV-ENEL



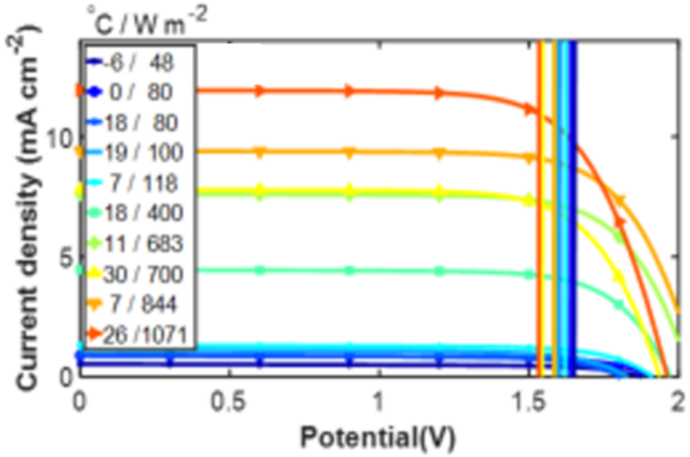
PV-FZJ



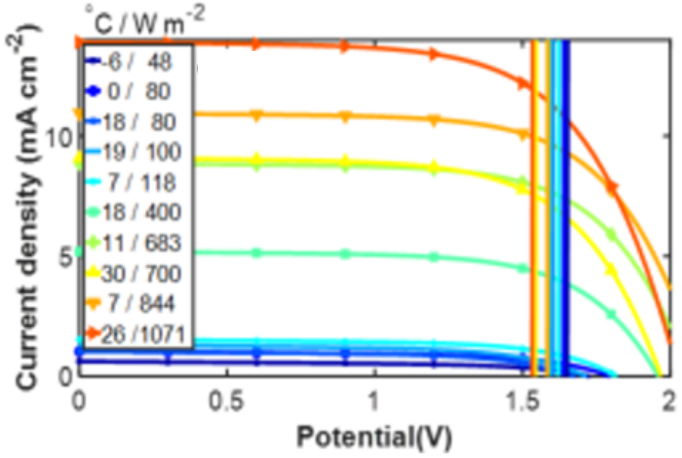
Simulation: Combining PV to Pt based EC (FZJ) Varying temperature and irradiation

EC-FZJ

PV-SRAB

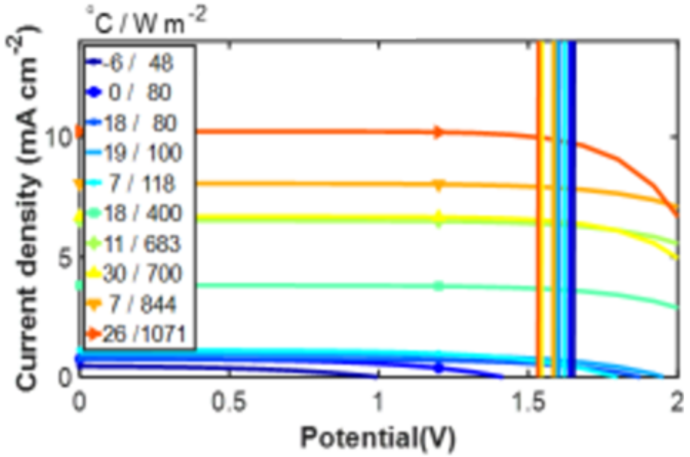


PV-HZB

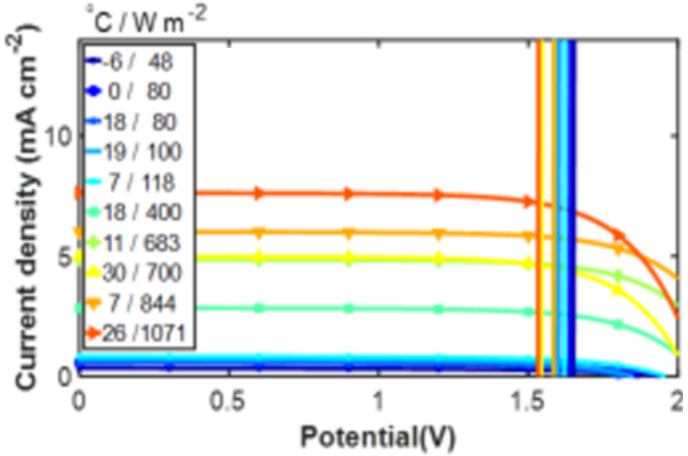


area of PV= area of EC

PV-ENEL



PV-FZJ

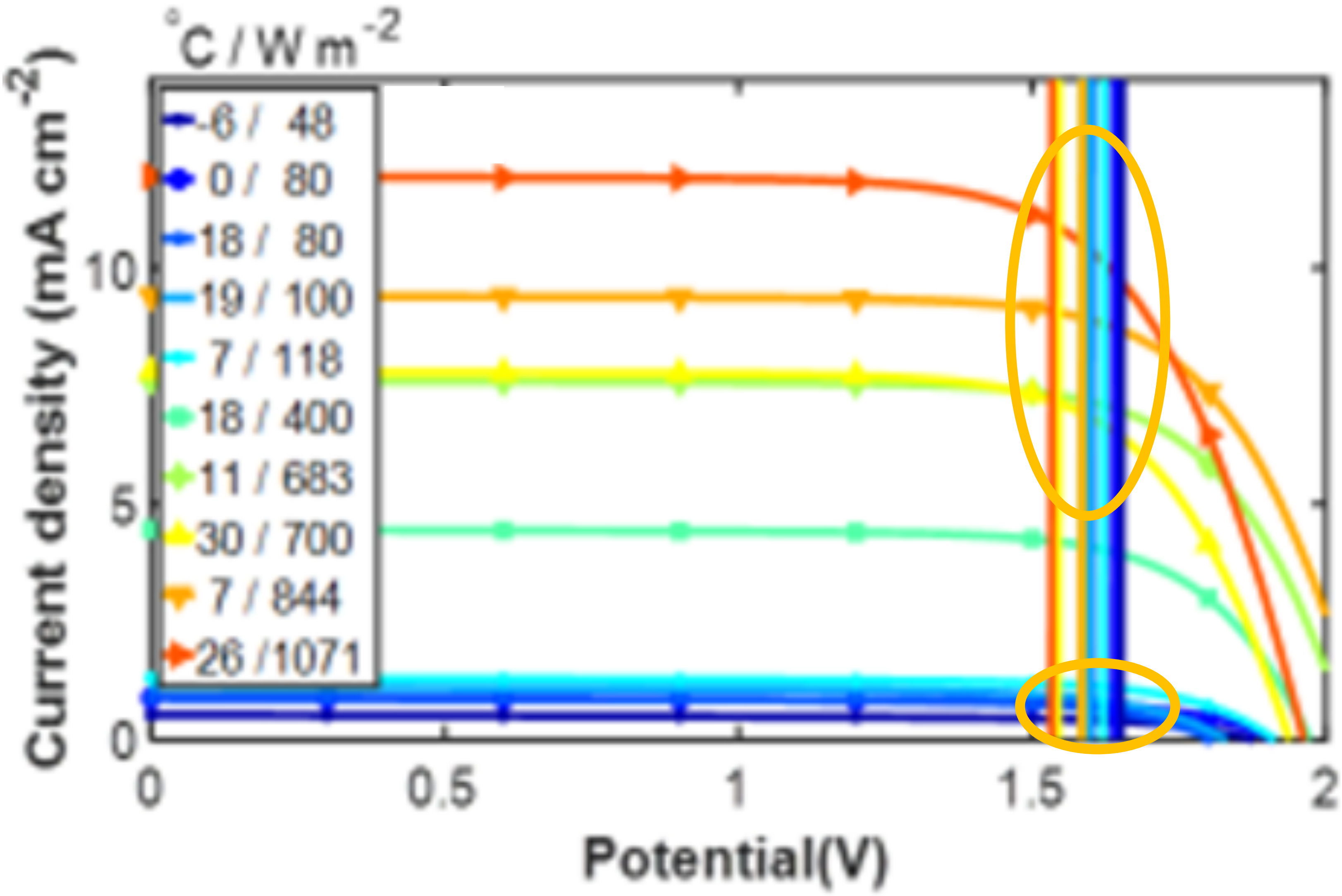


Marika.Edoff@angstrom.uu.se

WP6 – Accomplishments since May 2018

PV-SRAB

EC-FZJ



Cross over ≈ proportional to light intensity

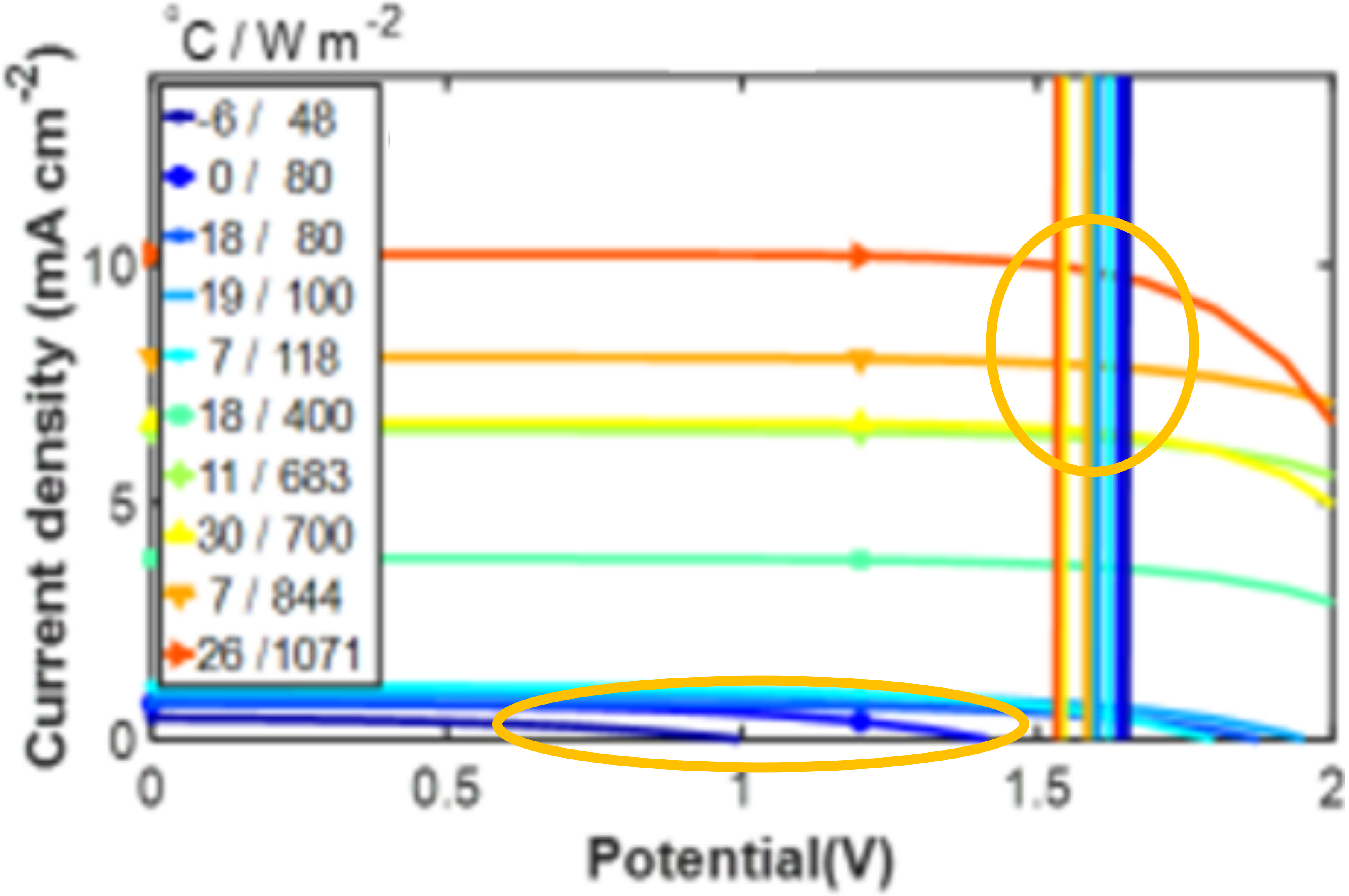
Good margin and match between PV and EC, also at low irradiance

Marika.Edoff@angstrom.uu.se

WP6 – Accomplishments since May 2018

PV-ENEL

EC-FZJ



Cross over ≈ proportional to light intensity

No hydrogen production at low irradiance

Modelling outcomes (all for Jülich data 2016)

- Energy yield and efficiency for PV
- Energy yield for different areas of PV-EC (varying EC area)
- Solar to hydrogen (STH) efficiency
- Electricity to hydrogen (ETH) efficiency
- *Assuming temperature for PV=temperature for EC*

Marika.Edoff@angstrom.uu.se

PV –EC (FZJ) Annual energy yield

PEM electrolyzer
Different PV devices

Different catalyst areas (A_{EC}=x A_{PV})

PV	EC	$E_{PV\text{-}EC}$ for various A_{EC} (kWh m^{-2})				
		0.01 A_{PV}	0.1 A_{PV}	A_{PV}	10 A_{PV}	100 A_{PV}
HZB_3cells	FZJ	109	117	117	117	117
SRAB_3cells		114	119	119	119	119
ENEL_4cells		98	99	99	99	99
FZJ_1cell		74	75	75	75	75

High PV efficiency, good match to EC

High PV efficiency, less good match to EC

Lower PV efficiency, good match to EC

Very similar results down to 1 % EC compared to PV area

Marika.Edoff@angstrom.uu.se

PV –EC (UU) Annual energy yield

Different catalyst areas (A_{EC}=x A_{PV})

alkaline electrolyzer
different PV devices

PV	EC	$E_{PV\text{-}EC}$ for various A_{EC} (kWh m^{-2})		
		0.01 A_{PV}	0.1 A_{PV}	A_{PV}
HZB_3cells	UU	27	79	116
SRAB_3cells		30	87	110
ENEL_4cells		70	92	95
FZJ_1cell		38	66	65

Match in area between EC and PV device
Smaller area leads to loss of yearly yield

Marika.Edoff@angstrom.uu.se


Volume 1
Number 3
May 2017
Pages 399-666

Sustainable Energy & Fuels

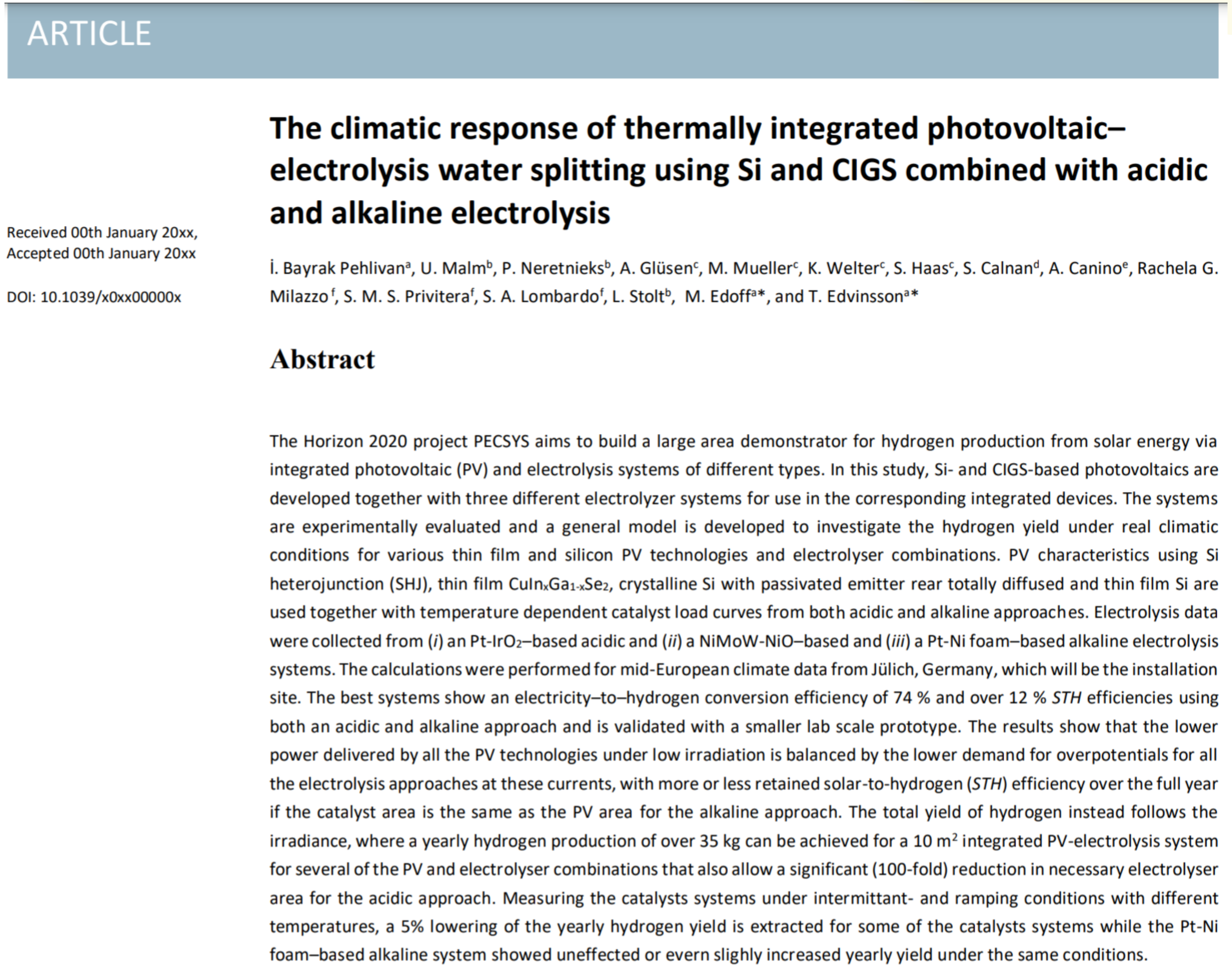
Interdisciplinary research for the development of sustainable energy technologies

rsc.li/sustainable-energy

ISSN 2398-4902

ROYAL SOCIETY OF CHEMISTRY

PAPER
Chengxiang Xiang, Nathan S. Lewis *et al.*
Evaluation of flow schemes for near-neutral pH electrolytes in solar-fuel generators


ARTICLE

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

The climatic response of thermally integrated photovoltaic–electrolysis water splitting using Si and CIGS combined with acidic and alkaline electrolysis

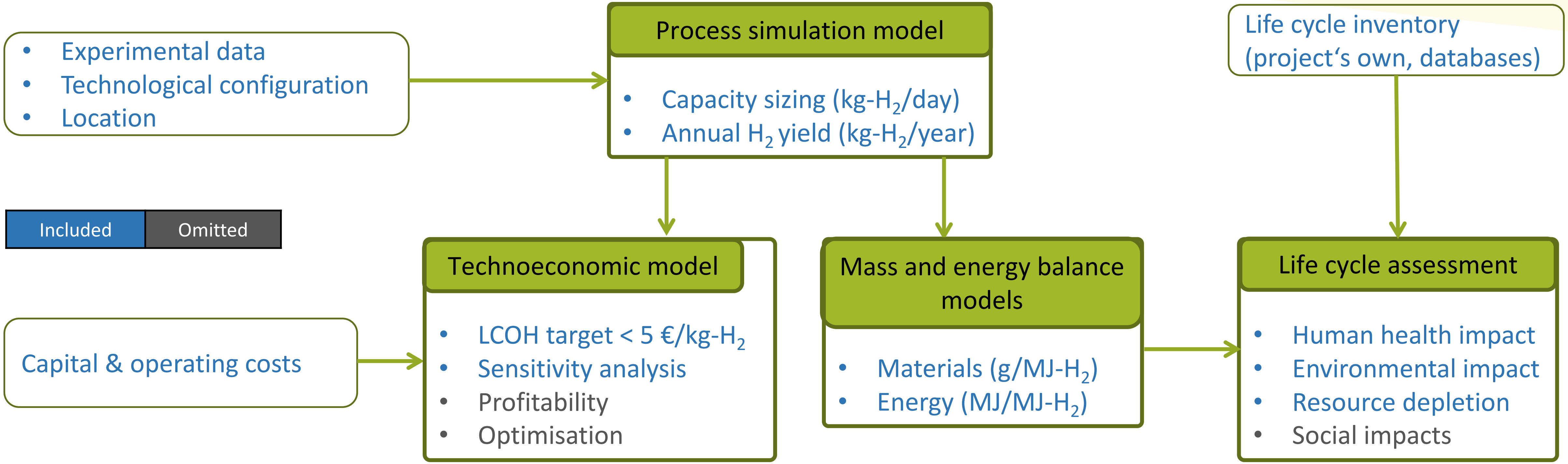
İ. Bayrak Pehlivan[a], U. Malm[b], P. Neretnieks[b], A. Glüsen[c], M. Mueller[c], K. Welter[c], S. Haas[c], S. Calnan[d], A. Canino[e], Rachela G. Milazzo[f], S. M. S. Privitera[f], S. A. Lombardo[f], L. Stolt[b], M. Edoff[a]*, and T. Edvinsson[a]*

Abstract

The Horizon 2020 project PECSYS aims to build a large area demonstrator for hydrogen production from solar energy via integrated photovoltaic (PV) and electrolysis systems of different types. In this study, Si- and CIGS-based photovoltaics are developed together with three different electrolyzer systems for use in the corresponding integrated devices. The systems are experimentally evaluated and a general model is developed to investigate the hydrogen yield under real climatic conditions for various thin film and silicon PV technologies and electrolyser combinations. PV characteristics using Si heterojunction (SHJ), thin film CuIn$_x$Ga$_{1-x}$Se$_2$, crystalline Si with passivated emitter rear totally diffused and thin film Si are used together with temperature dependent catalyst load curves from both acidic and alkaline approaches. Electrolysis data were collected from (*i*) an Pt-IrO$_2$–based acidic and (*ii*) a NiMoW-NiO–based and (*iii*) a Pt-Ni foam–based alkaline electrolysis systems. The calculations were performed for mid-European climate data from Jülich, Germany, which will be the installation site. The best systems show an electricity–to–hydrogen conversion efficiency of 74 % and over 12 % *STH* efficiencies using both an acidic and alkaline approach and is validated with a smaller lab scale prototype. The results show that the lower power delivered by all the PV technologies under low irradiation is balanced by the lower demand for overpotentials for all the electrolysis approaches at these currents, with more or less retained solar-to-hydrogen (*STH*) efficiency over the full year if the catalyst area is the same as the PV area for the alkaline approach. The total yield of hydrogen instead follows the irradiance, where a yearly hydrogen production of over 35 kg can be achieved for a 10 m^2 integrated PV-electrolysis system for several of the PV and electrolyser combinations that also allow a significant (100-fold) reduction in necessary electrolyser area for the acidic approach. Measuring the catalysts systems under intermittant- and ramping conditions with different temperatures, a 5% lowering of the yearly hydrogen yield is extracted for some of the catalysts systems while the Pt-Ni foam–based alkaline system showed uneffected or evern slighly increased yearly yield under the same conditions.

Marika.Edoff@angstrom.uu.se

Combined Technoeconomic and Life Cycle Analysis



- Experimental data
- Technological configuration
- Location

Process simulation model

- Capacity sizing (kg-H_2/day)
- Annual H_2 yield (kg-H_2/year)

Life cycle inventory (project‘s own, databases)

Included	Omitted

Capital & operating costs

Technoeconomic model

- LCOH target < 5 €/kg-H_2
- Sensitivity analysis
- Profitability
- Optimisation

Mass and energy balance models

- Materials (g/MJ-H_2)
- Energy (MJ/MJ-H_2)

Life cycle assessment

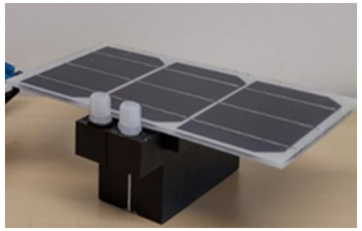
- Human health impact
- Environmental impact
- Resource depletion
- Social impacts

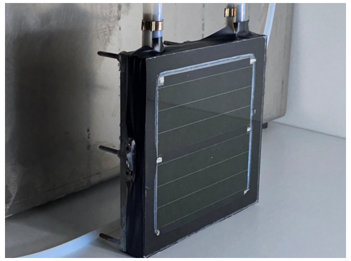
sonya.calnan@helmholtz-berlin.de

Main Results: Preliminary Technoeconomic Analysis

Hydrogen production capacity of 16g/h or 140 kg per year, 1 bar hydrogen, located in Jülich, Germany

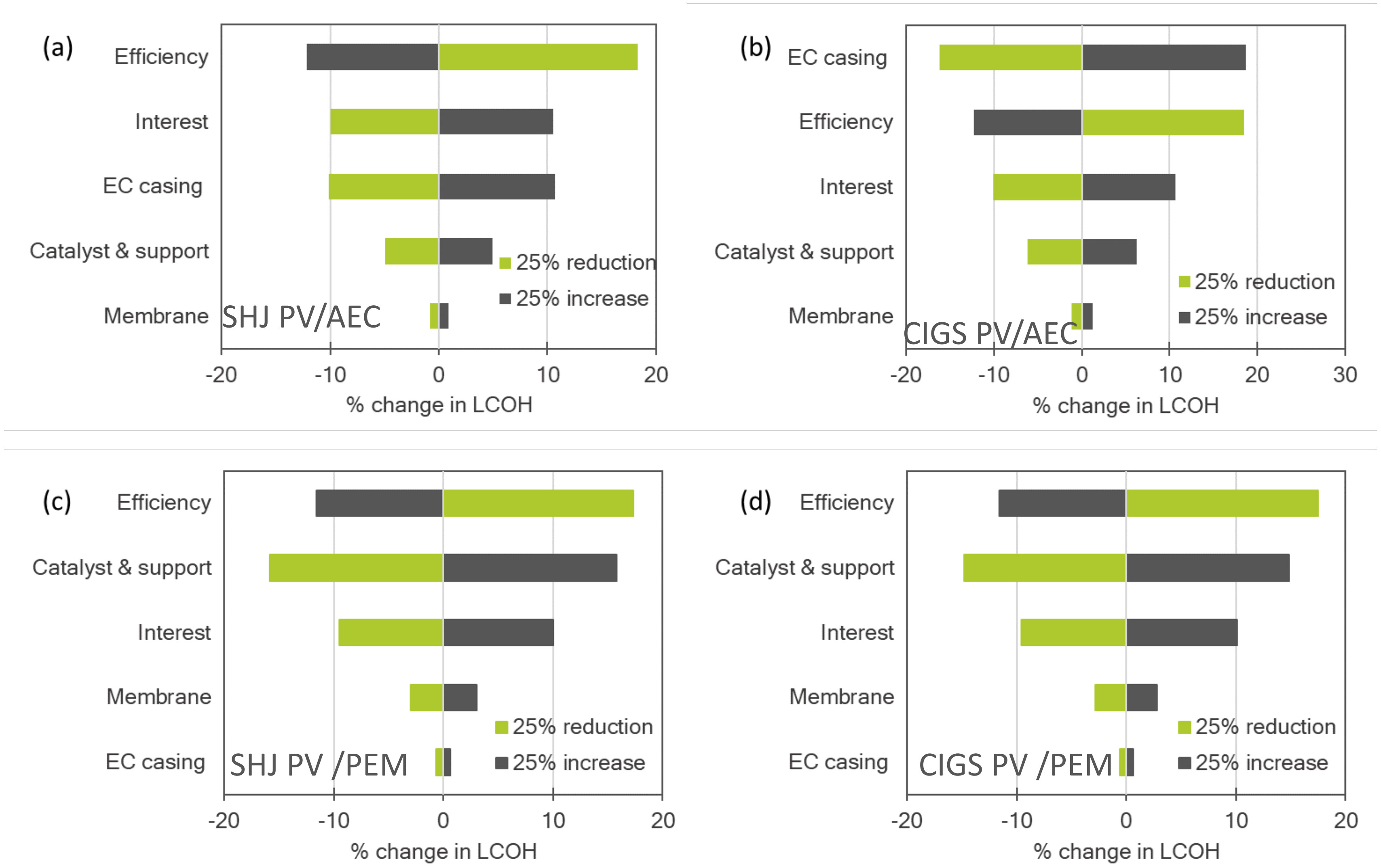
	Units	Components in thermal contact		Detached and thermally isolated	
		SHJ PV /AEC	CIGS PV /AEC	SHJ PV /PEMEC	CIGS PV /PEMEC
PV technology		SHJ	CIGS	SHJ	CIGS
Catalysts		NiFeO|NiMo	NiFeO|NiFeO	IrO_x|Pt	IrO_x|Pt
Electrolyser casing	-/-	Veroclear	Actual design uses Ni plate (calculations made assuming Veroclear)	Titanium and stainless steel plate	Titanium and stainless steel plate
Membrane	-/-	Zirfon PERL	Zirfon PERL	N212	Nafion N212
Economic assessment (for 16g/h or ~140 kg/year capacity)					
Annual CAPEX repayment	€/kg-H_2	6.47	9.52	6.12	3.96
Annual variable O&M costs	€/kg-H_2	0.20	0.20	0.35	0.35
Annual Fixed O&M costs	€/kg-H_2	0.25	0.41	0.16	0.10
LCOH annuity	**€/kg H_2**	6.92	**10.14**	**6.63**	**4.41**





Sonya.calnan@helmholtz-berlin.de

Main Results: Preliminary Technoeconomic Analysis



hydrogen production capacity of 16g/h or 140 kg per year

- Cost of electrolyser components dominate LCOH because there is no established supply chain for these materials and components similar to literature [1].
- Reports considering commercial electrolysers (1MW) indicate that PV capex is more dominant []
- The high impact of electrolyser and/or PV efficiency is in agreement with most studies [1,

[1] Grimm et al. (2020), International Journal of Hydrogen Energy, 45 (43): 22545-22555.

Sonya.calnan@helmholtz-berlin.de

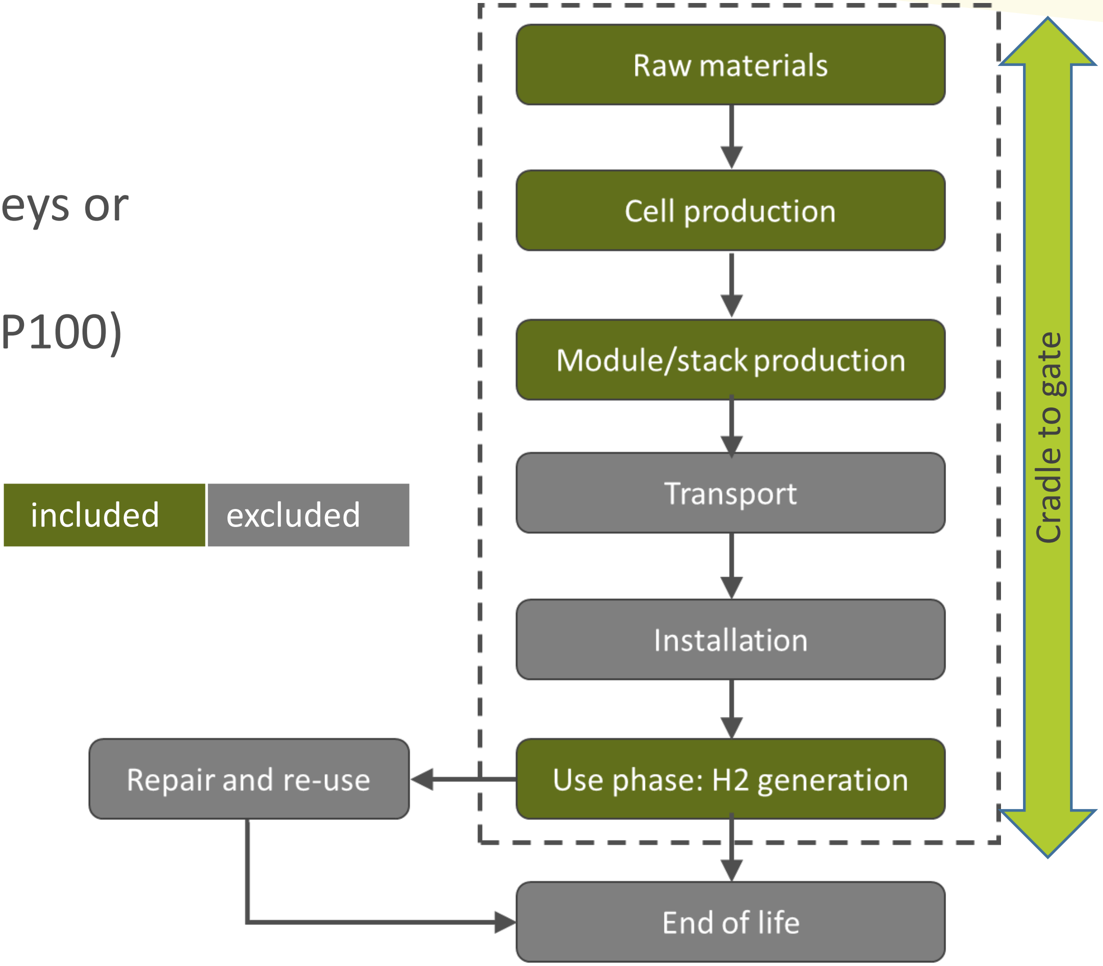
Main Results: Life Cycle Analysis approach

Methodology

- Software: OPENLCA
- Databases: ECOINVENT, NEEDS; missing data from own surveys or literature
- Impact Assessment method: RECiPE 2016 (Hierarchical, GWP100)
- Scope limited to cradle to gate for PECSYS systems

- Lifecycle stages which are the same for all production pathways to be omitted

- Gate to grave (end of life of H_2 generation systems) omitted as there is insufficient knowledge of recycling and disposal processes



sonya.calnan@helmholtz-berlin.de

Lifecycle analysis: energy and material flows

Life cycle analysis: Energy and material flows defined (essential flows to be identified)

		Significant components	Inputs	Output
Electrolyser stack	Core system	Anode, cathode, membrane, end plates, bipolar plates, seals, fasteners	Steel, Ti, Ni, Pt, Ir, Fe, Mo; PTFE; electricity, Nafion, Zirfon	emissions to the environment
	Balance of system	Pumps, compressor, purifiers	Materials to be determined from literature	emissions to the environment
	Process		Water; KOH (aq)	Hydrogen, oxygen, waste water
Photovoltaic module	Core system	Photoabsorber, metallic and transparent contacts; stringing ribbons, metalisation paste, glass	Si; Cu,In;Se, glass, EVA, PET; Cu(Sn60Pb40), ITO, Ag, Mo; process gases, electricity	emissions to the environment
	Balance of system	Mounting frame and fasteners, cables (for detached system)	Structural steel, aluminium, stainless steel	emissions to the environment
	Process		Solar energy	Electricity

- System emissions to the environment arise during material extraction processing, transport, system manufacture
- Flows for SMR and grid electricity shall be identified using data in existing databases and literature
- Use of essential flows reduces complexity of the calculation

Marika.Edoff@angstrom.uu.se

Progress beyond state of the art and impact

Progress beyond state of the art

- PV-EC combined and thermally integrated devices simulated using real climate data
  - No matching electronics included
  - Yearly hydrogen yield is highly dependent on accurate matching between series connected PV and EC
  - Reduction of voltage and efficiency of PV with high device operating temperature partly mitigated by higher EC efficiency

- Our TEA and LCA for integrated (PV) solar hydrogen devices and directly coupled PV-electrolysis differes from the following previous studies
  1. That use hypothetical systems and not actual prototype measurements to validate models [1,2]
  2. Study for was limited to TEA of directly coupled PV/EC and temperature dependence of device efficiencies not (explicitly) considered [2,3]
  3. Considers material and energy flows for the PV component in LCA unlike [4]

§

Expected impact

- Quantification of environmental as well as cost implications of directly coupled photovoltaic to water electrolysis systems

[1] Shaner et al. (2016), Energy Environ. Sci. 9: 2354–2371.
[2] Grimm et al. (2020), Int. Journal of Hydrogen Energy, 45 (43): 22545-22555.
[3] Yates et al., (2020), Cell Reports Physical Science 1:100209.
[4] Koj et al. (2015), Energy Procedia, 75:2871-2877.

Marika.Edoff@angstrom.uu.se

Conclusions and Outlook

Conclusions

- Modeling shows importance of match for PV-EC device for optimum yearly yield
- TEA and LCA values of solar hydrogen generation technologies can only be taken as indications with „large“ error bars because there is no established supply chain for materials and components
- Data for material and energy flows for the extraction and production of components (especially for the electrolysers) are not yet available in life cycle inventory databases
- Preliminary LCOH similar to other studies of silcion PV directly coupled to electrolysis (6.22 US$/kg-$H_2$ [1]; ~4 US$/kg-$H_2$ [2]) but comparisons are difficult because of differing locations and system specifications

Outlook

- Update TEA results once experimental data becomes available
- Complete life cycle inventories for compressors, balance of plant
- Calculate and analyse life cycle impacts
- Identify parameters for sensitivity analysis

[1] Grimm et al. (2020), Int. Journal of Hydrogen Energy, 45 (43): 22545-22555.
[2] Yates et al., (2020), Cell Reports Physical Science 1:100209.

Marika.Edoff@angstrom.uu.se

Thank you for your attention!

PECSYS

www.pecsys-horizon2020.eu

HZB Helmholtz Zentrum Berlin PVcomB

JÜLICH Forschungszentrum

UPPSALA UNIVERSITET

Consiglio Nazionale delle Ricerche

enel Green Power

FCH FUEL CELLS AND HYDROGEN JOINT UNDERTAKING

This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking under grant agreement No 735218. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation programme and Hydrogen Europe and N.ERGHY.
The project started on the 1st of January 2017 with a duration of 48 months.

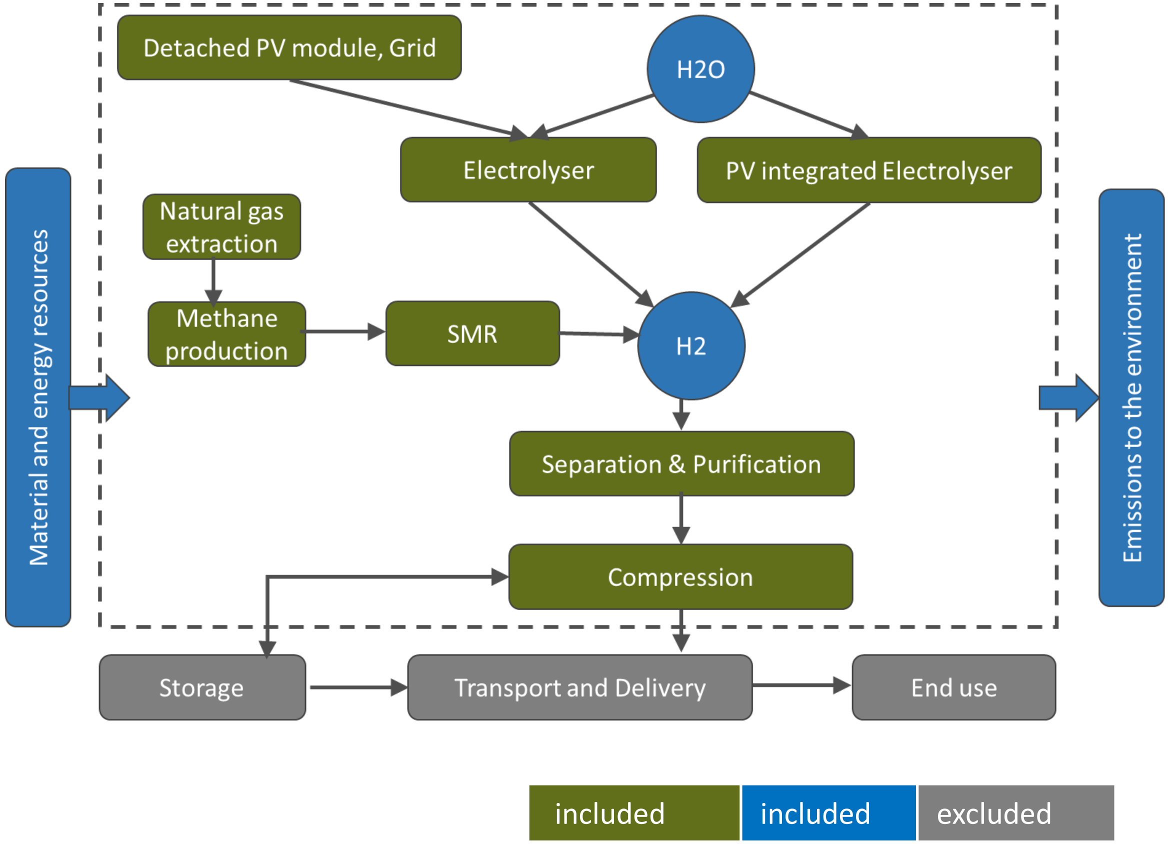
Lifecycle analysis: H_2 production pathways under consideration

- H_2 production pathways
  - i. Steam methanol reforming (pending consideration)
  - ii. Grid electricity and PEM electrolysis
  - iii. Direct coupled PV and PEM electrolysis (**PECSYS own**)
  - iv. PV thermally integrated to alkaline electrolysis (**PECSYS own**)
- Functional unit: 1MJ of H_2
- Reference flow: system size for production of 1 kg of H_2

Life cycle impact categories

- i. Human health
- ii. Ecological consequences (GWP, eutrophication, acidification, ozone depletion
- iii. Resource use: minerals, water, fossil fuels

System boundaries for H_2 production pathways



included	included	excluded

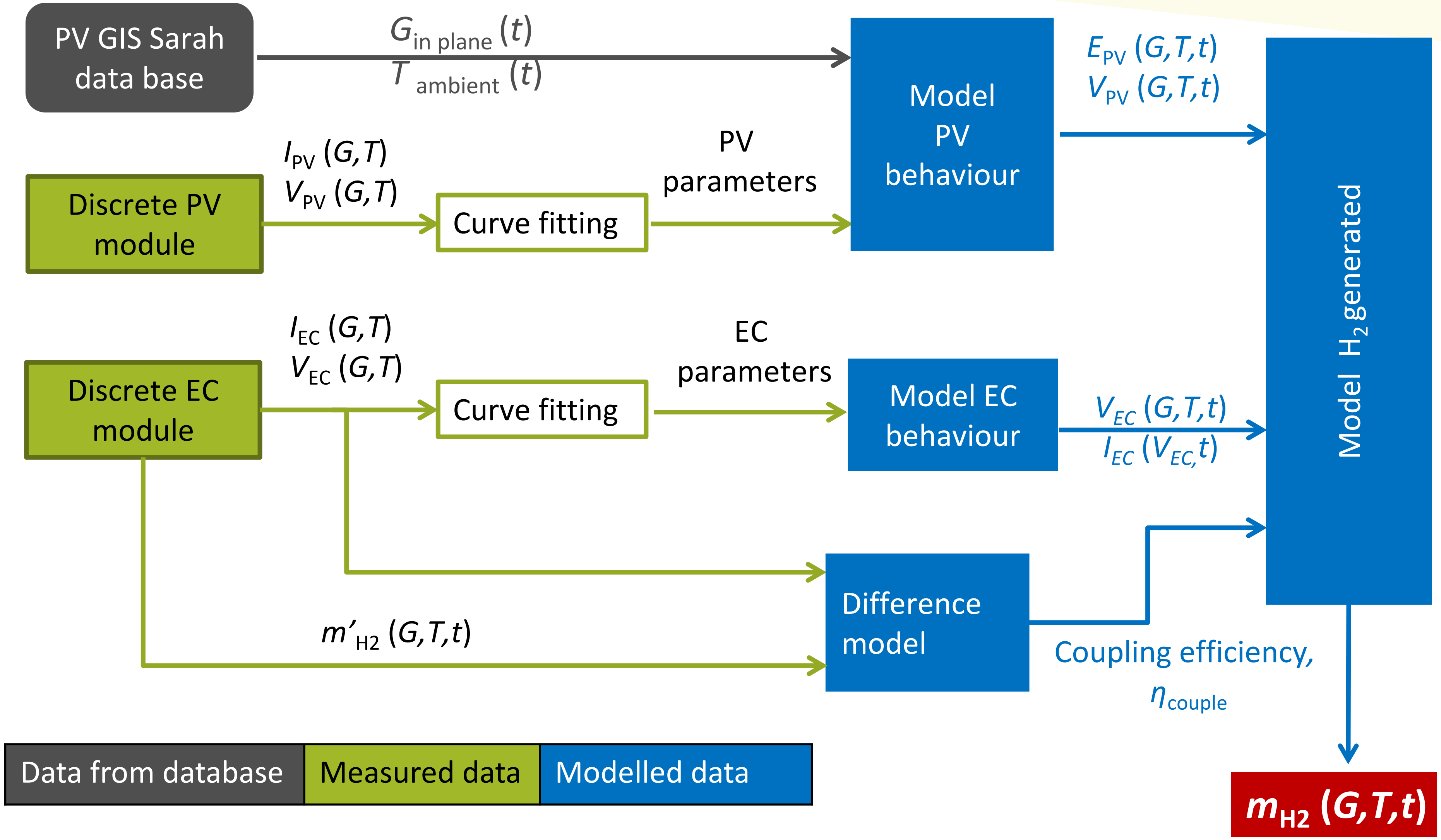
Data collection on-going

Sonya.calnan@helmholtz-berlin.de

Technical assessment: Annual performance model

Different from most models, Electrolyser is not operated at a fixed temperature, T_{EC} (T,t)

1. Discrete PV + discrete EC: T_{PV} (G,T,t) ≠ T_{EC} (T,t)
2. Integrated PV-EC with thermal integration: T_{PV} (G,T,t) ≠ T_{EC} (T,t) Except for near perfect heat transfer between PV and EC



PV GIS Sarah data base

$G_{\text{in plane}}$ (t)

T_{ambient} (t)

Discrete PV module

I_{PV} (G,T)

V_{PV} (G,T)

Curve fitting

PV parameters

Model PV behaviour

E_{PV} (G,T,t)

V_{PV} (G,T,t)

Discrete EC module

I_{EC} (G,T)

V_{EC} (G,T)

Curve fitting

EC parameters

Model EC behaviour

V_{EC} (G,T,t)

I_{EC} (V_{EC},t)

m'_{H2} (G,T,t)

Difference model

Coupling efficiency, η_{couple}

Model H_2 generated

m_{H2} (G,T,t)

Data from database	Measured data	Modelled data

Marika.Edoff@angstrom.uu.se

Methodology for economic analysis

System capital cost (*CAPEX*) calculation:

$$CAPEX_x = CAPEX_0 \times \left(\frac{Q_x}{Q_0}\right)^{-\alpha}$$

Q : the system's capacity,
0: index for base (prototype),
x: index for new (scaled- up) capacity,
α: learning parameter = **0.4** [1,2].

Assumptions for operating costs (OPEX)

- Electricity for balance of plant = **0.151 EUR/kWh** [3]
- (KOH) cost = **2.511 EUR/kg** [4]
- Water cost = **0.020 EUR/kg** [4]

$$C_{life} = \sum_{t=0}^{n} (CAPEX_t + OPEX_t)(1+r)^{-t}$$

- C_{life} [EUR/kg-H_2]: lifetime cost
- *r* [%]: annual discount rate for future cash flows = **5%**
- *n* [years]: economic lifetime of the investment = **20**

Annuity method

- Assumes constant annual payment over the economic service lifetime
- Ignores inflation and its effects on costs and income over time.
- Acceptable at prototype stage because cash inflows are unknown.

annuity factor, "*a*"

$$a = \frac{r\,(1+r)^n}{(1+r)^n - 1}$$

$$LCOH = \frac{(C_{life} \times a)}{m'}$$

m' [kg/year]: amount of hydrogen produced in a year

---

[1] B. van der Zwaan and A. Rabl, Solar Energy 74 (2003) 19.
[2] K. Schoots, et al., Int. J. Hydrogen Energy 33 (2008) 2630.
[3] Average electricity cost for mid-sized industry in Germany , Eurostats, 2018.
[4] W. Kuckshinrichs, et al, Frontiers in Energy Research 5(1),2017.