Ref. Ares(2024)4532231 - 24/06/2024

D14.1
Initial PDEC

Electrochemical oxidation of cyclic and biogenic substrates for high efficiency production of organic chemicals

eloxychem-horizon.eu
HORIZON-CL4-2023-TWIN-TRANSITION-01
1st January 2024 - 30th June 2028

ELOXYCHEM

Funded by
the European Union

Document control sheet

	ELOXYCHEM - Electrochemical oxidation of cyclic and biogenic substrates for high efficiency production of organic chemicals
Grant Agreement n°	101138376
Call identifier	HORIZON-CL4-2023-TWIN-TRANSITION-01
Type of action	HORIZON-RIA
Coordinator	SINTEF
Project start date	January, 1. 2024
Project duration	54 months
Work package n° and title	14 - Dissemination, communication and exploitation (RP1)
Work package leader	ETA
Dissemination level	PU - Public
Lead Beneficiary	ETA
Author	Claudia Batini, Emma Fromant, Álvaro Cabeza
Reviewer(s)	Bernd Wittgens, Theresa Rücker
Review date	18 June 2024
Due Date	30 June 2024

Statement of Originality
This deliverable contains original unpublished work except where clearly indicated otherwise. Acknowledgement of previously published material and of the work of others has been made through appropriate citation, quotation or both. This project has used a standard methodology already developed in BECOOL project (Grant Agreement number: 744821) and HYPER project (Grant Agreement number: 101091554), following EU recommendations. Ad hoc modifications were added to comply with the Grant Agreement conditions for ELOXYCHEM (Grant Agreement number: 101138376).

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This project has received funding from the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement No. 101138376.

Executive Summary

This document constitutes the preliminary version of the Dissemination, Exploitation and Communication Plan (PDEC) of ELOXYCHEM's results and it represents a strategic document to pave the impact pathway from the beginning of the project.

This first PDEC is an integrated Dissemination plan and Communication strategy, illustrating the most efficient measures to be carried out with reference to the targeted audiences. This document also provides a detailed schedule of activities to be implemented in the first year of the project (M1-M12). For the schedule of activities, please refer to the chapter "*6.Timeline for implementation (When?)*".

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List of Abbreviations

AI	Artificial Intelligence
ANN	Artificial Neural Network
BGIP	Background Intellectual Property = IP brought to the project by the partners
CAN	Controller Area Network
CAPE	Computer-Aided Process Engineering
CAPEX	Capital expenditure
CNN	Convolutional Neural Netwok
COCO	Cape Open to Cape Open
CPC	Cooperative Patent Classification
DAQ	Data Acquisition
DICA	Di-Carboxylic Acid
DNN	Deep Neural Network
DBNN	Deep Belief Neural Network
DT	Digital Twin
EC	Electrochemical
EIS	Electrochemical Impedance Spectroscope/Spectroscopy
EOP	Electrochemical Oxidation Process
FGIP	Foreground Intellectual Property = IP associated with the project results
FtO	Freedom to operate
IoT	Internet of Things
IPR	Intellectual Property Rights
KECA	Keto-Carboxylic Acid
KER	Key Exploitable Result
KPI	Key Performance Indicators
LCA	Life Cycle Assessment/Analysis
ML	Machine Learning
MOCA	Mono-Carboxylic Acid
NN	Neural Network
OEM	Original equipment manufacturers
OPEX	Operational expenditure
PDEC	Plan for dissemination, exploitation and communication
PINN	Physics-Informed Neural Network
PMC	Process Modelling Component
PME	Process Modelling Environment
RES	Renewable energy source
RTO	Research Technology Organization

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SCADA	Supervisory Control and Data Acquisition
SCLA	Social Life Cycle Assessment/Analysis
SME	Small and medium-sized enterprises
SOH	State of Health (of battery)
SotA	State of the Art
SOX	State of any battery parameter X
SWOT	Strengths, Weakness, Opportunities and Threats
TEA	Techno-Economic Assessment
T-FA	Tech-Futures Analysis
TOFA	Tall Oil Fatty Acid
TRL	Technology readiness level

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1. Definition and objectives

This document represents ELOXYCHEM preliminary plan for dissemination, exploitation and communication (PDEC) and its aim is to provide a guideline on how the project will be promoted and key results exploited to targeted audiences in an effective way.

To achieve this goal, ELOXYCHEM's pathway to impact is designed around the three pillars of Communication, Dissemination and support to Exploitation, as defined by the European Commission:

	Communication 	Dissemination 	Exploitation 
Objective	Engage with stakeholders and society and show the potential impacts and benefits of EU funded R&I activities, attracting the best experts and raising awareness of how public money is spent	Transfer knowledge and results to enable others to use and take up results, thus maximising the impact of EU funded research	Effectively use of project results through scientific, economic, political or societal exploitation routes aiming to turn R&I actions into concrete value and impact for society.
Focus	Inform about and promote the project and its impact on society	Focus on sharing results ensuring that they are made visible and available to be implemented in research, innovation and industries	Enable concrete use of research results - not restricted to commercial use
Target Audience	Audiences beyond the project's own community: stakeholders, media, citizens, broad public.	Audiences that might take an interest in the potential use of the results: scientists, industry, public authorities, policymakers, civil society, sectors of interest	Audiences - including project partners themselves - that may make concrete use of the project results: researcher, stakeholders, industry, (also SMEs), public authorities, industrial authorities, policymakers, sectors of interest, civil society

Figure 1 - Explanation of Communication, Dissemination, Exploitation

These three pillars should be conceived as integrated dimensions of the strategy to maximise the impact of the project. Therefore, while this document is focused on planning and implementing Communication and Dissemination activities, the outcomes achieved through the related measures will pave the way for exploitation actions as well.

Dissemination initiatives will be focused on raising awareness of the key stakeholders that could potentially uptake and further develop or utilize the project results at scientific, business or regulatory level.

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2. Dissemination and Communication strategy

This first dissemination and communication plan provides guidelines to promote ELOXYCHEM's initiatives and ensure impact from the project outcomes, with the aim to achieve effect of the generated results during the projects lifetime and beyond.

ELOXYCHEM PDEC is structured according to the following principles:

Who	Identify the **target groups** to address
What	Define **clear messages** to be conveyed, with a content in line with the profile of the target audience
How	Define and deploy the **appropriate tools** to convey the messages to the target audience
When	Plan the **appropriate time** to carry out both communication and dissemination activities, with respect to the project timeline.

Table 1 - Initial PDEC principles

2.1 Target audiences *(Who?)*

The first step in the communication strategy is to identify the relevant stakeholders. The identification and engagement with the target audience are crucial to ensure their needs are considered and to obtain maximum impact of the project's results. An effective stakeholder engagement can also amplify the chances of successful implementation and uptake of its results.

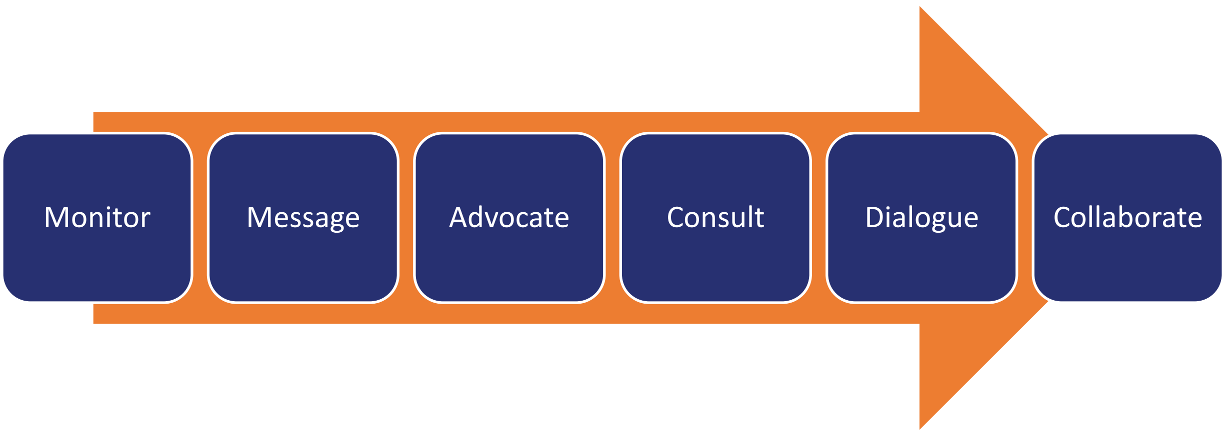

Figure 2 - Stakeholder engagement

Key stakeholders include individuals, groups or organizations with substantial interest in, or are impacted by, the project's goals, activities and outcomes.

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Target Group	Stakeholder
TG1: Research and scientific community	Universities and RTOs active in green chemistry, electrochemistry, biobased chemicals and waste stream, RES integration, AI, process control and in materials developments for electrodes
TG2: Industrial end users	Original equipment manufacturers (OEMs) and Tier 1 suppliers (polymer component manufacturers) in automotive, additive manufacturing, medical, electronics, oil & gas sectors and process industries under Processes4Planet (P4Planet) network
TG3: Financial actors	Industrial Investors in plants and renewable energy parks
TG4: Suppliers (equipment, materials)	Bio-based and recycle material suppliers, electrode manufacturers, cell manufacturers
TG5: General Public	Society interested in impact of project
TG6: Political	Policymakers, politicians, lobbyists
TG7: Energy providers	Renewable energy providers and utilities

Table 2 - Target stakeholders

2.2 Key messages (What?)

Proper and effective messages are vital for a successful communication campaign, especially when dealing with technical aspects, such as in the case of ELOXYCHEM project. The overall goal is to raise interest in learning more about the project and its endeavors. *Table 4* lists the identified key messages that will guide online communication activities.

Key Message	Target groups (as referred in *Table 3*)
KM1: Electrochemical conversion process information including coupling with RESs in terms of gains and pains	TG1, TG2, TG3, TG4, TG6
KM2: Green chemistry information	TG1, TG2, TG3, TG4, TG5, TG6
KM3: Environmental performance information	TG1, TG2, TG3, TG4, TG5, TG6
KM4: Techno-economic performance information	TG1, TG2, TG3, TG4, TG5, TG6
KM5: Implementation and investment requirements information	TG3, TG4
KM6: Exploitation framework and strategy information	TG3, TG4, TG6
KM7: Standards and commercialisation information	TG6
KM8: Supporting information to aid selection of sustainable products	TG6

Table 3 - Key messages

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3. Exploitation route

3.1 Introduction and goals

The definition of a strategy for the exploitation of the ELOXYCHEM outcomes is crucial to maximize the chances of future commercial implementations of ELOXYCHEM and its impact on society and the economy by: (1) contributing to electrifying the European chemical industry, (2) developing less energy-demanding solutions and with a lower environmental impact, (3) enhancing the integration with Renewable Energy Sources (RESs), and (4) developing AI-based digital with for optimal control and process maintenance.

The first step in this strategy is to identify the Key Exploitable Results (KER) before, during and after project execution, and their exploitation routes. Thus, Exploitation has a direct effect on Dissemination and Communication by defining those results that are worthy to be disseminated and communicated and, so, guaranteeing the efficiency of the related Dissemination and Communication actions.

To do so, an initial exploitation questionnaire and Intellectual Property (IP) register were done and shared with the consortium in M4. These documents include the aspects defined in the grant agreement (general information, innovation description, market description, financial and scale-up information, IPR, and Risks). However, the consortium was still involved in the discussion about the best approaches and in the identification of the Sensitive information before the submission of this deliverable and, for this reason, only partial information was available. Thus, an updated version will be available to the public through the project webpage once the complete feedback is provided (before M18). With the available information in this questionnaire, an initial exploitation plan and Tech-future analysis were drafted. Note that the Exploitation plant is a living document that will be continuously updated during the project (at least once per periodic report) and completed with a preliminary scale-up and Implementation plan (D15.2, M26). The final Exploitation plan will be ready in D16.4 (M54), also including a final exploitation roadmap (D16.5, M51), and the final scale-up & Implementation plan (D16.6, M54).

3.1.1. Exploitation plan goals

The **main goal** of the Exploitation plan drafted is to define the most adequate **steps for ELOXYCHEM results commercialisation**, also identifying alternative exploitation routes (related to Dissemination and Communication) for those results that cannot be commercially exploited. To do so, the proposed Exploitation plan includes the following sub-goals and time frame:

- The identification and evaluation of each KER by successive questionaries and the IP register (M6, M19, M38, and M48)
- The development of a business case (M54) and models (initial version in M6 and final models in M54)
- The development of the business plan (M54)
- The study of the market size and prospects, and route to market (draft version in M6 completed M54)
- The development and update of the Exploitation roadmap (initial draft in M6 and final version in M51)
- The identification of relevant stakeholders and the development of SWOT analysis (M6 and M54) in collaboration with ETA

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- The development of a risk evaluation for the project implementation (M6 and M54)
- The identification and definition of investment needs and funding options for the solution scale-up and market implementation (M6, M26 and M54)
- The establishment and update of the operational plan (M6, M19, M38, and M54)
- IP management and identification, including Tech-Futures (M6, and M54)

The preliminary Exploitation plan proposed is described in the subsequent sections, including the initial identification of the KERs, the exploitation roadmap, and the overall plan for the Exploitation activities. Updates based on the questionnaires will be done by IDE and ILL (M6, M19, M38, and M48) to define the final strategy plan in M54 (D16.4).

3.2 Exploitation questionnaire and innovation committee definition

The first step was to define an **innovation committee** composed of one representative from each partner to speed up the information exchange (see Table 4).

Partner number	Partner	Representative	Email
1	SINTEF AS	Theresa Rücker	theresa.rucker@sintef.no
2	MPI	Siegfried Waldvogel and Simon Trosien	siegfried.waldvogel@cec.mpg.de and simon.trosien@cec.mpg.de
3	EVONIK OPERATIONS GMBH	Jana Keupp	jana.keupp@evonik.com
4	IDENER	Álvaro Cabeza	alvaro.cabeza@idener.ai
5	ETA – ENERGIA	Stefano Capaccioli	stefano.capaccioli@etaflorence.it
6	Z PRIME GMBH	Ian Meakin	ian.meakin@z-prime.com
7	MEGARA RESINS S.A.	Poppy Krassa	p.krassa@megararesins.com
8	ESY-LABS GMBH	Annabella Kampfl	annabella.kampfl@esy-labs.de
9	IMPERIAL COLLEGE LONDON	Evina Katsou and David Renfrew	e.katsou@imperial.ac.uk and d.renfrew@imperial.ac.uk
10	ICONIQ INNOVATION LTD	Chris Hare	chris.hare@iconiqinnovation.com

Table 4 - ELOXYCHEM innovation committee

Once this committee was agreed, IDE and ILL prepared a questionnaire and IP register that was shared with the aforementioned representatives. The templates are provided in Annex -1. Exploitation questionnaire & IP register. Note that the filled document could not be

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included since there is not a clear definition of what information can be public yet. Once a public version is agreed, it will be available on the project webpage.

On the other hand, based on the available information (mainly from the proposal), **6 different KERs** could be defined and characterized:

- KER1: Industrially feasible metal-free electrochemical oxidation processes (EOPs) for the separate and combined conversion of cycloalkanes, cycloalkenes, and tall oil fatty acids (TOFA) to oxo-functionalization products, including mono- and dicarboxylic acids and cyclic ketones.

- KER2: Methodology for the scale-up from pilot to commercial scales, including future design options for commercialisation.

- KER3: EOP platform system for lab to demo and pilot scale process development.

- KER4: Machine-based learning methodology to optimize operating conditions for enhanced electrochemical performance (yield, lifetime, and reduction in CAPEX/OPEX cost).

- KER5: AI-based control & monitoring software for EOPs based on a Digital Twin.

- KER6: Strategy for integrating electrochemical processes with Renewable energy Sources (RESs), incorporating modelling and simulation tools.

Details about the related financial aspects, TRL changes, IP, exploitation model, route to market, risks, and market description were partially provided. Nevertheless, only partial information is available and, on the other hand, the definition of the sensitive aspects is not complete yet. For this reason, just an overall summary of the main aspect is provided below and in the following sections. Moreover, it should be noted that, despite this initial conservative definition of the exploitation strategy, the consortium follows the FAIR principles and, so a more complete version will published as soon as the exploitation options and the confidentiality are clearer.

All the KERs are related and allow the corrected development of KER1, which corresponds to the development of an electrochemical solution to produce polymer precursors. The overall project starts from a suitable technological base **(TRL3/4)** supported by the consortium IP and know-how (early-defined as Sensitive), which will allow an increase in the TRL **up to 6**. Moreover, some initial **estimates** (mainly Sensitive information) of the **financial aspects** were provided, which **foresees** a **feasible industrial development** of the solution. Also supported by the **wide different markets** where ELOXYCHEM could theoretically participate (see section 3.5). Regarding the exploitation model, **commercialisation** is the only initially defined, but from two different perspectives. The first one would be product selling (and, so, the route to market would be to produce the different precursors for several end users), while the second would be consultancy services to scale electrochemical processes at the industrial level (being the route to market following the internally defined steps to move from the concept to TRL9). Licensing would also be an option when fatty acids are used as a feedstock. Finally, for the risk assessment, see section 3.7.

A particular and critical aspect of the financial evaluation of each KER refers to the requirement for the scale-up. However, currently, the information is quite limited since the

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project is in its first stages. Despite this, some evaluations at reasonable scales were already provided, including the calculation of different economic estimates (like the net present value). All of them show a promising situation where the solution could provide profits at reasonable payback times assuming that the targets set for selectivity and current yield will be achieved. Detailed updates will be reported in D15.2 (M26) and D16.6 (M54).

3.3 Exploitation pathway and roadmap

Due to the current level of uncertainty (M6), the consortium indicated that a clear roadmap and pathway for exploitation cannot be correctly defined yet; especially with regard to the classification between sensitive and public information. Thus, although **initial versions** have been developed, this section was set as **SENSITIVE in this preliminary strategy**. However, a complete version will be provided in M51 (D16.5).

3.4 Preliminary business case and model

Similarly to section 3.3, the consortium is not still able to adequately define a completely clear business case and model(s). Thus, this section was also declared as **SENSITIVE.** Despite this, an initial **business model was drafted and internally shared. Likewise for the initial business case.**

3.5 The study of the market need, size, prospects, and route to market

A similar situation to sections 3.3 and 3.4 was defined for this section. In this sense, **a deep analysis of the market options was done based on the information provided in the Grant Agreement and the partner's knowledge.** Nevertheless, the degree of detail that can be currently achieved is limited, so, the consortium decided to initially keep this as **SENSITIVE.** The overall classification of the expected market and the main areas covered can be seen below.

3.5.1. Market(s) related to the electrochemical conversion

SENSITIVE.

Targeted customer(s)

SENSITIVE

Route to market

SENSITIVE

3.5.2. Market(s) related to consultancy services

SENSITIVE

Targeted customer(s)

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SENSITIVE

Route to market

SENSITIVE

3.6 Stakeholders and SWOT analysis

Stakeholders' identification is done inside the PDEC (see section 1), also including the key messages for each of them (see Table 4). However, stakeholders can also be **competitors** for the ELOXYCHEM solution. Thus it is a threat that must be also evaluated. In this sense, the questionnaires asked for any company that could have/develop a solution that would reduce the EXOLYCHEM process market opportunities or, even the freedom to operate. At this point, Evonik identified *Cathay Biotech* (captive use by Evonik) for DDDA production, and *Cathay Biotech*, *Emery Oleochemicals*, *Palmary Chemical*, and *Croda Int. Plc* when fatty acid and dicarboxylic acids different from DDDA are used. Similarly, IDENER reported that there are many consultant companies in the field of renewable energy (>10)[1]. However, they are usually focused on the integration of RESs with the grid rather than on evaluating the direct effect on a process. Nevertheless, aspects like intermittency and distributed power generation are covered. A remarkable company is the *INTEGRATION consulting group*[2], which has projects on Power to X and, can be a direct competitor for IDE, specifically for its worldwide activity. However, IDE expertise includes many fields, including process modelling, which makes it easier to understand the particular problem of the industry and develop tailored solutions. Despite this, the Tech-Futures Analysis (see section 3.8) based on the available patents reported that the freedom to operate would not be in a comprise, although several approaches developed by Chinese companies could affect EXLOCYHEM in the future. Thus, this feasible competitors' screening must continue during the whole project execution. To complete the threat evaluation, a **preliminary SWOT**[3] analysis was done in Figure 3.

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[1] https://jake-jorgovan.com/blog/renewable-energy-consultants-consulting-firms
[2] https://integration.org/
[3] SWOT (strengths, weaknesses, opportunities, and threats) analysis is a useful tool to evaluate the burdens and opportunities to exploit results. In addition, a clear definition of the strengths and opportunities allows a coherent identification of the base for exploitation and markets.

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STRENGTH	WEAKNESS
• Consortium composed by experts in the related fields (electrochemistry, downstream, AI, scale-up, and engineering) • Relevant industrial partners with direct access to the pointed-out markets (mainly, EVONIK and MEGARA) • Innovation solution to produce polymers precursors and specialty chemicals by electrochemical processes • Less energy and chemicals consumption than conventional thermochemical options and easiness to be supplied with renewable energy • Lower environmental impact • Digital twin for optimal maintenance and control	• Additional funding from other research calls or private is foreseen to achieve commercialization • Performance highly influenced by mass transfer limitations (e.g., oxygen dissolution) • Safety concerns about the organic solvents used in the electrochemical reactor in combination with oxygen (e.g., toxic gas released) • Scale-up limits due to technological barriers (e.g., electrodes has a maximum size)
OPPORTUNITIES	**THREATS**
• Training events and attendance to clustering activities • Collaboration with other EU projects • Alignment with EU industry electrification plans and carbon neutral economy • Society appealing of (more) sustainable products. Especially relevant for plastic	• Future patents (mainly from China) affecting some aspect of the ELOXYCHEM solution, reducing the freedom of operation • End-user reluctance to use new materials without an exhaustive verification • Extremely sensitive to fluctuations in the electricity market

Figure 3 - ELOXYCHEM preliminary SWOT analysis

3.7 Risk Assessment and Risk Map

Risk assessment is shared with the contingency plan. Thus, the update in the risk evaluation can be found in D17.2.

3.8 Tech-Futures Analysis.

The complete (T14.6) Tech-Future Analysis by partner IIL is a stand-alone report can be found in Annex-2. It is a comprehensive document and relates strongly to exploitation. The key summaries are noted here:

Executive Summary

The main technological development aims of the ELOXYCHEM project are defined in Grant Agreement (PDF p62):

- ELOXYCHEM will establish a commercially relevant electrochemical oxidation process that will become a strategic development to replace existing chemical conversion processes that are heavily reliant on imported materials such as nitric acid and imported fossil-fuels such as natural gas.
- ELOXYCHEM will promote a credible pathway for Europe's twin transition (green and digital) by demonstrating: (i) a new transformational electrochemical conversion platform process at a pilot scale consisting of reactors and downstream separation to final products with marketable specification to reliably achieve TRL6; (ii) drop-in replacement technology for chemical conversion.
- ELOXYCHEM will also optimise the process to demonstrate versatility of the process to multiple feedstocks ranging from current feedstocks and future bio-based and biogenic sources. Using AI strategies for optimisation, the pilot plant will aim to improve electrochemical performance, improve lifetime and reduce cost; prove viability of integrating with renewable energy sources considering intermittency and potential to offer demand-response flexibility; integrate process design, including

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materials, reactor/cell, and separation methods, from the process intensification and cost perspectives.

The purpose of this 1st Iteration ELOXYCHEM Tech-Futures Analysis [T-FA] is to assess the potential of the proposed outputs of the ELOXYCHEM project [FGIP] for patent-protection and exploitation, IIL has carried out this review into patenting activity in Electrochemical Oxidation Process [EOP] technology, the 1st Iteration T-FA, to:
- update the State of the Art [SotA] in each ELOXYCHEM project technology development area
- identify any new competing technologies that have been published since the ELOXYCHEM proposal was prepared in March 2023
- identify no-go areas where project technology developments might lead to third-party patent infringements
- establish current Freedom to Operate [FTO] with the planned technology developments.

The analysis was carried out as described in Section 2 of the F-TA report. Key words, phrases and acronyms were used along with Cooperative Patent Classification codes [CPC codes] in T-FA activities to identify the most recent and relevant granted patents and patent applications. The results of those activities are presented and analysed and are summarised here:
- Overall conclusions on the SotA for ELOXYCHEM technology developments
  - ✓ No patent application or granted patent discovered in the T-FA searches discloses technology that appears to duplicate, in detail, the characteristics of the proposed ELOXYCHEM electrochemical system for the conversion of organic substrates to high added-value chemicals;
  - ✓ None of the patents or applications discovered appears to infringe the partners' IPRs in their own technology patents.

- Overall conclusion regarding FTO with the ELOXYCHEM project results:
  From the observations made above, it may be inferred that the project partners can seek patent protection for their developments in electrochemical oxidation processes [EOPs], powered from renewable energy sources [RESs] and designed for the conversion of organic substrates to high added-value chemicals. However, it is important to note that any patent search is only ever a snapshot of the patent database(s) on the day and at the time it is carried out. Therefore, the partners should continually monitor developments in the relevant technology sectors, perhaps as suggested in Section 6 of the T-FA report.

Further summaries from the body of the report:

Overall summary of the SotA for each KER
Below are collated the overall summaries from Section 3.1.1 through Section 3.1.6 (of the T_FA report) regarding the SotA for each KER.
- KER1 – Metal-free EOPs for conversion of cycloalkanes, cycloalkenes and TOFA to oxo-functionalisation products:
  It is clear that each of the 16 publications listed in the T-FA report (Table 3.1.) discloses one or more inventions that show some degree of overlap with the electrochemical oxidation process [EOP] technology developments that the partners plan to make during the ELOXYCHEM project. However, none discloses all of them. In particular the use of cycloalkanes, cycloalkenes and TOFA as substrates for EOPs was not found to be disclosed in any publication.

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- KER2 – Methodology for the scale-up of EOP chemical production from pilot to commercial scales:
  Whilst publications were identified that disclose means for scaling up electrochemical processes e.g. WO2023161695 (A1) that discloses scale-up of an electrochemical process for making nanocrystalline carbons to the level of mass-production, no patents or patent applications were found that disclose the scale-up of electrochemical oxidation processes [EOPs].
- KER3 – EOP platform system for lab to demo and pilot scale process development:
  Whilst publications were identified that disclose electrochemical technology platforms e.g. EP3453064 (B1) that discloses an advanced electrode technology platform for electrochemical reduction of COX (cyclooxygenase) species, no patents or patent applications were found that disclose such a platform for electrochemical oxidation processes [EOPs].
- KER4 – ML methodology to optimise operating conditions for enhanced EOP performance:
  No publications were found that disclose the application of machine learning to the optimisation of electrochemical oxidation processes or the devices/reactors/cells in which they are carried out.
- KER5 – AI-based control and monitoring software for EOPs based on a Digital Twin:
  Numerous publications were found that disclose the application of artificial intelligence, especially neural networks of different types to data from non-destructive monitoring of electrochemical systems (especially lithium ion batteries) and/or to the creation of digital twins of such systems. However, no publication was found that specifically discloses the application of AI to electrochemical oxidation processes for the conversion of organic substrates to high added-value chemicals and/or the creation of Digital Twinss thereof for EOP optimisation.
- KER6 – Strategy for integrating EOPs with RES, incorporating modelling and simulation tools
  Although several publications were found that disclose the modelling of energy systems that include RESs for powering of electrochemical systems and several were found that disclose the application of RES-derived electricity to the electrochemical oxidation of organic chemicals, no patent or patent application was discovered that discloses both.

In summary, having reviewed each KER collated above, it is obvious that the partners in the ELOXYCHEM project are currently working at the very cutting edge of technology in each of the relevant technology sectors.

Summary of the FTO with the ELOXYCHEM project results
Should they be lucky enough to be eventually awarded a patent for their invention(s), the partners should then have freedom to operate [FTO] with it (them) on markets in that jurisdiction and in any other where a patent is granted .
As far as FTO with the actual ELOXYCHEM project results is concerned, this cannot be judged as it appears that none of the processes/products is completed and, therefore, their potential for patentability and/or infringing third party IPRs cannot be properly assessed at this time.
What can be said is that of the relevant patents or patent applications found during the searches for this 1st Iteration T-FA, listed in F-TA report, Table 3.1.1 through Table 3.1.6, 78% of them are from Chinese enterprises and are for Chinese national patents or national utility model patents only. This means that, so long as they do not attempt to launch any related product on Chinese markets, the partners cannot infringe the IPRs in the inventions disclosed in those publications. However, the teachings of all of them now form part of the

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prior art and must be taken into account should the partners decide to seek patent protection for their own inventions arising during the ELOXYCHEM project.
That said, there appears to be very little overlap between published EOP systems powered from renewable energy sources and the proposed technology developments in the ELOXYCHEM project meaning that the partners may well be able to get patent protection for their own inventions made during the project and eventually enjoy FTO with them.
N.B. As pointed out above, it will be essential for the partners to continue to monitor competitor patenting and commercial activity throughout the remainder of the project and beyond (Section 6 of the T-FA report has suggestions as to how this might be achieved).

Potential competitors identified in searches for the T-FA
As noted above, 78% of the publications listed in the F-TA tables are from Chinese enterprises. Of these, UNIV GUILIN TECHNOLOGY has published the most that are relevant to the technology developments anticipated in the ELOXYCHEM project: ELOXY1-04, ELOXY1-05, ELOXY1-12 and ELOXY1-19. This may mark them out as potential competitors and it may be worthwhile to maintain a watching brief on them and their published patent applications.
From the conclusions in the F-TA report Section 3.3 and in Section 4, it seems that there is a global lack of competitors offering EOP systems for the conversion of cycloalkanes, cycloalkenes and TOFA into high added value chemicals that are powered from RESs. However, as pointed out above, it will be essential for the partners to continue to monitor competitor patenting and commercial activity throughout the remainder of the project and beyond (Section 6 of the T-FA report has suggestions as to how this might be achieved).

Conclusions
The conclusions from the T-FA report are clearly laid out in Section 3 and Section 4 of the report and summarised Executive Summary.
In summary, this 1st Iteration T-FA report has provided a timely update of the SotA in technology sectors relevant to the six anticipated Key Exploitable Results [KERs] of the project, whilst simultaneously providing an indication of the patentability of the projects results and the partners' freedom to operate [FTO] with those results now and in future.
This report will be followed by reports on two further iterations of T-FA – one towards the middle of the project and one towards the end of the project.

3.9 Operational Plan

In order to fulfil the exploitation goals, i.e. to promote the successful exploitation of the project results by adequate strategies, several actions are considered for the 54 months of project execution (see Table 5).

Objective	Strategy	Timeframe	Responsible	Progress
Development of an adequate and efficient plan for results Exploitation	Collection of all the relevant information from internal (exploitation questionnaires and IP register) and external sources (e.g., patents bases and market)	The complete project: -M6: preliminary exploitation plant and first questionary & IP register (D14.1) - M19: intermediate questionary & IP register -M38: second intermediate	IDENER, IIL, All	Initial draft in D14.1

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Objective	Strategy	Timeframe	Responsible	Progress
		questionary & IP register -M48: final questionary & IP register -M51: final exploitation roadmap (D16.5) -M54: final exploitation plant (D16.4)		
To create a business plan, case and models	Analyse the competitors and improve the value proposition, focusing on the different feasible end users for the solution(s) developed in ELOXYCHEM	The whole project: -M54: final exploitation plant (D16.4)	IDENER, IIL, All	Not started as detailed information on the process and its performance (technical, economic, and environmental) is needed for its development
To engage any relevant stakeholders	Follow the dissemination plan, events participation, website, and social media update	The whole project: -See sections 2 and 4. -Especially remarkable events: workshops associated with D15.1 (M24), and D16.1 (M42).	ETA, ALL	Initial draft in D14.1
Scale-up and implementation	Monitor and evaluate the cost related to the ELOXYCHEM solution(s) scale-up and implementation	The whole project: -M26: initial Implementation plan (D15.2) -M54: final scale-up & Implementation plan (D16.6)	IDENER, all	Not enough information yet

Table 5 - ELOXYCHEM exploitation operational plan

Finally, it should be noted that the operational plan for the 5-10 years after the project end will be in the final exploitation plan (D56.5, M54), focusing on the key activities required for commercialisation.

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4. Dissemination and Communication tools *(How?)*

4.1 Visual identity

ELOXYCHEM visual identity represents an **easy-to-recognize** tool to present the project at events, conferences, workshops and other activities to the European Commission, as well as to the scientific audience, industrial entities and general public. The visual identity includes logos for different backgrounds, fonts, color palette and graphic elements, and templates for project presentations, documents and posters, leaflet and the website.

The project logo consists of two electrical wires (power supply) with sockets that create a hexagonal shape, referring to an cyclohexane/cyclohexene - a representative of the cyclic alkane/alkene family and the lightning to electricity as renewable energy carrier. The shapes of lettering take up the concept of electrical circuit, revisited in a modern way, while the blue and orange colors refer to the electrical world.

Figure 4 - ELOXYCHEM logos on different screens

The colours palette ensures consistency in visual identity, creating a pleasant and user-friendly interface.

Figure 5 - ELOXYCHEM colours palette and fonts

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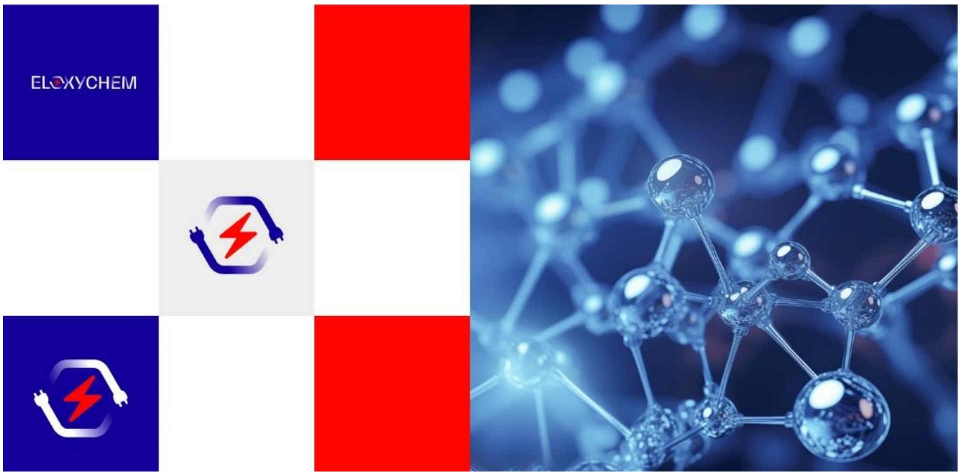

Figure 6 - ELOXYCHEM graphic elements

As the elaboration of the logo and colors palette have been completed, a series of templates have been designed in compliance with the visual identity and made available to all partners on the project shared area – "*Shared Point*" managed by SINTEF. The templates include:

- Presentation slides (ppt)
- Minutes of meeting (word doc)
- Deliverable report (word doc)

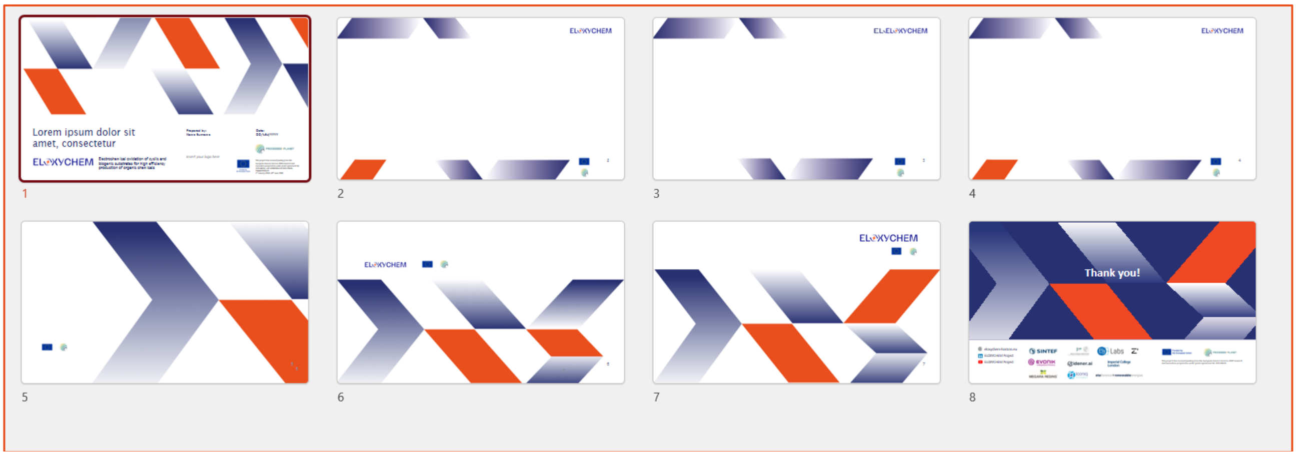

Figure 7 - ELOXYCHEM slides template

This project has received funding from the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement No. 101138376.

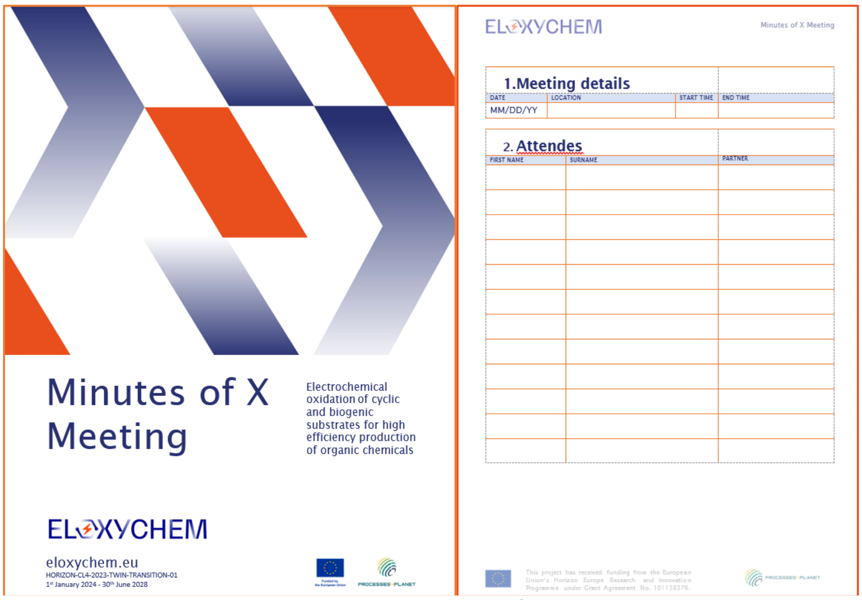

Figure 8 - ELOXYCHEM minutes of meeting template

Figure 9 – ELOXYCHEM deliverable template

This project has received funding from the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement No. 101138376.

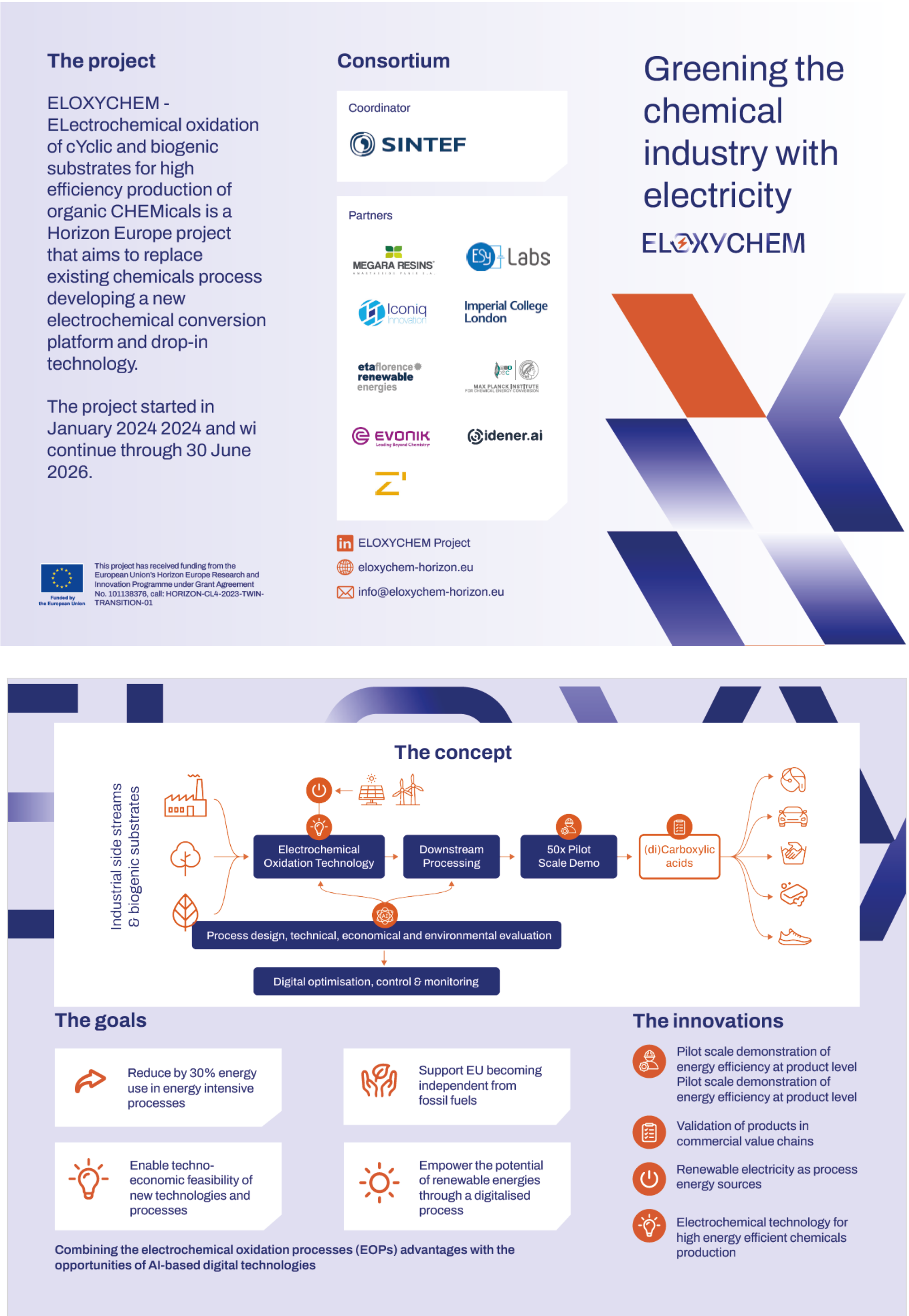

Figure 10 – ELOXYCHEM leaflet

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4.2 Online presence

ELOXYCHEM website is the main digital hub of the project during its lifetime and beyond. To ensure the project's best visibility, the website is accessible with an intuitive URL: https://www.eloxychem-horizon.eu/

The ELOXYCHEM website has been developed in line with the project characteristics and following this structure:

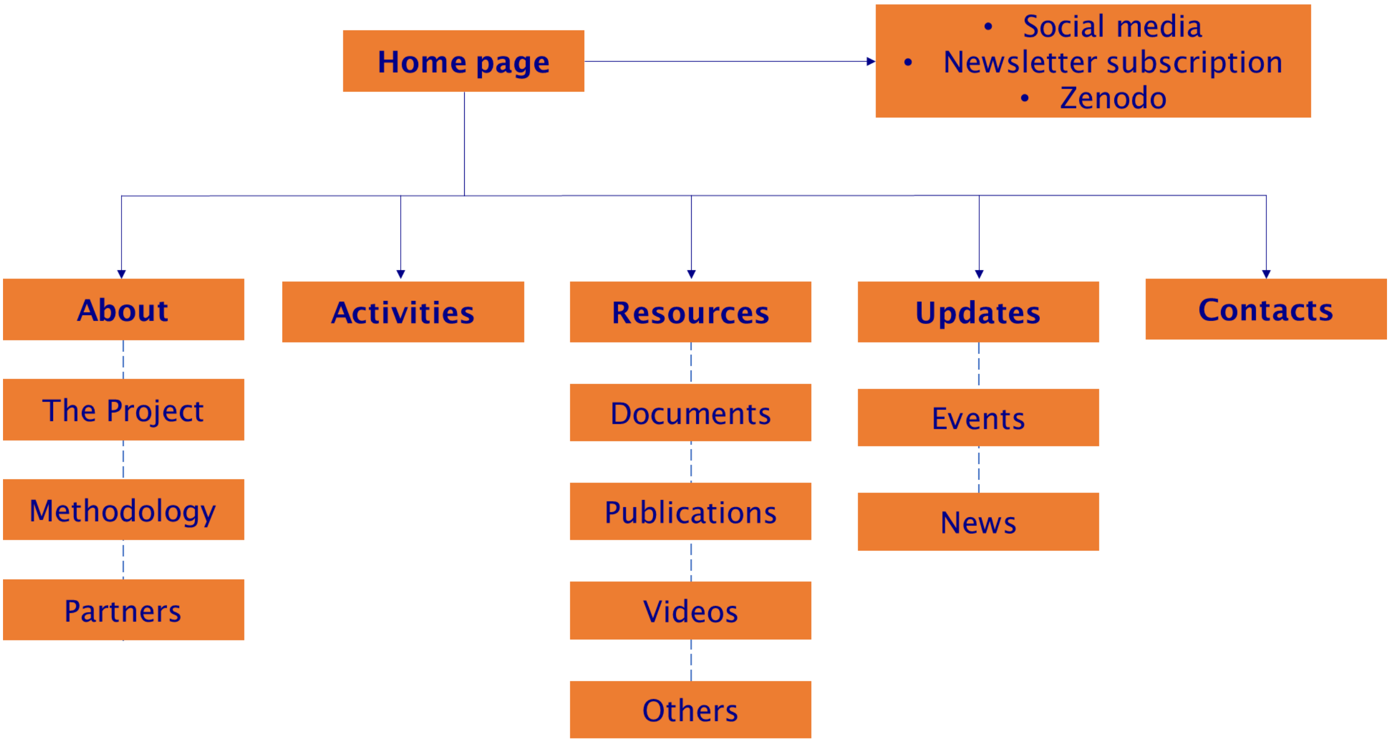

Figure 11 – ELOXYCHEM website structure

Figure 12 - ELOXYCHEM Homepage (https://www.eloxychem-horizon.eu/)

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4.3 Social Media

ELOXYCHEM social media channels will actively boost the key messages 2-4 to these key stakeholders as identified in Table 2 - Target stakeholders. During the initial phase of the project, the social medias channels will be focused on raising awareness of the project and paving the way to cluster with stakeholders and related initiatives.

Therefore, **LinkedIn** will be used as the main tool to build the widest possible audience of entities interested in the project, promoting the participation and/or organization of research activities, events and workshops, and events undertaken by ELOXYCHEM.

Figure 13 – ELOXYCHEM LinkedIn page (https://www.linkedin.com/company/eloxychem-project/)

YouTube will instead be used as repository for ELOXYCHEM videos, regarding key messages 2-4.

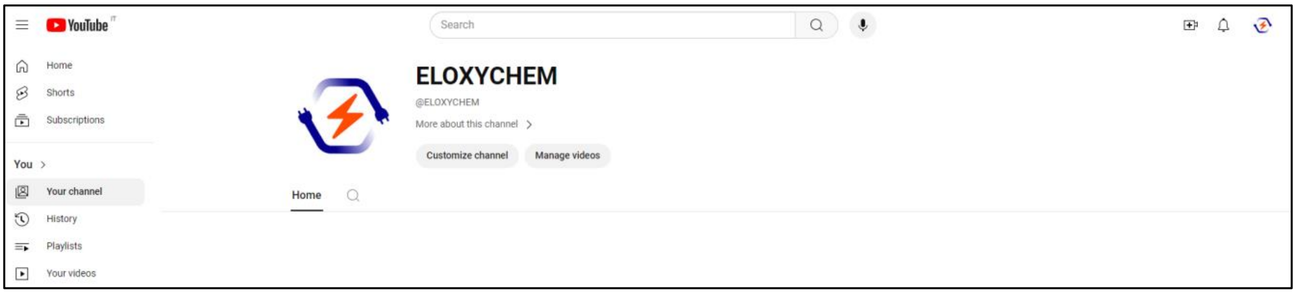

Figure 14 – ELOXYCHEM YouTube account (@ELOXYCHEM)

4.4 Events

The presence at scientific events is crucial for the proper dissemination of ELOXYCHEM and its outcomes. For this reason, the following list constitutes the preliminary plan for project specific events:

- **2 cross – cutting issue workshops** organized by SINTEF and supported with input from all partners, at M18 and M36; in the M36 the Max-Planck Institute (MPI) will

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organize a capacity building session to present main conclusions, results, pilot and future activities;
- 1 project-specific event at MPI at M12;
- **1 day-final event** (at M54) event will be organized in Germany and hosted by Evonik. At which, MPI will organize a capacity building session (as a workshop) to present the main conclusions.

Within the first year, the ELOXYCHEM team has identified the following international events as relevant platforms to potentially present the project at:

- International Society of Electrochemistry (ISE) – annual and topical meetings;
- EUROCORR – Next conference, 1-5 September 2024, Paris;
- ACHEMA – Next conference: 10 -14 June 2024, Frankfurt, Germany;
- CphI – Next conference: 8-10 October 2024, Milan;
- EUBCE – Next conference: 24-27 June 2024, Marseille;
- **Processes4Planet/A.SPIRE events** –often arranged as networking events in collaboration with other EU funded projects.

4.5 Digital initiatives

Several digital materials will be developed during the lifetime of the project and beyond. ETA will oversee producing:

- At least one video with **short interviews of partners** during project meetings, to present the different institutions and their role within ELOXYCHEM;
- **One** project **video** introducing the **concept of the project**, guiding public use – by M12;
- At least **one project video** related to the plant demonstration at M35.

The format of the above-mentioned videos can consider different techniques, such as animations and infographics, to successfully convey scientific content to a wide audience.

ELOXYCHEM videos will be shared on the project website and social channels, as well as at conferences and exhibitions across Europe.

4.6 Publications

All consortium partners will try to use all opportunities to generate publications to disseminate project results according to open access requirements.

At least 5 **press releases** will be produced: the first one to announce ELOXYCHEM's launch, the second at M12 to promote the project's progress, the third in M24 and the fourth in M36 (if the project progress allows it), while at M52 a final press release will be published.

At the end of the project, a **white paper** will be prepared within the *D16.4 – Final PDEC including white paper (M54)*, to examine the ELOXYCHEM research methodology and experiments performed. The white paper will constitute a valuable and publicly available document and will be available in digital versions (downloadable from ELOXYCHEM website and social channels) and printed as handouts for the final event. The paper will constitute one of the principal tools to enable and assure the creation of impact beyond the project end, supporting the escalation of the ELOXYCHEM project recognition.

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ELOXYCHEM's scientific papers will be published in peer-reviewed and green or gold model open access papers, targeting journals such as ACS sustainable chemistry and engineering, ChemSusChem, Green Chemistry, and more (M36).

5. Key Performance Indicators (KPIs)

This table lists the KPIs relevant to dissemination and communication work packages for the ELOXYCHEM project.

Dissemination Measures	Who?	How?	What?	KPIs?
To disseminate scientific findings that would benefit further R&I activities	• TG1 • TG2	• Peer-reviewed publications (M36) • Attendance at conferences and events (M12, M54) • Course materials	• KM1 • KM2 • KM3 • KM4	• 8 accepted publications • At 20 events (physical and online) • Academic course (35 credit hours) on electrochemistry and industrial applications in at least 2 universities
To establish synergies with other relevant projects and stakeholders	• TG1 • TG2 • TG3 • TG4	• Targeted Communications • Direct engagement at conferences and events	• KM1 • KM2 • KM3 • KM4 • KM5 • KM6	• Engagement with at least 20 relevant association members • Participation of 15 conferences and events (physical and online)
To demonstrate technology to the stakeholders from industry and policy makers	• TG1 • TG2 • TG4 • TG6	• Capacity building sessions	• KM1 • KM2 • KM3 • KM4 • KM5 • KM6	• 2 capacity building sessions • 2 workshops with 60 participants – held in conjunction with ELOXYCHEM scientific events
To engage relevant experts for the ELOXYCHEM advisory board	• TG1 • TG2 • TG3 • TG4 • TG6 • TG7	• Dissemination and Exploitation Manager will support the project coordinator and project partners to form a proper Experts Advisory Board (EAB)	• KM1 • KM2 • KM3 • KM4 • KM5	• Recruitment of at least 3 experts by M12
Communication Measures	• TG5 • TG6	• Project website, videos, social media • Press releases • Other multi-media outputs	• KM2 • KM3 • KM4	• At least 10,000 search hits from at least 10 countries in Y1 • 1,500 unique visits to the website in Y1 • 1,000 views total across all project videos • Average of 24 social media posts per year (2 per month, 108 in total) • 1,000 followers across all social medias

Table 6 - ELOXYCHEM KPIs

6. Timeline for implementation *(When?)*

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Dissemination and communication activities during the first 18 months of the ELOXYCHEM will be focused on **rising awareness** and interest on the project and its goals, connecting with the key stakeholders. To reach this goal, an effective dissemination of early results is essential, and it will be done through social medias and website, participation in conferences, scientific publications, along with workshops and webinars. During the period from M19 to M36, the dissemination and communication activities will be focused on **transferring the knowledge** between the project partners and the key stakeholders, together with keep high the awareness about ELOXYCHEM and create consensus and interest on large scale. In the last phase of the project, from M37 to M54, the activities will be aimed at **transferring results**, conveying the main results and facilitating their replication, as well as consolidating synergies with relevant EU initiatives and exploiting the results. After the end of the project, dissemination and communication will continue to play their role to build the long-term impacts of the projects, maintaining the website and following up with exploitation by key stakeholders.

M1-M18	M19-M36	M37-M54	>M54
Raise awareness	**Transfer knowledge**	**Replicate**	**Build impacts**
Develop ELOXYCHEM's dissemination and communication tools	Disseminate the first results to key stakeholders	Communicate ELOXYCHEM's outcomes	Maintain ELOXYCHEM website
Design and update website and social media channels	Engage with stakeholders to address information gaps	Disseminate and demonstrate achievements	Continue present project results and promote achievements
Map stakeholders	Convey information to create awareness on social benefits	Plan and execute exploitation of project results	Follow-up with exploitation to uptake Key Exploitable Results (KERs)
Setup Expert Advisory Board (EAB)	Press release update at least at M24 and M36	Press release update at least at M52	
Communicate ELOXYCHEM goals and activities with social media updates	Enhance synergies and liaisons with relevant EU initiatives		
Attendances at European events and conferences			
At least 2 press releases to promote progress (M2, M12)			
Build a cluster of related initiatives (EU-funded projects, institutions, etc.)			

Table 7 - Dissemination and Communication timeline

A preliminary schedule of the main topics that will be communicated and disseminated has been developed in Table7. For each topic, the proper communication tool and target audiences have been identified. Table7 constitutes a non-exhaustive list.

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Period	Topic	D&C channels						Audience
		Social channels	Press releases/ Newsletter	Video	Slide presentation	Webinars/ Events	Article/ Paper	
M1-M18	D14.2 Communication materials	x			x			TG1, TG2, TG3, TG4, TG5, TG6, TG7
	D14.3 1st project video	x		x		x		
M19-M36	D13.1 Social acceptance review	x	x		x	x		TG1, TG3, TG5, TG6
	D15.1 1st stakeholder workshop	x			x			TG1, TG2, TG3, TG4, TG5, TG6, TG7
	D18.1 Initial gender, diversity and inclusion plan	x	x		x			TG1, TG5
	D3.1 Optimization approaches for TOFA conversion					X	x	TG1, TG3, TG4, TG7
	D3.2 Products and by-products from TOFA conversion						x	TG1, TG3, TG4, TG7
	D15.3 2nd project video	x		x		x		TG1, TG2, TG3, TG4, TG5, TG6, TG7
M37-M54	D16.2 2nd stakeholder workshop	x			x		x	TG1, TG2, TG3, TG4, TG5, TG6, TG7
	D4.1 Optimization approaches for other substrates					x	x	TG1, TG3, TG4, TG7
	D16.2 Education & training materials	x	x	x	x			TG1, TG5,
	D19.1 Final gender, diversity and inclusion plan	x			x	x	x	TG1, TG5
	D4.2 Products and by-products from conversion of other substrates						x	TG1, TG2, TG3,
	D8.2 TOFA future design options & commercial assessment						x	TG1, TG2, TG3
	D16.3 Brochure on environmental credentials	x			x			TG1, TG2, TG5, TG7
	D12.2 Validation of products	x	x				x	TG1, TG2, TG6
	D13.2 LCA, circularity & environmental impact assessment	x	x	x	x	x	x	TG1, TG2, TG3, TG4, TG5, TG7
	D13.3 Social impact assessment	x			x	x	x	
	D12.1 Commercial feasibility report	x	x	x	x	x	x	TG2, TG3, TG4, TG6, TG7

Table 8 – Preliminary plan of expected main project outputs relevant for dissemination and communication

This table displays a plan of the first year-project dissemination and communication activities to be carried out:

Activity	Planned Period
1st project press release	M3
Design visual identity and dissemination tools	M6
Launch of website and social media	M4-M6
Education and training: summer schools, webinars and modules for educating students on the benefits of electrochemistry	M6-M8
Social media campaign to raise project awareness and connect to stakeholders	M4-M18
1st project newsletter	M6-M9
First joint online introductory webinar with similar research project (topic to be discussed)	M8-M12
Project participation at international conferences (e.g. ACHEMA, EUBCE, EUROCORR, CphI, etc.)	M6, M9, M10
2nd project press release	M12
1st project video	M12

Table 9 – Plan of activities during first year of the project (M1-M12)

7. Internal communications

In this project there will be additional steps for checking and approving public deliverables and all communication and dissemination material prior to publication. Two protocols have been set up for the flow of information in this project.

Flow of Information Protocol 1 – Public Deliverable or Scientific Abstract/ Publication

- A deliverable or transcript must be submitted to ALL
- 45 days review and acceptance
- After this the reviewed and accepted document cannot be changed without starting the review process again
-

This is a Consortium Agreement requirement. The following Table 9 is a list of all the public deliverables that will follow the review process as set out above.

WP	Deliverable	Deliverable Name	Lead	Level	Due Date
WP3	D3.1	Optimisation approaches for TOFA conversion	JGU	PU	31 Mar 2026
WP3	D3.2	Products and by-products from TOFA conversion	JGU	PU	30 Sep 2026
WP4	D4.1	Optimisation approaches for other substrates	JGU	PU	30 Sep 2027
WP4	D4.2	Products and by-products from conversion of other substrates	JGU	PU	31 Mar 2028
WP8	D8.2	TOFA future design options & commercial assessment	SINTEF	PU	30 Apr 2028
WP12	D12.1	Commercial feasibility report	EVO	PU	30 Jun 2028
WP12	D12.2	Validation of products	MEG	PU	31 May 2028

WP	Deliverable	Deliverable Name	Lead	Level	Due Date
WP13	D13.1	Social acceptance review	ICL	PU	31 Dec 2025
WP13	D13.2	LCA, circularity & environmental impact assessment	ICL	PU	31 May 2028
WP13	D13.3	Social impact assessment	ICL	PU	31 May 2028
WP14	D14.1	Initial PDEC	ETA	PU	30 Jun 2024
WP14	D14.2	Communications materials	ETA	PU	30 Jun 2024
WP14	D14.3	1st project video	ETA	PU	31 Dec 2024
WP15	D15.1	1st Stakeholder workshop	ETA	PU	31 Dec 2025
WP15	D15.3	2nd project video	ETA	PU	30 Nov 2026
WP16	D16.1	2nd Stakeholder workshop	ETA	PU	30 Jun 2027
WP16	D16.2	Education & training materials	JGU	PU	31 Dec 2027
WP16	D16.3	Brochure on environmental credentials	ETA	PU	30 Apr 2028
WP16	D16.4	Final PDEC including white paper	ETA	PU	30 Jun 2028
WP17	D17.1	Contingency plan	SINTEF	PU	30 Jun 2024
WP18	D18.1	Initial gender, diversity and inclusion plan	SINTEF	PU	31 Dec 2025
WP19	D19.1	Final gender, diversity and inclusion plan	SINTEF	PU	31 Dec 2027

Table 10 – All public deliverables

Flow of Information Protocol 2 – Public Information
Including but not limited to:

- 'News', Social media post, Press Release, outreach articles, Project info Presentations, etc.

The process is as follows:

1. Comms agenda points in every WPL meeting.
2. Partners should say if they have any info to share.
3. This written info will be shared with ALL.
4. Once shared, 3 days allowed for review and acceptance.
5. Thereafter, no edits allowed without starting review again.

8. Activity and Impact monitoring

Activity and impact monitoring will be carried out in conjunction with WP14, WP15, and WP16. This monitoring will take place in the form of a shared 'live' excel spread, accessible in the ELOXYCHEM shared area, under WP14 > T14.4 Impact monitoring and assessment: events_control_v2.xlsx

There are three tabs to fill in different information. All partners are requested to review and complete Tab 1 – Events and Tab 2 – Publications monthly in conjunction with the Monthly WP Leaders meetings.

Tab 3 – Impact Monitoring should be filled in every 3 months, predominantly by ETA, with website and social media data, such as: number of visits, interactions, countries of the visitors, views, posts, interactions, and downloads of the public material (Zenodo), etc.

9. Conclusion

This document must be considered a reference document, reflecting an open, ongoing dialogue with potential users and related networks during the project. ETA as lead beneficiary will continuously review and update the timeline of deliverables and task outputs, to ensure the best possible outcomes. The final version of this plan will be delivered at M54 at the end of the project and will be considered as a summary of the project's dissemination and communication activities and will include a plan only for exploitation after the project has ended.

10. Partners

KER X					
General Information					
Owner(s)					
Location					
Short description					
Related project aim(s)					
Related expected result(s)					
Exploitation model*					
Innovation Description					
Current TRL (1-9)			**TRL end of project (1-9)**		
Market Description					
Market size 2024			**Expected market growth to 2030**		
Description (how well established, current position of the partner in the market, barriers to innovation)					
Targeted customer(s)					

Route to market			
Time to market (years after the project)			
Competitors			
Financial information			
Additional funding needed for commercialisation? (Yes/No)		**Founding sources (choose as many as relevant)**	- Internal sales ☐ - Loans ☐ - Business Angels ☐ - Venture Capital ☐ - Industrial Investors ☐ - EU funding programs ☐ - National funding programs ☐ - Follow-up/parallel projects ☐ -Other ☐ -Not known ☐
Expected revenue from innovation at end of project		**Expected revenue from innovation 5 years after end of project**	
Expected profit from innovation at end of project		**Expected profit from innovation 5 years after end of project**	
Expected employment growth at end of project		**Expected employment growth 5 years after end of project**	
Description			
Scale-up and implementation		.	
Risks identified in the proposal			
Other risks (add as many as needed)			
Risk 1			
Type**		**Description**	

Likelihood (1-10)		**Criticality*** (1-10)**	
Mitigation measure		**Intervention (1-10)**	

*New research, Standard (knowledge to update current legislation), Internal adoption, or Commercial exploitation; **Technical Risks, Management Risks, Sustainability and Environmental Risks, or Exploitation Risks; *** It shows the capacity of the consortium to answer and solve any of the identified risks

Table 11 – Exploitation questionnaire

Date	Revision number	Made by	Changes made
01.04.2024	1	IIL	First Issue
10.04.2024	2	IIL	Background info added for EVONIK, MPI, ESL, MEGARA. Example text added to Foreground tab.
06.05.2024	3	EVONIK	Updated & revised background IP info for Evonik

Revision log | Background IP Register | Foreground IP Register

Figure 15 – ELOXYCHEM IP register

ANNEX 2

1st Iteration Tech-Futures Analysis

Contributing to:

Deliverable D14.1: Initial PDEC

Electrochemical oxidation of cyclic and biogenic substrates for high efficiency production of organic chemicals

eloxychem-horizon.eu
HORIZON-CL4-2023-TWIN-TRANSITION-01
1st January 2024 - 30th June 2028

This project has received funding from the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement No. 101138376.

ELOXYCHEM

Project	**ELOXYCHEM - Electrochemical oxidation of cyclic and biogenic substrates for high efficiency production of organic chemicals**
Grant Agreement n°	101138376
Call identifier	HORIZON-CL4-2023-TWIN-TRANSITION-01
Type of action	HORIZON-RIA
Coordinator	SINTEF
Project start date	1 January 2024
Project duration	54 months
Work package # and title	WP14 – Dissemination, communication & exploitation (RP1)
Work package leader	ETA
Dissemination level	PU- Public
Lead Beneficiary	ETA SRL
Author	Iconiq Innovation Ltd (IIL)
Reviewer(s)	Stephen Ryley (IIL), Emma Fromant (ETA), Theresa Rucker
Review date	08/05/2024
Due Date	30/06/2024

ELOXYCHEM

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List of Tables

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List of Abbreviations

AI	Artificial Intelligence
ANN	Artificial Neural Network
BGIP	Background Intellectual Property = IP brought to the project by the partners
CAN	Controller Area Network
CAPE	Computer-Aided Process Engineering
CNN	Convolutional Neural Netwok
COCO	Cape Open to Cape Open
CPC	Cooperative Patent Classification
DAQ	Data Acquisition
DICA	Di-Carboxylic Acid
DNN	Deep Neural Network
DBNN	Deep Belief Neural Network
EC	Electrochemical
EIS	Electrochemical Impedance Spectroscope/Spectroscopy
EOP	Electrochemical Oxidation Process
FGIP	Foreground Intellectual Property = IP associated with the project results
IoT	Internet of Things
KECA	Keto-Carboxylic Acid
KER	Key Exploitable Result
KPI	Key Performance Indicators
LCA	Life Cycle Assessment/Analysis
ML	Machine Learning
MOCA	Mono-Carboxylic Acid
NN	Neural Network
PINN	Physics-Informed Neural Network
PMC	Process Modelling Component
PME	Process Modelling Environment
SCADA	Supervisory Control and Data Acquisition
SCLA	Social Life Cycle Assessment/Analysis
SOH	State of Health (of battery)
SotA	State of the Art
SOX	State of any battery parameter X
TEA	Techno-Economic Assessment
T-FA	Tech-Futures Analysis
TOFA	Tall Oil Fatty Acid

Executive Summary

Principal objectives of the ELOXYCHEM project

Electrochemical oxidation of cyclic and biogenic substrates for high efficiency production of organic chemicals

The main technological development aims of the **ELOXYCHEM** project are defined in this extract from the Project Summary in the Grant Agreement (PDF p62):

> **ELOXYCHEM** will establish a commercially relevant electrochemical oxidation process that will become a strategic development to replace existing chemical conversion processes that are heavily reliant on imported materials such as nitric acid and imported fossil-fuels such as natural gas.
>
> **ELOXYCHEM** will promote a credible pathway for Europe's twin transition (green and digital) by demonstrating: (i) a new transformational electrochemical conversion platform process at a pilot scale consisting of reactors and downstream separation to final products with marketable specification to reliably achieve TRL6; (ii) drop-in replacement technology for chemical conversion.
>
> **ELOXYCHEM** will also optimise the process to demonstrate versatility of the process to multiple feedstocks ranging from current feedstocks and future bio-based and biogenic sources. Using AI strategies for optimisation the pilot plant will be targeted improve electrochemical performance, improve lifetime and reduce cost; prove viability of integrating with renewable energy sources considering intermittency and potential to offer demand-response flexibility; integrate process design, including materials, reactor/cell, and separation methods, from the process intensification and cost perspectives.

Purpose of this 1st Iteration ELOXYCHEM Tech-Futures Analysis [T-FA]

To assess the potential of the proposed outputs of the **ELOXYCHEM** project [FGIP] for patent-protection and exploitation, **IIL** has carried out this review into patenting activity in Electrochemical Oxidation Process [EOP] technology, the **1st Iteration T-FA**, to:

- ✓ update the State of the Art [SotA] in each **ELOXYCHEM** project technology development area
- ✓ identify any new competing technologies that have been published since the **ELOXYCHEM** proposal was prepared in March 2023
- ✓ identify no-go areas where project technology developments might lead to third-party patent infringements
- ✓ establish current Freedom to Operate [FTO] with the planned technology developments.

The analysis was carried out as described in **Section 2** below. Key words, phrases and acronyms were used along with Cooperative Patent Classification codes [CPC codes] in **T-FA** activities to identify the most recent and relevant granted patents and patent applications. The results of those activities are presented and analysed in **Section 3** and summarised in **Section 4** thereafter. Results of that analysis are summarised here:

Overall conclusions on the SotA for ELOXYCHEM technology developments

- ✓ No patent application or granted patent discovered in the **T-FA** searches discloses technology that appears to duplicate, in detail, the characteristics of the proposed **ELOXYCHEM** electrochemical system for the conversion of organic substrates to high added-value chemicals;
- ✓ None of the patents or applications discovered appears to infringe the partners' IPRs in their own technology patents.

Overall conclusion regarding FTO with the ELOXYCHEM project results

From the observations made above, it may be inferred that the project partners can seek patent protection for their developments in electrochemical oxidation processes [EOPs], powered from renewable energy sources [RESs] and designed for the conversion of organic substrates to high added-value chemicals. However, it is important to note that any patent search is only ever a snapshot of the patent database(s) on the day and at the time it is carried out. Therefore, the partners should continually monitor developments in the relevant technology sectors, perhaps as suggested in **Section 6** of this report.

1. Introduction

1.1 Principal objectives of the ELOXYCHEM project

The main technological development aims of the **ELOXYCHEM** project are defined in this extract from the Project Summary in the Grant Agreement (PDF p62):

> **ELOXYCHEM** will establish a commercially relevant electrochemical oxidation process that will become a strategic development to replace existing chemical conversion processes that are heavily reliant on imported materials such as nitric acid and imported fossil-fuels such as natural gas.
>
> **ELOXYCHEM** will promote a credible pathway for Europe's twin transition (green and digital) by demonstrating: (i) a new transformational electrochemical conversion platform process at a pilot scale consisting of reactors and downstream separation to final products with marketable specification to reliably achieve TRL6; (ii) drop-in replacement technology for chemical conversion.
>
> **ELOXYCHEM** will also optimise the process to demonstrate versatility of the process to multiple feedstocks ranging from current feedstocks and future bio-based and biogenic sources. Using AI strategies for optimisation the pilot plant will be targeted improve electrochemical performance, improve lifetime and reduce cost; prove viability of integrating with renewable energy sources considering intermittency and potential to offer demand-response flexibility; integrate process design, including materials, reactor/cell, and separation methods, from the process intensification and cost perspectives.

1.2 Anticipated results of the ELOXYCHEM project

The main technological developments anticipated in the **ELOXYCHEM** project are summarised in the Grant Agreement (PDF pp122-123) as these **K**ey **E**xploitable **R**esults [**KER**s]:

KER1: Industrially feasible metal-free EOPs for the separate and combined conversion of cycloalkanes, cycloalkenes and TOFA to oxo-functionalisation products, including cyclic ketones, monocarboxylic acids [MOCAS], dicarboxylic acids [DICAS], ketocarboxylic acids [KECAs], and alkyl-substituted DICAs [ALKYL-DICAs].

> **KER1a: Line CYCLIC ALKENES – Conversion of cycloalkanes/cycloalkenes to cyclic ketones and DICAs**
>
> **KER1b: Line TOFA – Conversion of Tall Oil Fatty Acids to MOCAs and DICAs**
>
> **KER1c: Line SIDES – Conversion of biogenic substrates and/or industrial side streams to KECAs and ALKYL-DICAs**

KER2: Methodology for scale-up of EOP chemical production from pilot to commercial scales

KER3: EOP platform system for lab to demo and pilot scale process development

KER4: ML methodology to optimise operating conditions for enhanced EOP performance

KER5: AI-based control and monitoring software for EOPs based on a Digital Twin

KER6: Strategy for integrating EOPs with RES, incorporating modelling and simulation tools

1.3 Purpose of this 1st Iteration ELOXYCHEM Tech-Futures Analysis [T-FA]

To assess the potential of the proposed outputs of the **ELOXYCHEM** project [FGIP] for patent-protection and exploitation, **IIL** has carried out this review into patenting activity in Electrochemical Oxidation Process [EOP] technology, the **1st Iteration T-FA**, to:

- ✓ update the State of the Art [SotA] in each **ELOXYCHEM** project technology development area
- ✓ identify any new competing technologies that have been published since the **ELOXYCHEM** proposal was prepared in March 2023
- ✓ identify no-go areas where project technology developments might lead to third-party patent infringements
- ✓ establish current Freedom to Operate [FTO] with the planned technology developments.

The analysis was carried out as described in **Section 2** below. Key words, phrases and acronyms were used along with Cooperative Patent Classification codes [CPC codes] in **T-FA** activities to identify the most recent and relevant granted patents and patent applications. The results of those activities are presented and analysed in **Section 3** and summarised in **Section 4** thereafter.

1.4 Positioning of the Deliverable

This report provides a benchmark for the state of the art [SotA] of the different technologies that underpin the developments that will lead to the realisation of the six anticipated **K**ey **E**xploitable **R**esults [**KER**s] of the **ELOXYCHEM** project.

Two further iterations of **T-FA** will be undertaken, one towards the middle of the project and one close to its end. The middle iteration will not only enable an update of the SotA in each of those technologies but will also enable an assessment of the progress in the project developments versus the benchmark provided in this report.

The third and final iteration will allow an assessment of the partners' freedom to operate [FTO] with their, hopefully completed, technology developments. In addition, the analysis will enable an assessment of the value of the partners' foreground intellectual property [FGIP] and how that may be exploited using the **RAPID** strategy outlined in the Grant Agreement (PDF pp150-151).

2. Methodology

2.1 Tech-Futures Analysis [T-FA]

This report is based on the use of **Tech-Futures Analysis** [T-FA]. A **T-FA** includes, *inter alia*, a review of the current State of the Art (SotA) in each relevant technology sector, set alongside prior art and FTO analyses. **IIL** will carry out three iterations of **T-FA** for the **ELOXYCHEM** project – together contributing to Deliverable **D16.4** – Final PDEC including white paper.

To identify key patents relevant to development of the **ELOXYCHEM** electrochemical oxidation process system along with current Freedom To Operate [FTO] in the relevant technology sectors, we have enhanced the usual keyword searches by using a citation analysis technology that is proprietary to Ambercite Pty Ltd and Griffith Hack, both of Melbourne, Australia. Together they developed powerful spring algorithms for the analysis of patent citations which enable filtering, grouping, ranking and charting of cited patents and applications – Amberscope [AS]. In addition, they developed AI algorithms that enable an analysis of the similarities (and hence the differences) between the inventions disclosed in patents.

2.2 Searching by key words, phrases and acronyms

Searching the various patent databases, such as Google Patents, Espacenet and the USPTO database, using key words, phrases and acronyms alone can lead to lack of accuracy. It is easy to miss patents and applications because of misspellings, alternative spellings, specific usage of words and phrases unknown to the researcher, etc. However, such searches can be useful if they identify key patents which can in turn be used to identify Cooperative Patent Classification codes [CPC codes] applicable to the technologies being researched. Those technologies are summarised in the following figure taken from the Grant Agreement:

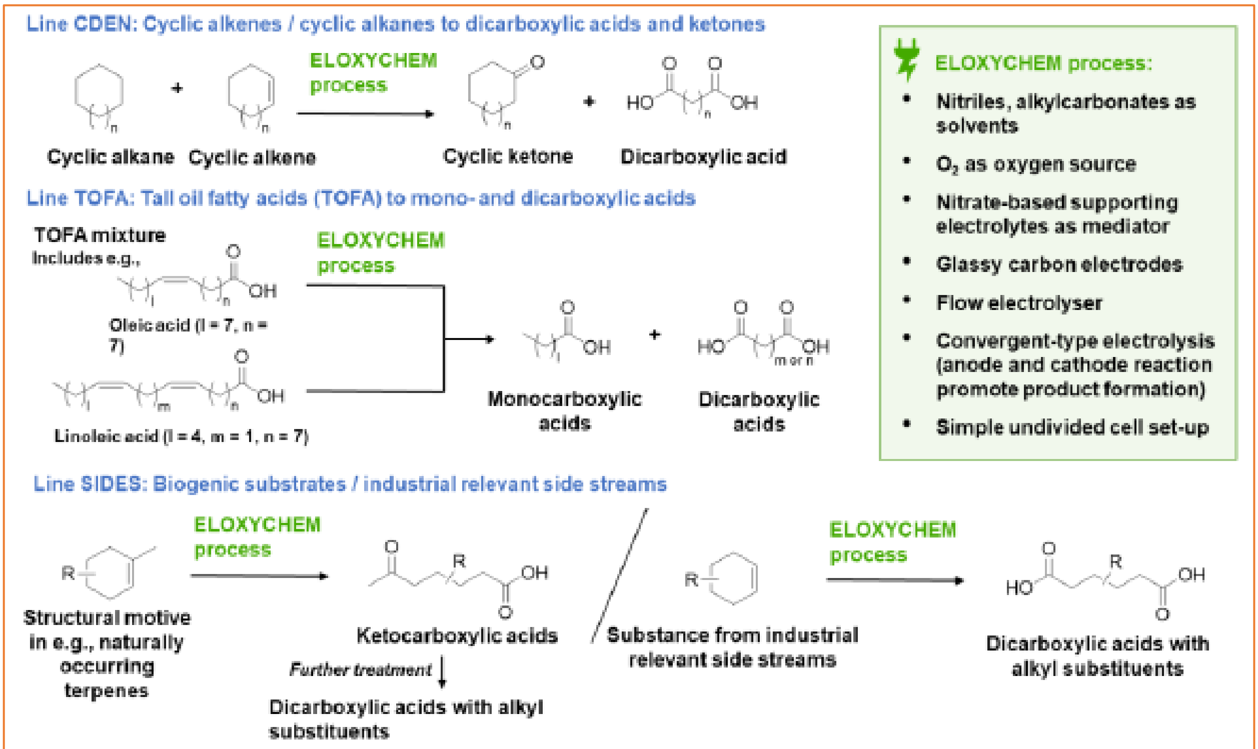


Figure 5. Overall electro-synthetic methodology of the ELOXYCHEM project with its application lines.

For the purposes of this 1st **Iteration T-FA**, Google Patent and Espacenet databases were interrogated using key words, phrases and acronyms relevant to the processes outlined in the figure. These included, but were not limited to:

'electrochemical oxidation, process, metal-free, galvanostatic, constant current, flow cell, biogenic substrate, cycloalkane, cycloalkene, tall oil fatty acid, TOFA, mono-, di-, keto-, carboxylic acid, cyclic ketone, terpene, oxidation, glassy carbon, electrode, anode, cathode, electrolyte, ammonium tetrabutyl nitrate, life cycle assessment/analysis, LCA, techno-economic assessment, TEA, artificial intelligence, AI, machine learning, ML.*

*N.B. The * operator picks out all words with the same trunk e.g., process, processes, processed, processing*

ELOXYCHEM

2.3 Searching by Cooperative Patent Classification [CPC] codes

The Cooperative Patent Classification [CPC] system enables all filed patents and applications in e.g. the Espacenet and USPTO databases to be searched logically and rapidly. To the right is an example of a CPC code:

B	29	C	39	/023
Section	Class	Sub-class	Group	Sub-Group

Following our initial searches using a range of key words and phrases, the key CPC codes that define the anticipated **ELOXYCHEM** inventions were identified. These are exemplified by C25B 15/02:

Symbol	Classification and description
C	CHEMISTRY; METALLURGY
	METALLURGY
C25	ELECTROLYTIC OR ELECTROPHORETIC PROCESSES; APPARATUS THEREFOR
C25B	ELECTROLYTIC OR ELECTROPHORETIC PROCESSES FOR THE PRODUCTION OF COMPOUNDS OR NON-METALS; APPARATUS THEREFOR (anodic or cathodic protection C23F 13/00; single-crystal growth C30B)
C25B 15/00	Operating or servicing cells
C25B 15/02	• Process control or regulation

2.4 Patent database searches for this ELOXYCHEM T-FA

The chosen key CPC codes, words and phrases were then entered into the ESPACENET Advanced Search engine to identify the most recent and relevant published patents and patent applications. The search results were then assessed for their relevance to this study's objectives by:

- ✓ checking the status of each patent application at the relevant intellectual property office;
- ✓ checking the Background to each invention;
- ✓ examining the Description and Claims in the published documents for relevance;
- ✓ checking the Assignees/Applicants vs their record in this technology sector.

3. Results of the ELOXYCHEM T-FA searches – SotA

3.1 SotA for the six principal ELOXYCHEM technology developments

The main intention of the **1st Iteration T-FA** searches presented here is to update the State of the Art in the six principal technological developments to be made in the **ELOXYCHEM** project.

Date range for the searches – This **1st Iteration T-FA** report includes mostly publications made since the SotA was reviewed for the **ELOXYCHEM** proposal that was prepared and submitted in March 2023. Earlier publications that are deemed to be particularly relevant to the **ELOXYCHEM KER**s are also included. From **Section 1.2** above, those technical developments can be summarised as:

KER1: Industrially feasible metal-free EOPs for the separate and combined conversion of cycloalkanes, cycloalkenes and TOFA to oxo-functionalisation products, including cyclic ketones, monocarboxylic acids [MOCAS], dicarboxylic acids [DICAS], ketocarboxylic acids [KECAs], and alkyl-substituted DICAs [ALKYL-DICAs].

> **KER1a: Line CYCLIC ALKENES – Conversion of cycloalkanes/cycloalkenes to cyclic ketones and DICAs**
>
> **KER1b: Line TOFA – Conversion of Tall Oil Fatty Acids to MOCAs and DICAs**
>
> **KER1c: Line SIDES – Conversion of biogenic substrates and/or industrial side streams to KECAs and ALKYL-DICAs**

KER2: Methodology for scale-up of EOP chemical production from pilot to commercial scales

KER3: EOP platform system for lab to demo and pilot scale process development

KER4: ML methodology to optimise operating conditions for enhanced EOP performance

KER5: AI-based control and monitoring software for EOPs based on a Digital Twin

KER6: Strategy for integrating EOPs with RES, incorporating modelling and simulation tools

The most relevant patents and patent applications discovered in the **T-FA** searches are presented in **Table 3.1.1** through **Table 3.1.6** in the following **Sections 3.1.1** through **3.1.6.** The number of the start page in this document of each of those sections is provided in the following table:

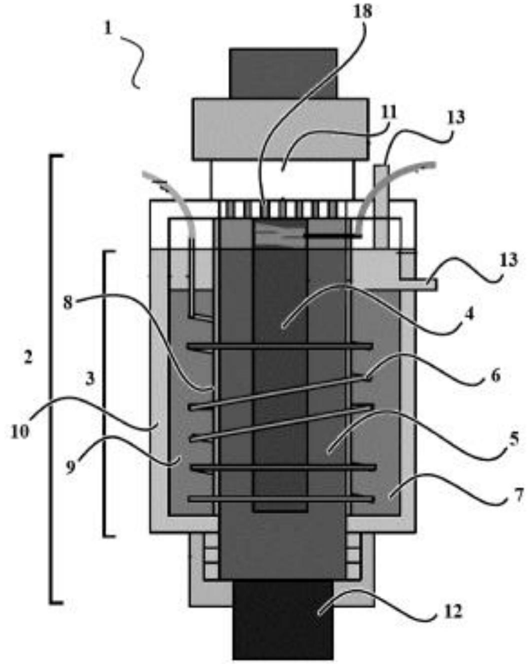
Section	Section title	Starts
3.1.1	Metal-free EOPs for conversion of cycloalkanes, cycloalkenes and TOFA to oxo-functionalisation products	p12
3.1.2	Methodology for scale-up of EOP chemical production from pilot to commercial scales	p30
3.1.3	EOP platform system for lab to demo and pilot scale process development	p31
3.1.4	ML methodology to optimise operating conditions for enhanced EOP performance	p32
3.1.5	AI-based control and monitoring software for EOPs based on a Digital Twin	p36
3.1.6	Strategy for integrating EOPs with RES, incorporating modelling and simulation tools	p45

Each publication listed in each of the tables has an associated Report Ref. #, **ELOXY1-XX**, which is used throughout this document. The reference numbers can be found in **Column 1** of the lists in each table. The following details of each patent or patent application are also provided in each table:

Report Ref #	Publication # Priority date Applicants/Assignees Publication date	TITLE Abstract/extract Status Comment (if appropriate)	Figure (s) Extract (s)

The results are presented in each table in order of **Priority date** from the earliest to the most recent.

ELOXYCHEM – Table 3.1.1 – Patents and applications on metal-free EOPs for conversion of cycloalkanes, cycloalkenes and TOFA to oxo-functionalisation products

Report Ref #	Publication # Priority date Applicants/Assignees Publication date	TITLE Abstract/extract Status Comment (if appropriate)	Figure (s) Extract (s)
KER1: Metal-free EOPs (ultimately undivided flow cell processes)			
ELOXY1-01	**WO2019028560 (A1)** **Aug 10th 2017** **BOUDREAU, J** **[CA]** **Feb 14th 2019**	**ELECTROCHEMICAL REACTOR FOR GENERATING ACTIVE COMPOUNDS FROM PRECURSORS** Devices for **electrochemically activating precursor compound through oxidation (or reduction) to produce active compound** are provided. Devices may include **an electrochemical reactor having an electrochemical cell including an anode and a cathode housed in a shared compartment, with or without a dividing membrane, wherein the anode and cathode form an electrical circuit in the presence of electrolyte solution**; and a sealed housing enclosing the electrochemical cell, the housing including a precursor compound input in communication with the anode/cathode/shared compartment, for inputting precursor compound, an active compound output in communication with the anode/cathode/shared compartment for outputting activated compound following activation, and a gas release and/or liquid overflow port; a power supply powering the electrochemical reactor; and, optionally, a pump or valve controlling flow rate of the assembly. **Status** Granted so far as: **CA3035406 (C)** – Aug 10th 2021 **US11198943 (B2)** – Dec 14th 2021	 An electrochemical reactor (2), electrochemical cell (3), anode (4) anode compartment (5), cathode (6), cathode compartment (7), membrane divider (8), electrolyte solution (9), sealed housing (10) precursor input port (11), active compound output port (12), gas release and/or liquid overflow port elements (13).

ELOXY1-02	**CN115044923 (A)** **Jun 1st 2022** **UNIV YANCHENG TEACHERS [CN]** **Sep 13th 2022**	**METHOD FOR PREPARING 2-ARYL-3-THIOCYANO-BENZOTHIOPHENE BY ELECTROCHEMICAL REACTION** The method comprises the following steps of: **exciting thiocyano free radicals through electrochemical anodic oxidation** by taking cheap and easily available thiocyanate as a functional reagent through a reaction substrate 2-aryl ethynyl phenyl methyl sulfide with active alkyne, so as to prepare the 2-aryl-3-thiocyano-benzothiophene. Intramolecular cyclization is initiated by addition of thiocyano free radicals to alkyne, and the purpose of preparing the 2-aryl-3-thiocyano-benzothiophene is achieved through a bi-functionalization reaction of active alkyne. According to the method, **a green electrochemical oxidation means is utilized, construction of a thiophene ring is efficiently achieved under the conditions of no transition metal catalyst and no exogenous oxidizing agent, the aryl and thiocyano disubstituted benzothiophene is obtained**, and the method is easy to operate, low in cost, environmentally friendly and good in industrial application prospect. **Status** Granted as **CN115044923 (B)** – May 5th 2023	**No particularly informative figure available**

ELOXY1-03	**CN114990590 (A)** **Jul 15th 2022** **UNIV JIANGXI NORMAL [CN]** **Sep 2nd 2022**	**NEW METHOD FOR ELECTROCATALYTIC METAL-FREE TRANSAMIDATION REACTION** The method comprises the following steps of: **synthesizing a tertiary amide product through constant-current electrochemical oxidation** by taking a platinum electrode as a cathode and an anode of the reaction, an amide twist and tertiary amine as raw materials, **n-tetrabutylammonium bromide as an electrolyte**, ammonium sulfate as an additive and dichloromethane as a solvent. Wherein the molar ratio of the amide twist to the n-tetrabutylammonium bromide to the ammonium sulfate to the tertiary amine is 4: 3: 3: 24. **Compared with a traditional method for synthesizing tertiary amide, transition metal catalysis is not needed**, the reaction is promoted by directly utilizing an electrochemical condition, the condition is mild, the operation is simple, the yield is high, separation and purification are convenient, the method is green and environment-friendly, and the substrate application range is wide. **Status** Granted as **CN114990590 (B)** – Aug 18th 2023	**No figure provided**

ELOXY1-04	**CN115584518 (A)** **Oct 24th 2022** **UNIV GUILIN TECHNOLOGY [CN]** **Jan 10th 2023**	**ELECTROCHEMICAL METHOD FOR PREPARING N-ALKYLAMIDE** The method comprises the following steps: **in an air atmosphere, adding an aliphatic amine compound and alpha-ketonic acid into a reactor** according to a molar ratio of 1: 1.2, adding electrolyte tetrabutylammonium fluoride, and adding a mixed solution of dichloromethane and tetrahydrofuran according to a ratio of 4: 1; and stirring the mixture by using a magnetic stirring device to dissolve the mixture, **inserting two electrodes, electrifying for 8 mA for 2 hours by using a graphite electrode as a positive electrode and a platinum sheet electrode as a negative electrode**, after the reaction is finished, evaporating to remove the solvent under reduced pressure to obtain a crude product, and purifying by column chromatography to obtain the N-alkylamide compound. **Compared with the traditional synthesis method**, the method has the advantages that the reaction condition is mild, and the reaction can be smoothly carried out at room temperature; the operation is simple, and all operations can be carried out in an open system; **current is used as an oxidation method in the reaction, so that pollution of transition metal or a chemical oxidant is avoided**; the raw materials are easy to obtain, the functional group compatibility is good, and the substrate application range is wide. **Status** Under examination	**No particularly informative figure available**

ELOXY1-05	**CN115896824 (A)** **Oct 24th 2022** **UNIV GUILIN TECHNOLOGY [CN]** **Apr 4th 2023**	**ELECTROCHEMICAL METHOD FOR PREPARING ALPHA-KETOAMIDE COMPOUND** An electrochemical method for preparing an alpha-keto amide compound comprises the following steps: adding a sulfoximine compound and alpha-keto acid into a reactor according to a molar ratio of 1: 3 in an air atmosphere, and adding an acetonitrile solution into the reactor without electrolyte; stirring the mixture by using a magnetic stirring device to dissolve the mixture, inserting two electrodes, **electrifying for 4mA for 6h by using a graphite electrode as a positive electrode and a stainless steel electrode as a negative electrode**, after the reaction is finished, evaporating to remove the solvent under reduced pressure to obtain a crude product, and purifying by column chromatography to obtain the alpha-ketoamide compound. Compared with the traditional synthesis method, the method has the advantages that **the reaction condition is mild, and the reaction can be smoothly carried out at room temperature; the operation is simple, and all operations can be carried out in an open system; current is used as an oxidation method in the reaction, so that pollution of transition metal or a chemical oxidant is avoided**; the raw materials are easy to obtain, the functional group compatibility is good, and the substrate application range is wide. **Status** Under examination	**No particularly informative figure available**

ELOXY1-06

CN115652343 (A)

Oct 25th 2022

UNIV SOUTHWEST [CN]

Jan 31st 2023

METHOD FOR ESTERIFYING ALKYL AROMATIC HYDROCARBON AND AMIDE THROUGH POLARITY REVERSAL OF BENZYL FREE RADICALS

Through electrochemical anodic oxidation, a transient free radical is constructed on a benzyl C (sp3)-H bond, and then the free radical is oxidized to obtain benzyl carbocations, so that the polarity reversal process of the free radical is realized; then amide attacks carbocations to generate an imine intermediate, and C-N bonds are broken after hydrolysis, so that synthesis of the benzyl ester compound is realized.

According to the method, **the use of transition metal, high-temperature, high-pressure and stoichiometric dangerous oxidizing agents and reducing agents is avoided**, good functional group tolerance is established, various substrates are expanded, and a supplementary scheme is provided for synthesis of benzyl ester compounds under mild conditions.

Status

Under examination

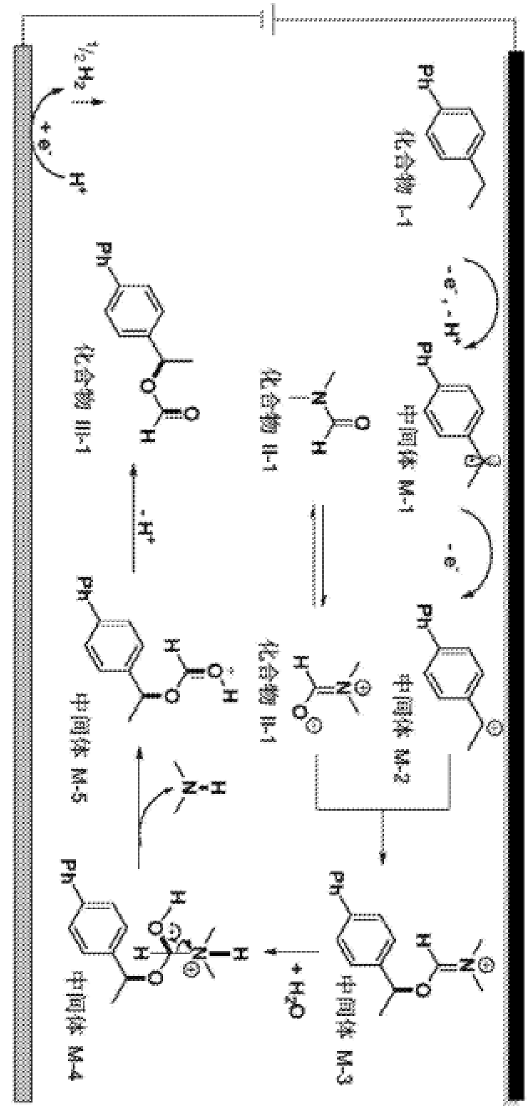
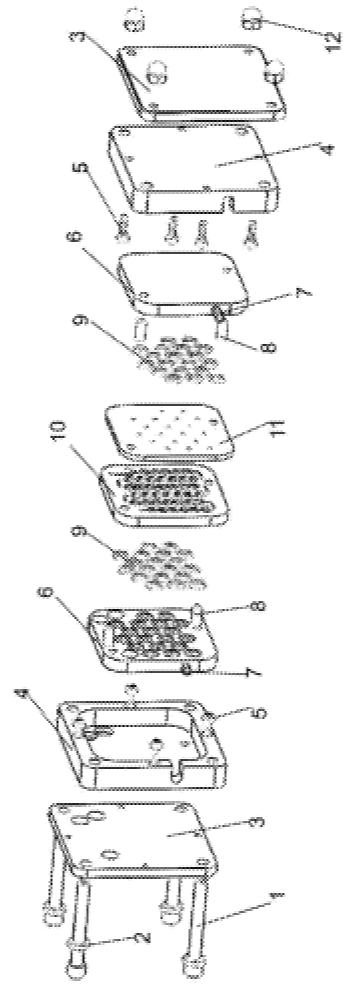


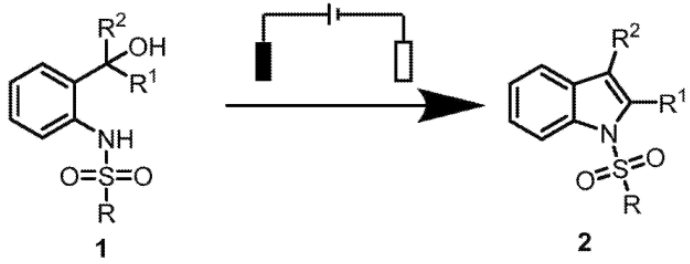
FIG.3 is the reaction mechanism of the method for esterifying alkyl aromatic hydrocarbons and amides by polarity inversion of benzylic free radicals in the present invention.

ELOXY1-07	**CN115449825 (A)** **Oct 27th 2022** **UNIV LISHUI [CN]** **Dec 9th 2022**	**METHOD FOR SYNTHESIZING FLUORINE-CONTAINING ISOXAZOLE DERIVATIVE THROUGH ELECTROCHEMICAL OXIDATION** The method comprises the steps that beta, gamma-unsaturated ketoxime and inorganic salt sodium trifluoromethanesulfinate serve as starting raw materials, **under the condition that C (+)/Pt (-) serves as an electrode, the reaction is conducted for 3 h at the room temperature under the current of I = 10 mA, and the fluorine-containing isoxazole derivative is obtained**; according to the present invention, the trifluoromethyl group in the inorganic salt can be successfully introduced into the organic substrate, and the trifluoromethylated isoxazole product is generated through the intramolecular nucleophilic cyclization reaction, **such that the inorganic fluoride is ingeniously introduced into the isoxazole ring skeleton under the condition of no metal and no additional oxidizing agent**. **Status** Under examination	**No particularly informative figure available**

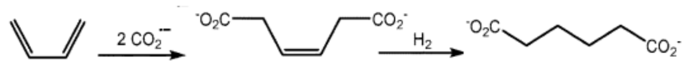
ELOXY1-08	**CN116479446 (A)** **Oct 27th 2022** **UNIV LISHUI [CN]** **Jul 25th 2023**	**GREEN SYNTHESIS METHOD OF ELECTROCHEMICAL CATALYSIS SULFONYLATION ISOXAZOLE DERIVATIVE** According to the method, beta, gamma-unsaturated ketoxime and p-toluene sulfonyl hydrazide are used as initial raw materials, **under the condition that C (+)/C (-) is used as an electrode, the current is I = 10mA, the room temperature reaction is performed for 4 hours, the oxidative sulfonylation reaction of an alkenyl oxime substrate can be smoothly realized, and the sulfonylated isoxazole derivative is obtained.** The method comprises the following steps: carrying out single electron oxidation on a p-toluene sulfonyl hydrazide anode to generate sulfuryl free radicals, then carrying out free radical addition on alkenyl oxime to generate benzyl free radicals, and further carrying out a benzyl free radical oxidation reaction and an intramolecular nucleophilic cyclization reaction on the anode to generate a sulfonylated isoxazole product. Compared with the traditional synthesis scheme, **the sulfuryl group can be introduced into the skeleton of the isoxazole ring under the electrochemical condition only by adding the inorganic electrolyte as a conductive medium and without adding metal and additional oxidizing agent under the mild condition**; and the constructed aryl alkyl sulfone compound widely exists in medical and bioactive products and materials, and has important biological and synthetic research values. **Status** Under examination	**No particularly informative figure available**

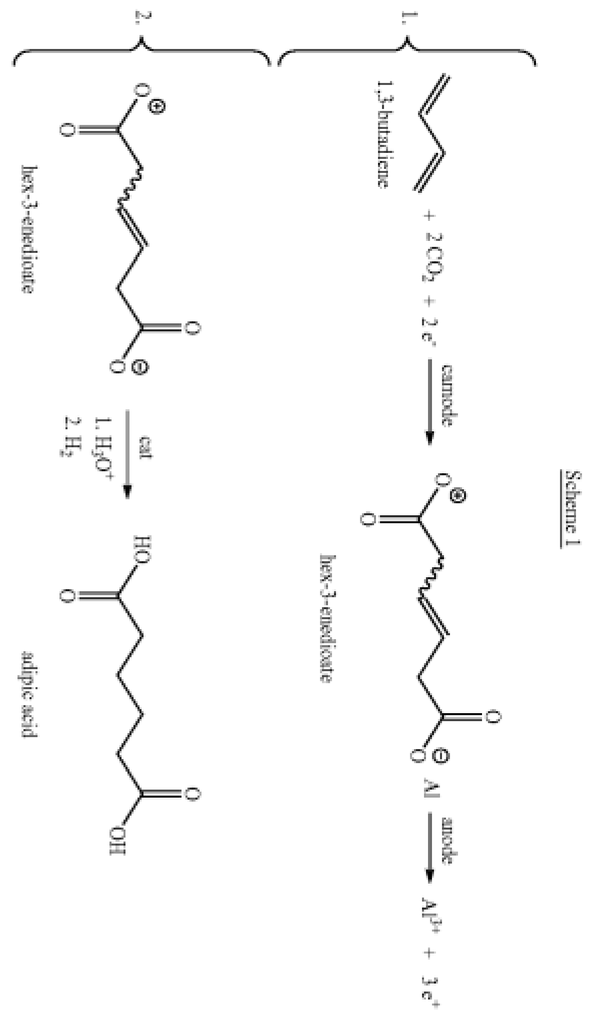
ELOXY1-09	**CN115613060 (A)** **Nov 11th 2022** **UNIV ZHEJIANG TECHNOLOGY [CN]** **Jan 17th 2023**	**METHOD FOR SYNTHESIZING C-3 PHOSPHORYLATED 2H-INDAZOLE COMPOUND THROUGH DIRECT ELECTROCHEMICAL OXIDATION** The invention relates to **a method for synthesizing a C-3 phosphorylated 2H-indazole compound through direct electrochemical oxidation**, and the C-3 phosphorylated 2H-indazole compound. The method comprises the following steps: by taking a 2H-indazole compound as shown in a structural formula (II) and a trialkyl phosphite compound as shown in the structural formula (II) as reaction substrates, **carrying out electrolytic reaction by adopting a two-electrode system**, and after the reaction is finished, carrying out separation treatment to obtain the C-3 phosphorylated 2H-indazole compound as shown in the structural formula (I). The method has the main beneficial effects that **(1) clean electric energy is used as an oxidizing agent, so that the environmental cost is reduced;** (2) the universality of a reaction substrate is good; (3) reaction conditions are mild; and (4) a class of novel C-3 phosphorylated 2H-indazole compounds are provided, and a basis is provided for screening of new drugs. **Status** Under examination	**No particularly informative figure available**

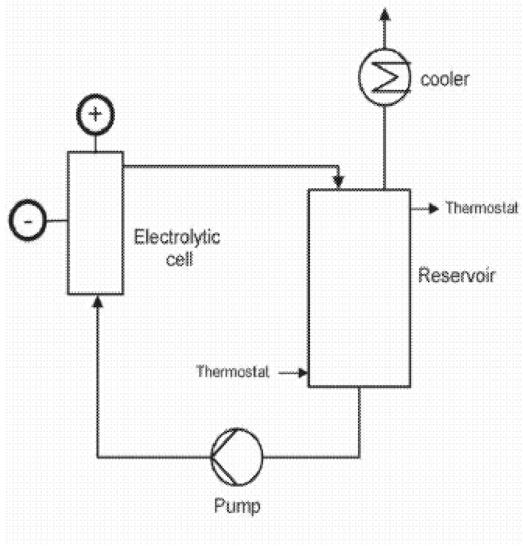
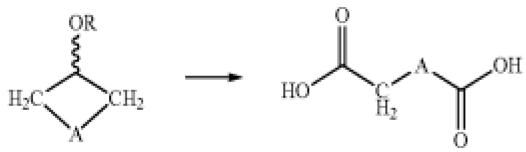
ELOXY1-10	**CN116036908 (A)** **Nov 23rd 2022** **UNIV NANJING SCIENCE & TECH [CN]** **May 2nd 2023**	**ELECTROCHEMICAL REACTOR CAPABLE OF SIMULTANEOUSLY REALIZING STATIC MIXING AND ELECTROCHEMICAL REACTION** **The electrochemical reactor comprises two graphite polar plates, a planar static mixer and the like.** According to the plane static mixer, fluid diversion and vortex generation are promoted through obstacles in a pipeline and rapid changes of the pipe diameter, and the mixing quality is improved. According to the reactor and the reaction method disclosed by the invention, electrochemical oxidation can be completed under the conditions of small current gradient and no addition of electrolyte through the large surface area of the graphite polar plate and small electrode spacing. **The efficient preparation of HNS is successfully realized by using the electrochemical reactor**. The TNT solution and the NaClO solution are fully mixed to form the HNS, meanwhile, the by-product HNBB is subjected to electrochemical dehydrogenation to be converted into the HNS, the reaction is carried out for 30 min, and the yield can reach 50.85%. According to the device, static mixing and electrochemistry are carried out at the same time, so that the yield of HNS is improved. **Status** Under examination	 FIG.2 is a structural composition diagram of the electrochemical reactor. 1 is a cylindrical head screw, 2 is a gasket, 3 is a stainless steel plate, 4 is a heat insulation layer, 5 is a fixing screw, 6 is a graphite plate, 7 is a copper stud connected to electricity, 8 is a fixed cylinder, 9 is a sealing washer, 10 is a plane static mixer, 11 is a bonding plate, and 12 is an ark nut.

ELOXY1-11	CN115807233 (A) Dec 12th 2022 UNIV SOUTHWEST [CN] Mar 17th 2023	**METHOD FOR ELECTROCHEMICAL SYNTHESIS OF SUBSTITUTED INDOLE FROM GAMMA-HYDROXYLAMINE** The method comprises the following steps: mixing a substrate, an organic additive, an electrolyte and a solvent to obtain a homogeneous solution, adding the homogeneous solution into **an electrochemical reaction device with a carbon cloth anode and a platinum cathode**, and synthesizing the substituted indole through an electro-catalysis one-step method. **The synthesis of substituted indole by gamma-hydroxylamine is combined with an organic electrocatalysis technology, and the oxidation-reduction reaction is realized by using clean electric energy, so that the use of an oxidation or reduction reagent is avoided.** The electrochemical indole synthesis strategy has excellent functional group, water and air tolerance. Compared with the prior art, the synthesis method disclosed by the invention is efficient and economical, free of metal residues in products, short in reaction time, simple and easily available in raw materials and high in yield; the application of the material in the field of biomedical materials is more competitive. **Status** Under examination	 FIG.1 is the reaction equation of the present invention synthetic substituted indole compound.

ELOXY1-12	**CN115799484 (A)** **Dec 29th 2022** **UNIV GUILIN TECHNOLOGY [CN]** **Mar 14th 2023**	**ELECTROCHEMICAL METHOD FOR PREPARING N-ARYL SULFIMIDE COMPOUND** An electrochemical method for preparing an N-aryl sulfimide compound comprises the following steps: **in an air atmosphere, adding a sulfoximine compound and alpha-ketonic acid into a reactor according to a molar ratio of 1: 2**, adding an electrolyte tetrabutylammonium tetrafluoroborate and a catalyst nickel bromide, and then adding an acetone solution; stirring the mixture by using a magnetic stirring device to dissolve the mixture, **inserting two electrodes, electrifying for 3h at 6mA by using a graphite electrode as a positive electrode and a platinum sheet electrode as a negative electrode**, after the reaction is finished, evaporating to remove the solvent under reduced pressure to obtain a crude product, and purifying by column chromatography to obtain the N-aryl sulfonimide compound. Compared with the traditional synthesis method, the method has the advantages that the reaction condition is mild, and the reaction can be smoothly carried out at room temperature; the operation is simple, and all operations can be carried out in an open system; **the reaction uses current as an oxidation method, so that the pollution of a chemical oxidant is avoided**; the raw materials are easy to obtain, the functional group compatibility is good, and the substrate application range is wide. **Status** Under examination	**No particularly informative figure available**

KER1a:	Line CYCLIC ALKENES – Conversion of cyclic alkanes/cyclic alkenes to cyclic ketones and DICAs		
ELOXY1-13	**US20200181782 (A1)** **Jul 28th 2017** **UNIV MICHIGAN STATE [US]** **Jun 11th 2020**	**ELECTROCHEMICAL REDUCTIVE CARBOXYLATION OF UNSATURATED ORGANIC SUBSTRATES IN IONICALLY CONDUCTIVE MEDIUMS** The unsaturated organic substrate is electrochemically reduced with a carbon dioxide reactant in an ionically conductive, water-immiscible reactant medium to form the dicarboxylic organic product. The dicarboxylic organic product is recovered in an aqueous product medium. Example dicarboxylic organic products include **phthalic acid**, naphthalene dicarboxylic acid, furan-2,5-dicarboxylic acid, thiophene-2,5-dicarboxylic acid, pyrrole-2,5-dicarboxylic acid, **adipic acid**, suberic acid, sebacic acid, and **1,12-dodecanedioic acid.** **Status** Granted as **US11851778 (B2)** – Dec 26th 2023	 FIG. 11 illustrates the synthesis of **adipic acid** by electrocarboxylation of 1,3-butadiene

ELOXY1-14	**US20220251717 (A1)** **Jul 10th 2019** **UNIV BERLIN TECH [DE]** **Aug 11th 2022**	**METHOD FOR ELECTRO-DICARBOXYLATION OF AT LEAST ONE ALKENE WITH CARBON DIOXIDE CO2 IN THE PRESENCE OF HYDROGEN H2** The person invention relates to **a method for the electro-dicarboxylation of at least one diene with carbon dioxide in the presence of hydrogen, forming at least one unsaturated dicarboxylic acid.** The reaction is carried out in a reactor comprising at least one cathode (e.g. of graphite) as the working electrode for the cathodic activation of CO_2, at least one anode (e.g. of platinum) as the counter-electrode for the anodic oxidation of H_2, with a volumetric ration of hydrogen H_2 to carbon dioxide between 1:1 and 1:3, a total pressure in the reactor between 2 and 4 MPa, particularly preferably between 3 and 4 MPa, and an average current density j between 5 and 15 mA/cm2, particularly preferably between 10 and 12.5 mA/cm2. **Status** Granted as **US11913127 (B2)** – Feb 27th 2024 **Comment –** The method is intended to provide a cleaner alternative route to adipic acid production as shown in Scheme 1 to the right	

ELOXY1-15	**WO2021249775 (A1)** **Jul 10th 2020** **EVONIK OPERATIONS GMBH [DE]** **Dec 16th 2021**	**METHOD FOR ELECTROCHEMICALLY PRODUCING ALKANE DICARBOXYLIC ACIDS BY MEANS OF A RING-OPENING OXIDATION USING A DOPED NI(O)OH FOAM ELECTRODE** The invention relates to a method for electrochemically producing alkylene dicarboxylic acids by means of a ring-opening oxidation using a doped Ni(O)OH foam electrode in an aqueous alkaline solution. **Status** Granted so far as: **EP4165236 (B1)** – Dec 27th 2023	 FIG.1 shows the schematic design of a continuous flow reaction cell. **[0014]** In the method according to the invention, preference is given to preparing alkanedicarboxylic acids (DC) according to scheme (I) Scheme (I)  where ∿∿ represents a single or double bond, R accordingly being present or not,

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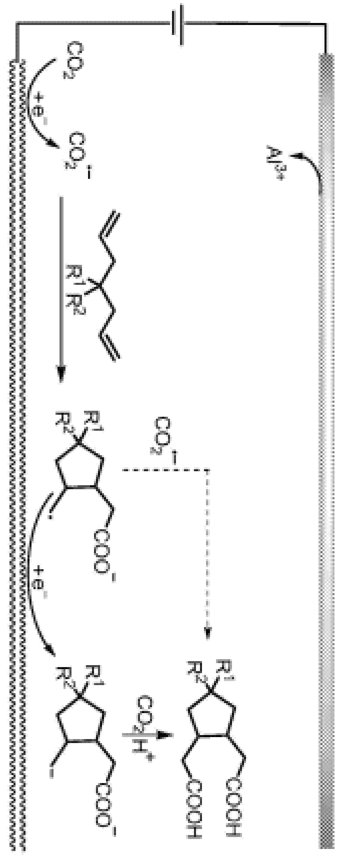
ELOXY1-16	**CN117210834 (A)** **Jun 10th 2022** **UNIV SICHUAN [CN]** **Dec 12th 2023**	**METHOD FOR PROMOTING CO2 TO SYNTHESIZE DICARBOXYLIC ACID COMPOUND BASED ON ELECTROCHEMISTRY** The invention discloses **a method for promoting CO_2 to synthesize dicarboxylic acid compounds based on electrochemistry, and belongs to the technical field of organic synthesis**. The method mainly comprises the following steps that a substrate, alkali and an additive are added into a reaction container, then a solvent is added in the CO_2 atmosphere, an electrolytic reaction is conducted at the temperature of 20-50 DEG C, after the reaction is finished, a product is separated and purified, and the dicarboxylic acid compounds are obtained. The method has the characteristics of mild reaction conditions, simplicity and convenience in operation, cheap and easily available raw materials, excellent selectivity and high atom economy. **The preparation method disclosed by the invention is wide in applicability, various substrates such as non-conjugated dienes, 1, 3-butadiene derivatives and heterocyclic aromatic hydrocarbons can be efficiently subjected to dicarboxylation reaction, and accurate construction of various novel diacid monomers is rapidly realized**. **Status** Under examination **Comment** – Proposes the use of renewable electric energy to power the electrochemical cell. Also proposes the possibility of using meshed glassy carbon for the anode.	 FIG.1 is a reaction mechanism diagram of the present invention.

KER1b: Line TOFA – Conversion of Tall Oil Fatty Acids to MOCAs and DICAs
None found
KER1c: Line SIDES – Conversion of biogenic substrates/ind. side streams to KECAs and ALKYL-DICAs
None found

Summary of Table 3.1.1 – Patents and patent applications on metal-free EOPs for conversion of cycloalkanes, cycloalkenes and TOFA to oxo-functionalisation products

The **ELOXYCHEM** system preferably includes **(1)** a transition metal-free (2) two electrode **(3)** undivided **(4)** flow cell (**5**) operable at constant current **(6)** powered by RES and utilising **(7)** parallel glassy carbon electrode plates for **(8)** EOP of cycloalkenes, **(9)** EOP of cycloalkanes and **(10)** EOP of TOFA.

The characteristics of the systems disclosed in the publications listed in **Table 3.1.1** above are compared to those of the **ELOXYCHEM** system, numbered **(1)** through **(10)** above, in the following summary table:

ELOXYCHEM ⇨	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
ELOXYCHEM Ref # ⇩	**(1)**	**(2)**	**(3)**	**(4)**	**(5)**	**(6)**	**(7)**	**(8)**	**(9)**	**(10)**
ELOXY1-01	-	✓	-	✓	✓	-	-	-	-	-
ELOXY1-02	✓	✓	✓	-	✓	-	-	-	-	-
ELOXY1-03	(✓)	✓	✓	-	✓	-	-	-	-	-
ELOXY1-04	(✓)	✓	✓	-	✓	-	-	-	-	-
ELOXY1-05	(✓)	✓	✓	-	✓	-	-	-	-	-
ELOXY1-06	✓	✓	(✓)	-	(✓)	-	(✓)	-	-	-
ELOXY1-07	✓	✓	(✓)	-	✓	-	-	-	-	-
ELOXY1-08	(✓)	✓	(✓)	-	✓	✓	-	-	-	-
ELOXY1-09	(✓)	✓	(✓)	-	✓	✓	-	-	-	-
KEY	✓ = Specifically disclosed in the patent or application - = Not specifically disclosed (✓) = Partly disclosed or implied									

ELOXYCHEM

The **ELOXYCHEM** system preferably includes **(1)** a transition metal-free (**2**) two electrode **(3)** undivided **(4)** flow cell (**5**) operable at constant current **(6)** powered by RES and utilising **(7)** parallel glassy carbon electrode plates for **(8)** EOP of cyclic alkenes, **(9)** EOP of cyclic alkanes and **(10)** EOP of TOFA.

ELOXYCHEM ⇨	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
ELOXYCHEM Ref # ⇩	**(1)**	**(2)**	**(3)**	**(4)**	**(5)**	**(6)**	**(7)**	**(8)**	**(9)**	**(10)**
ELOXY1-10	(✓)	✓	(✓)	-	✓	-	-	-	-	-
ELOXY1-11	✓	✓	✓	-	(✓)	(✓)	-	-	-	-
ELOXY1-12	✓	✓	(✓)	-	(✓)	(✓)	-	-	-	-
ELOXY1-13	(✓)	✓	-	(✓)	✓	-	-	(✓)	-	-
ELOXY1-14	-	✓	✓	-	(✓)	-	-	(✓)	-	-
ELOXY1-15	✓	✓	✓	✓	(✓)	-	-	-	(✓)	-
ELOXY1-16	✓	✓	✓	-	✓	✓	✓	(✓)	-	-
KEY	✓ = Specifically disclosed in the patent or application - = Not specifically disclosed (✓) = Partly disclosed or implied									

Table 3.1.1.1 Summary of the inventions disclosed in the publications listed in Table 3.1.1

Summary of the SotA regarding KER1 – Metal-free EOPs for conversion of cycloalkanes, cycloalkenes and TOFA to oxo-functionalisation products

Overall summary – From **Table 3.1.1.1** above, it is clear that each publication listed in **Table 3.1.1** discloses one or more inventions that show some degree of overlap with the EOP technology developments that the partners plan to make during the **ELOXYCHEM** project. However, none discloses all of them. In particular the use of cycloalkanes, cycloalkenes and TOFA as substrates for electrochemical oxidation processes was not found to be disclosed in any publication.

3.1.2 Methodology for scale-up of EOP chemical production from pilot to commercial scales

Table 3.1.2 – Patents and patent applications on methodology for scale-up of EOP chemical production from pilot to commercial scales

Report Ref #	Publication # Priority date Applicants/Assignees Publication date	TITLE Abstract/extract Status Comment (if appropriate)	Figure (s) Extract (s)
None found			

Summary of the SotA regarding KER2 – Methodology for scale-up of EOP chemical production from pilot to commercial scales

Overall summary – Whilst publications were identified that disclose means for scaling up electrochemical processes e.g. **WO2023161695 (A1)** that discloses scale-up of an electrochemical process for making nanocrystalline carbons to the level of mass-production, no patents or patent applications were found that disclose the scale-up of electrochemical oxidation processes [EOPs].

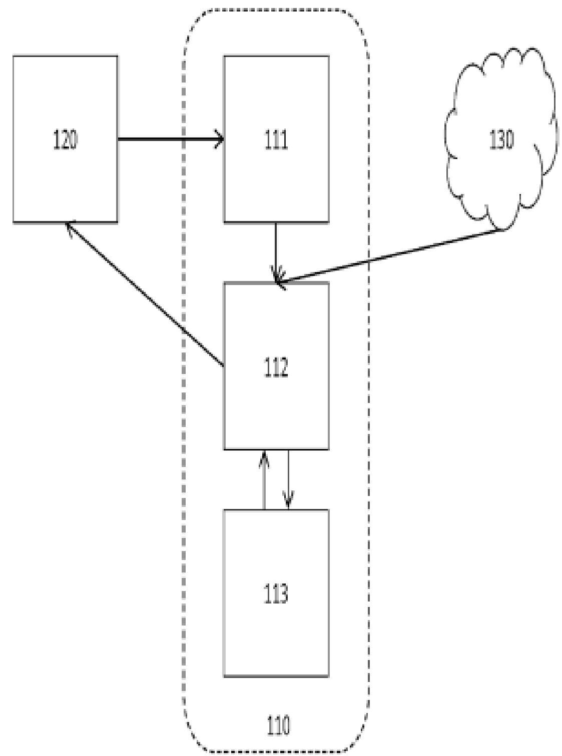
3.1.3 EOP platform system for lab to demo and pilot scale process development

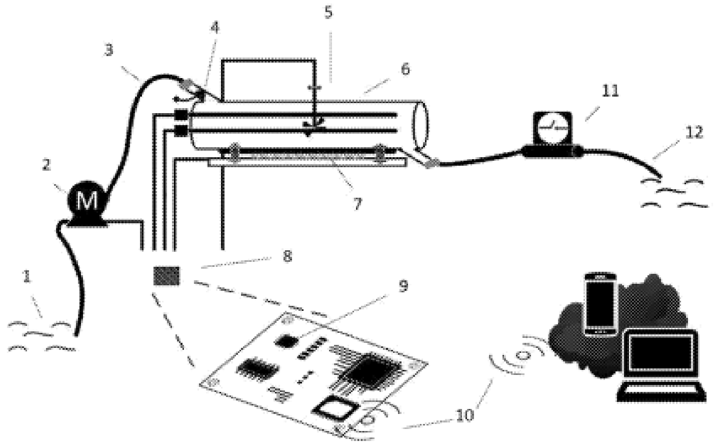
Table 3.1.3 – Patents and patent applications on EOP platform system for lab to demo and pilot scale process development			
Report Ref #	Publication # Priority date Applicants/Assignees Publication date	TITLE Abstract/extract Status Comment (if appropriate)	Figure (s) Extract (s)
None found			

Summary of the SotA regarding KER3 – EOP platform system for lab to demo and pilot scale process development

Overall summary – Whilst publications were identified that disclose electrochemical technology platforms e.g. **EP3453064 (B1)** that discloses an advanced electrode technology platform for electrochemical reduction of CO_x species, no patents or patent applications were found that disclose such a platform for electrochemical oxidation processes [EOPs].

Table 3.1.4 – Patents and patent applications on ML methodology to optimise operating conditions for enhanced EOP performance

Report Ref #	Publication # Priority date Applicants/Assignees Publication date	TITLE Abstract/extract Status Comment (if appropriate)	Figure (s) Extract (s)
ELOXY1-17	US10925192 (B1) Oct 14th 2018 MODIUS INC [US] Feb 16th 2021	**USING PREDICTIVE ANALYTICS IN ELECTROCHEMICAL AND ELECTROMECHANICAL SYSTEMS** Machine learning techniques provide predictions of computer system load and cooling requirements, allowing cooling systems to anticipate, prepare for, and ameliorate, those requirements. Techniques provide confirmation or denial that the computer and cooling systems are operating as expected, allowing those systems to determine if any parts are failing. **Techniques provide information regarding likely effect due to proposed changes.** **Techniques provide probabilistic predictions, well in advance, of whether parts will fail or degrade.** Techniques provide probabilistic predictions whether parts will fail or degrade, responsive to degrees of redundancy, set points for of cooling, or set points when cooling starts or ends. **Status** Granted patent **Comment –** ‘Ensemble of Random Trees Model’ lies at the heart of the ML system.	 FIG.1 shows a conceptual drawing of a system 100. 111-Virtual machine; 120-Data center; 112-Second virtual machine; 113-GUI; 130-Cloud.

ELOXY1-18	**CN113740406 (A)** **Sep 9th 2021** **UNIV NANKAI [CN]** **Dec 3rd 2021**	**PORTABLE MINIATURIZED COD (CHEMICAL OXYGEN DEMAND) ELECTROCHEMICAL MEASUREMENT DEVICE AND MEASUREMENT METHOD THEREOF** The measurement method includes the steps that firstly, a software and hardware system used for environmental ecology is constructed. The hardware system comprises a cylindrical electrochemical experiment pool, a small electrochemical workstation, a circulating pump, an electromagnetic valve, an electric stirrer, an infrared detector, a working electrode, a reference electrode and a counter electrode. **The software system is composed of an artificial intelligence algorithm based on a Support Vector Regression [SVR] model**, wherein the small electrochemical workstation is based on an electrochemical analog front end AD5941, a single chip is integrated with a complete three-electrode system chain, and the system is a novel solution which is high in precision and low in power consumption and can be expanded into a multi-parameter measurement system. **The working electrode is a boron-doped diamond [BDD] electrode and can generate a large number of hydroxyl radicals with strong oxidizing property to thoroughly oxidize organic matters in the solution, and the electric quantity passing through the working electrode in the oxidation process is linearly related to the quantity of the organic matters in the solution.** **The main controller calculates a COD value and completes precision compensation through a Support Vector Machine [SVM] model**, and data is transmitted to a self-built database through NB-IoT for a user to check in real time. **Status** Under examination	 FIG.1 is a schematic diagram of the present invention; 1-water quality sampling point; 2-circulating pump; 3-sampling pipeline; 4-infrared detector; 5-electric stirrer; 6-cylindrical electrochemical experiment cell; 7-working electrode; 8-control Circuit; 9-electrochemical analog front end; 10-narrowband Internet of Things; 11-solenoid valve; 12-drainage pipeline

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ELOXY1-19	CN113884935 (A) Nov 2nd 2021 UNIV GUILIN ELECTRONIC TECH [CN] Jan 4th 2022	**SOH ESTIMATION SYSTEM AND METHOD BASED ON ONLINE ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY MEASUREMENT OF LITHIUM BATTERY** The method comprises the following steps of: measuring electrochemical impedance spectra and open-circuit voltages of the battery under different aging cycle times of the battery; **performing feature selection on the electrochemical impedance spectra by using a grey correlation degree;** **establishing and training a machine learning model;** and collecting data of the tested battery to carry out SOH estimation. According to the SOH estimation method, related characteristic parameters are obtained by analyzing the electrochemical impedance spectra of the battery and parameter identification of a complex equivalent circuit model is avoided. By adopting the SOH estimation method, the electrochemical impedance spectroscopy measurement of the battery and the estimation of the SOH of the battery can be completed, and the integration level and the reliability of the system are improved. **Status** Notification of grant of patent – Apr 19th 2024	**No particularly informative figure available**

Summary of the SotA regarding KER4 – machine learning [ML] methodology to optimise operating conditions for enhanced EOP performance

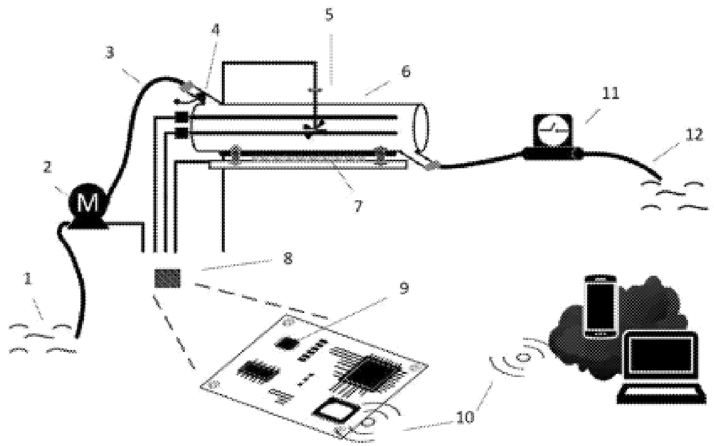
Whilst published well outside the chosen date range, **ELOXY1-17** is included here as an early example of the application of ML to electrochemical [EC] processes. Note that application to EOPs is not specifically disclosed in that document.

Whilst plenty of publications were found that disclose application of ML to optimisation of electrochemical oxidation of organic matter in waste water, exemplified by **ELOXY1-18**, no publication was found that discloses use of ML for optimising EOPs for conversion of organic substrates to high added-value chemicals.

Numerous publications were found that disclose use of ML in optimising various operational parameters for batteries and other electrochemical energy storage means, exemplified by **ELOXY1- 19**, but none was found that discloses its use in optimising EC cell function for conversion of organic substrates to high added-value chemicals.

Overall summary – No publication was found that discloses the application of machine learning to the optimisation of electrochemical oxidation processes or the devices/reactors/cells in which they are carried out.

Table 3.1.5 – Patents and patent applications on AI-based control and monitoring software for EOPs based on a Digital Twin

Report Ref #	Publication # Priority date Applicants/Assignees Publication date	TITLE Abstract/extract Status Comment (if appropriate)	Figure (s) Extract (s)
ELOXY1-18	CN113740406 (A) Sep 9th 2021 UNIV NANKAI [CN] Dec 3rd 2021	**PORTABLE MINIATURIZED COD (CHEMICAL OXYGEN DEMAND) ELECTROCHEMICAL MEASUREMENT DEVICE AND MEASUREMENT METHOD THEREOF** The measurement method includes the steps that firstly, a hardware and software system used for environmental ecology is constructed. The hardware system is shown to the right: **The software system is composed of an artificial intelligence algorithm based on a Support Vector Regression [SVR] model**, wherein the small electrochemical workstation is based on an electrochemical analog front end AD5941, a single chip is integrated with a complete three-electrode system chain. **The working electrode is a boron-doped diamond [BDD] electrode and the electric quantity passing through the working electrode in the oxidation process is linearly related to the quantity of the organic matters in the solution.** **The main controller calculates a COD value and completes precision compensation through a Support Vector Machine [SVM] model**, and data is transmitted to a self-built database through NB-IoT for a user to check in real time. **Status** Under examination	 FIG.1 is a schematic diagram of the present invention; 1-water quality sampling point; 2-circulating pump; 3-sampling pipeline; 4-infrared detector; 5-electric stirrer; 6-cylindrical electrochemical experiment cell; 7-working electrode; 8-control Circuit; 9-electrochemical analog front end; 10-narrowband Internet of Things; 11-solenoid valve; 12-drainage pipeline

ELOXY1-20	**CN113793649 (A)** **Sep 13th 2021** **UNIV TONGJI [CN]** **Dec 14th 2021**	**ALKALINE ELECTROLYTIC CELL OPERATION CHARACTERISTIC DIGITAL TWINBORN MODEL CONSTRUCTION METHOD** The method comprises the following steps: 1) constructing an alkaline electrolytic cell impedance characteristic digital twinborn model by taking a cell temperature as a unique twinborn correlation variable according to related tests and working mechanisms of an alkaline electrolytic cell; and 2) **based on the digital twinning model of the impedance characteristic of the alkaline electrolytic cell, fusing the mathematical driving model and the electrochemical mechanism model, and realizing digital twinning modeling of the operating characteristic of the alkaline electrolytic cell** by taking the characteristic characterization parameters of the total voltage, the total current, the cell body temperature, the operating power and the hydrogen yield of the electrolytic cell as observation variables, the characteristics specifically comprise temperature rise characteristics, power regulation characteristics, hydrogen production efficiency characteristics and separation tank characteristics. Compared with the prior art, the method has the advantages of being high in universality, simple in process, high in accuracy, high in engineering availability and the like. **Status** Granted as **CN113793649 (B)** – Feb 27th 2024	**No particularly informative figure available**

ELOXY1-21	**CN114062786 (A)** **Jan 7th 2022** **UNIV BEIHANG [CN]** **Feb 18th 2022**	**EIS ONLINE MEASUREMENT METHOD BASED ON DIGITAL TWINNING AND PROGRAMMABLE RESISTORS** The method comprises the steps: achieving the online measurement of medium and high frequency bands of an EIS through a programmable resistor at a vehicle end and an IGBT switch; transmitting the impedance information of the medium and high frequency bands to a cloud battery management system; **inputting the medium and high frequency band information into a neural network algorithm deployed in the digital twin model of the cloud battery management system**; **estimating the low frequency band information of the EIS**; **and forming an electrochemical impedance spectrum of a complete frequency band to update the digital twin battery model of the cloud battery management system to obtain accurate battery state information.** The state detection of the mechanism level of the power battery and the iterative updating of the digital twinborn model are realized. **Status** Granted as **CN114062786 (B)** – Apr 1st 2022	**No particularly informative figure available**

ELOXY1-22	**CN114154429 (A)** **Feb 10th 2022** **YANGTZE RIVER THREE GORGES GROUP CO LTD [CN]** **Mar 8th 2022**	**DIGITAL TWIN CONSTRUCTION METHOD AND DEVICE OF ENERGY STORAGE SYSTEM AND STORAGE MEDIUM** The method comprises the following steps: establishing an electrochemical mechanism model according to cell data of the energy storage system; building a building information model corresponding to the energy storage system based on the energy storage system data; **building a digital twin model according to the relationship between the two models**; based on data monitored and collected by the energy storage system, a data relation model and a simulation calculation analysis model of the energy storage system are established according to the electrochemical mechanism model and the building information model; and, **based on the digital twin scenario, establishing a digital twin model of the energy storage system according to the data relation model and the simulation calculation analysis model.** By implementing the method, the electrochemical mechanism model and the BIM model are established, and meanwhile, **a multi-physical field simulation calculation model which needs to be integrated for establishing the digital twin model of the energy storage system is fully considered, so that static and dynamic data are fused and analyzed, and the method is closer to an electrochemical energy storage power station entity.** **Status** Granted as **CN114154429 (B)** – Jun 14th 2022	**No particularly informative figure available**

ELOXY1-23	**CN114371409 (A)** **Mar 7th 2022** **SHANGHAI ROSUKENG ENERGY STORAGE SCIENCE AND TECH LIMITED COMPANY [CN]** **Apr 19th 2022**	**TRAINING METHOD OF BATTERY STATE PREDICTION MODEL, AND BATTERY STATE PREDICTION METHOD AND DEVICE** The method comprises the following steps: acquiring an electrochemical model, wherein the electrochemical model is constructed by measurement operation data and attribute data of a battery; performing charge and discharge simulation based on the electrochemical model to obtain simulation operation data of the battery under different simulation conditions; **taking the simulation operation data and the measurement operation data as training samples, inputting the training samples into a neural network, adjusting network parameters of the neural network and model parameters of the electrochemical model according to an output result of the neural network**; and determining the neural network meeting an iteration stop condition as a battery state prediction model. According to the invention, **the training samples of the neural network are expanded and enriched by means of the electrochemical model, and the electrochemical model is optimized based on the output result of the neural network, so that the electrochemical model provides more accurate training samples for the neural network, and the accuracy of model training is improved.** **Status** Granted as **CN114325403 (B)** – Jul 4th 2023	**No particularly informative figure available**

ELOXY1-24	**CN115097321 (A)** **Aug 29th 2022** **UNIV BEIHANG [CN]** **Sep 23rd 2022**	**LITHIUM BATTERY EIS AND SOH ESTIMATION METHOD BASED ON DIGITAL TWINNING** The invention relates to the technical field of battery state parameter estimation and SOX prediction, and provides a lithium battery EIS and SOH estimation method based on digital twinning. The method comprises the following steps: **constructing a lithium battery cloud digital twinning model based on a fractional order differential equation**; **continuously transmitting twinning data of open-circuit voltage of a voltage sensor and working current collected by a current sensor to a cloud server through a vehicle-mounted TBOX**; carrying out iterative optimization on state parameters and constructing a state parameter filter to obtain an estimated electrochemical impedance spectrum; and **establishing a regression model of electrochemical impedance growth of the lithium battery, introducing the regression model into a non-parameterized particle filter framework, and estimating the SOH of the lithium battery to obtain the SOH of the lithium battery.** The method is high in detection precision, provides reference for the calculation of the maximum output power SOP of the battery, improves the estimation precision of the state parameters and the health degree of the battery, and can accurately simulate the recession change process of the battery. **Status** Granted as **CN115097321 (B)** – Nov 15th 2022	**No particularly informative figure available**

ELOXY1-25	**CN117393060 (A)** **Nov 6th 2023** **SHANGHAI HEERMOSI TECH CO LTD [CN]** **SHANGHAI APOLLO MACHINERY CO [CN]** **Jan 12th 2024**	**METHOD FOR DETERMINING ELECTROLYSIS CONTROL DATA OF TARGET METAL BASED ON NEURAL NETWORK** The invention relates to a method for determining electrolysis control data of target metal based on a neural network, a method for electrolytic extraction of the target metal and a method for electrolytic extraction of lithium. The method comprises the following steps: **constructing a depth potential energy model to fit the interatomic interaction potential of a structural unit of target metal molten salt or electrolyte**; **training the constructed deep potential energy model based on the determined target loss function**; acquiring characteristic data of a structural unit of the target metal molten salt or electrolyte, so as to determine electrochemical property data of ions through a deep potential energy model; and **based on the candidate electrolysis control data and the electrochemical property data, through an electrolysis parameter prediction model, predicting candidate target metal electrolysis effect characterization data for determining target electrolysis control data.** Thus, **the present invention makes it possible to efficiently, accurately and adaptively perform electrolysis control even in a complex system** containing a plurality of electrolytes or in a case where the components of the electrolytes change. **Status** Under examination	**No particularly informative figure available**

ELOXY1-26	**CN117592365 (A)** **Nov 21st 2023** **SHANGHAI MAKESENS ENERGY STORAGE TECH CO LTD [CN]** **Feb 23rd 2024**	**METHOD AND SYSTEM FOR SOLVING ELECTROCHEMICAL MODEL BASED ON PHYSICAL INFORMATION NEURAL NETWORK** The method comprises the steps: **building the physical information neural network [PINN] according to a partial differential equation set in a to-be-trained electrochemical model**; according to the loss function of the PINN, adjusting the weight and bias of the PINN to train it; when the loss function is smaller than a preset value, obtaining a trained PINN system by simultaneously establishing the trained PINN corresponding to each partial differential equation set; iteratively solving the PINN system according to the loss function of the PINN system to obtain a trained PINN system; and **according to the trained PINN system, solving to obtain the electrochemical model**. **Status** Under examination	**No particularly informative figure available** **Extract –** In recent years, the development of artificial intelligence in many fields has provided new ideas. In particular, the rapid development of deep learning technology makes it possible to model and predict complex nonlinear systems through neural networks. However, **traditional neural networks mainly rely on large amounts of data for training, and there are certain limitations in their application for systems such as batteries where the internal state is difficult to directly measure**. **Physics-Informed Neural Networks [PINNs] provide a possible solution to this problem**. A PINN is a special neural network, which is characterized by incorporating some prior knowledge of physics during the training process, for example, some physical laws (such as conservation laws) or physical properties (such as continuity, smoothness, etc.). In this way, **a PINN can guarantee the physical rationality of the model output to a certain extent, especially when the data is sparse or incomplete**. Therefore, a PINN-based method is needed to solve the partial differential equations of the P2D model representing the internal physical processes of the electrochemical system (in this case, a battery).

Summary of the SotA regarding KER5 – AI-based control and monitoring software for EOPs based on a Digital Twin

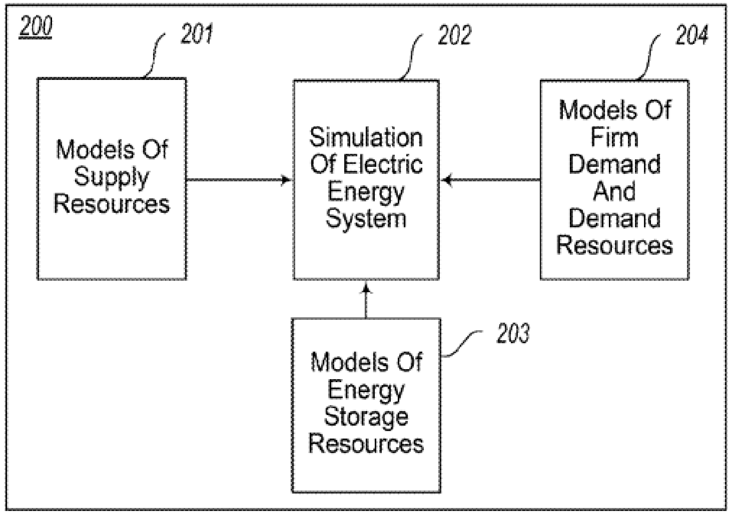
ELOXY1-18 discloses the application of artificial intelligence [AI] to the determination of chemical oxygen demand [COD] in waste water treated using an electrochemical [EC] system.

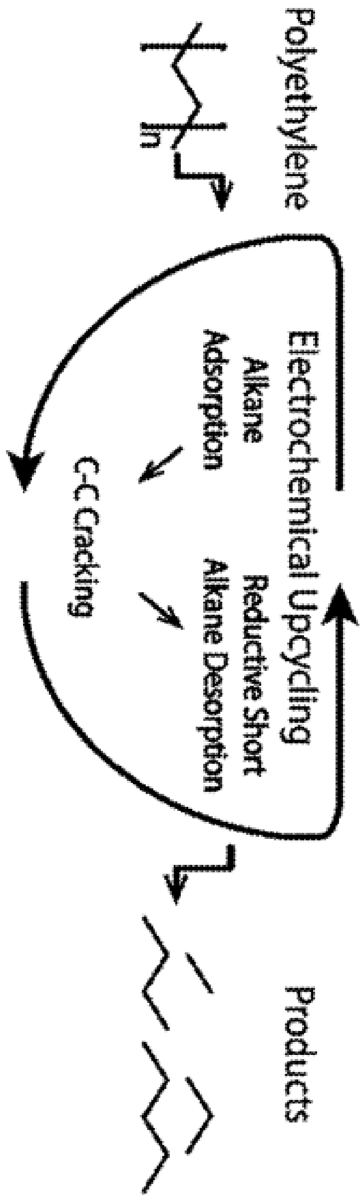
Each of **ELOXY1-20, ELOXY1-21, ELOXY1-22** and **ELOXY1-24** discloses the generation of digital twins of electrochemical processes for the purpose of optimising such.

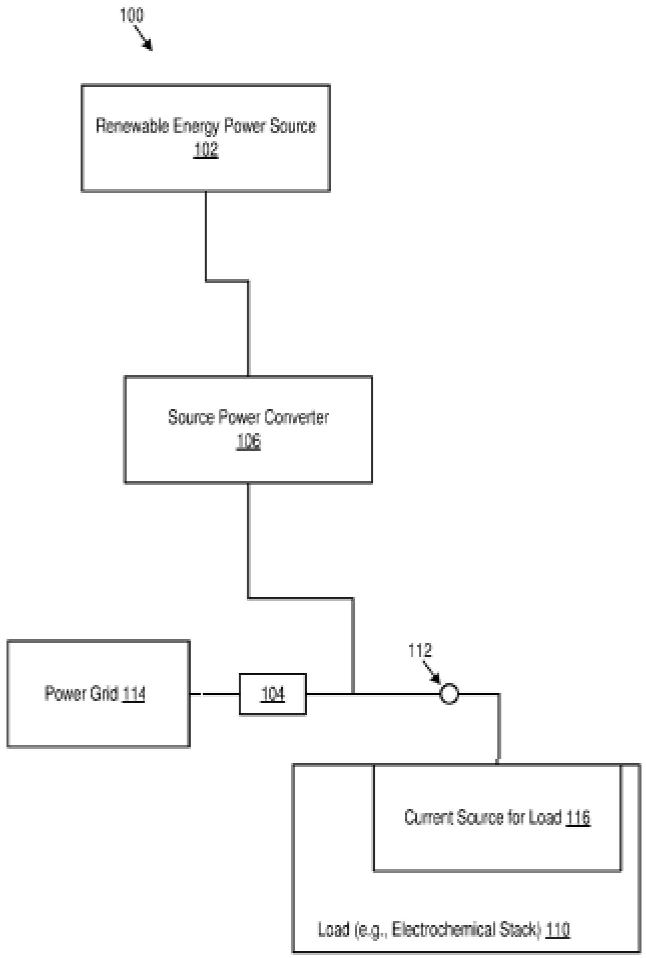
Numerous publications were found that apply AI means to the non-destructive monitoring of electrochemical system, particularly battery, operating parameters including battery SOXs, such as their State of Health [SOH]. These are exemplified by **ELOXY1-21**, **ELOXY1-23** and **ELOXY1-26.**

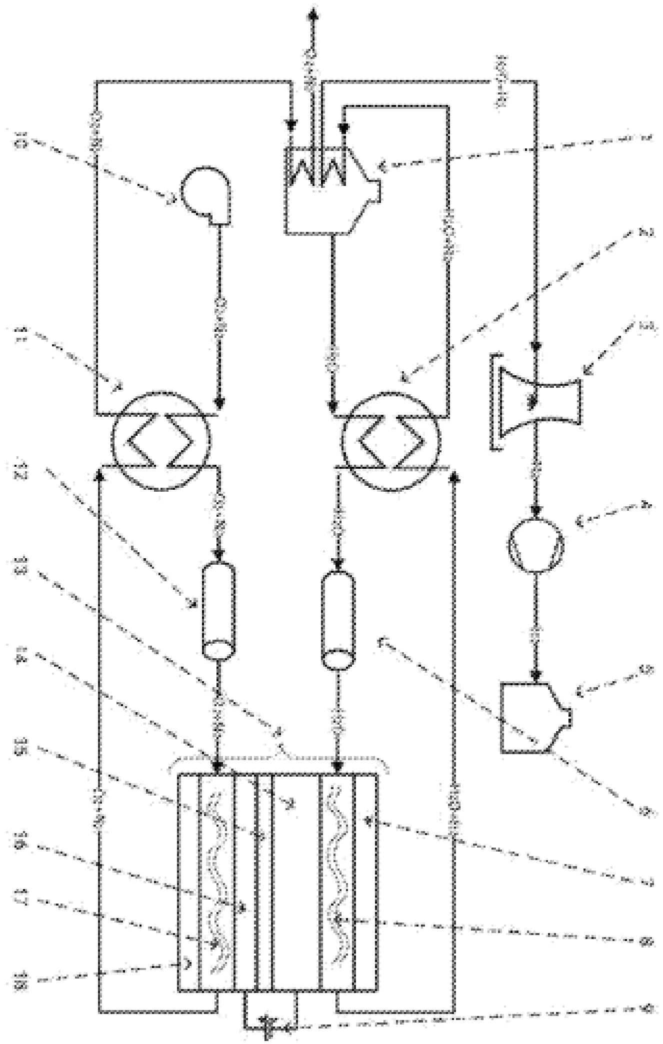
ELOXY1-25 is included as the only example found of a publication that discloses monitoring of the state of the electrolyte in an electrochemical cell rather than its SOH, etc.

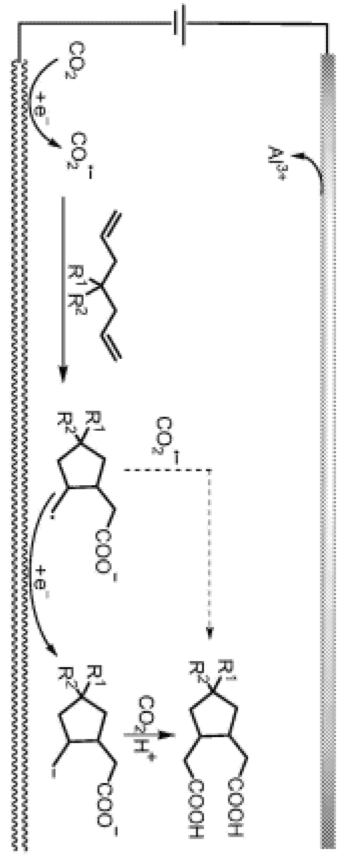
Overall summary – Numerous publications were found that disclose the application of artificial intelligence, especially neural networks of different types, to data from non-destructive monitoring of electrochemical systems (especially lithium ion batteries) and/or to the creation of digital twins of such systems. However, no publication was found that specifically discloses the application of AI to electrochemical oxidation processes for the conversion of organic substrates to high added-value chemicals and/or the creation of DTs thereof for EOP optimisation.

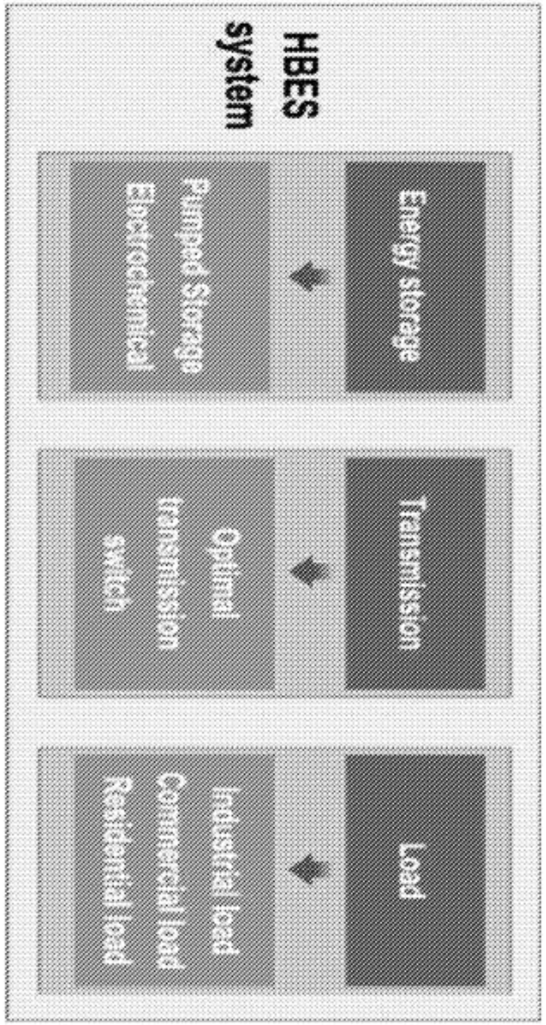
ELOXYCHEM – Table 3.1.6 – Patents and patent applications on strategy for integrating EOPs with RES, incorporating modelling and simulation tools			
Report Ref #	Publication # Priority date Applicants/Assignees Publication date	TITLE Abstract/extract Status Comment (if appropriate)	Figure (s) Extract (s)
ELOXY-27	US20160077507 (A1) Sep 11th 2014 SHEBLE GB [US] Mar 17th 2020	**RESOURCE CONTROL BY PROBABILITY TREE CONVOLUTION PRODUCTION COST VALUATION BY ITERATIVE EQUIVALENT DEMAND DURATION CURVE EXPANSION (AKA. TREE CONVOLUTION)** **A method, system and program product for quantifying risk of unserved energy in an energy system using a digital simulation.** An energy demand forecast is generated based at least in part on a weather model for near term future periods. A plurality of energy supply resources are committed to meet the plurality of energy demand assisted by a plurality of storage devices and associated ancillary services. A probable operating status is specified for each committed energy supply resource in the energy system. **Renewable energy resources such as wind, solar cells, and biofuels are also included in the models for energy supply sources.** A determination is made as to whether or not the committed supply resources and storage devices are sufficient to meet the energy demand as well as determine the cost of production above a prespecified LODP and EUE. **Status** Granted as **US10770899 (B2)** – Sep 8th 2020	

ELOXY1-28	US20230106006 (A1) Oct 4th 2021 WISCONSIN ALUMNI RES FOUND [US] Apr 6th 2023	**ELECTROCHEMICAL BREAKING OF C-C BONDS** Electrochemical systems and methods for cleaving C—C bonds are disclosed. In performing the method, a reactant adsorption electrical potential, a C—C bond breaking electrical potential, and a desorption electrical potential are sequentially applied to an electrode pair contacting a composition initially containing a target chemical reactant, such as a polymer or alkane. **As a result of performing the method, one or more desired chemical products, such as smaller alkane-containing molecules, are released from the electrode into the region between the electrode pairs.** **The method may be performed at ambient temperatures using renewable electricity.** **Status** Under examination	

ELOXY1-29	**WO2023129480 (A1)** **Dec 27th 2021** **ELECTRIC HYDROGEN CO [US]** **Jul 6th 2023**	**POWER SUPPLY SYSTEM FOR AN ELECTROCHEMICAL STACK** The system may support operation in at least two modes: a first where power for the electrochemical stack originates from a renewable energy (e.g., an on-site) power source; and a second mode where power for the electrochemical stack is supplied at least in part from a power grid interconnection. **A source power converter may adjust its operating voltage to select between prioritizing power from the on-site source and/or drawing power from the electrochemical stack at least in part from the power grid.** **Status** Written Opinion of the International Search Authority* Novelty: Claims 3-5, 10-20: YES; The rest: NO Inventive Step: Claims 4-5, 12-20: YES; The rest: NO Industrial Applicability: Claims 1-20: YES *For more information on this See ANNEX 1 of this document.	

ELOXY1-30	**CN114781188 (A)** **May 31st 2022** **LIYANG RESEARCH INSTITUTE SOUTHEAST UNIV SOUTHEAST [CN]** **Jul 22nd 2022**	**DYNAMIC MODELING METHOD FOR SOLID OXIDE ELECTROLYTIC HYDROGEN PRODUCTION SYSTEM ORIENTED TO FLUCTUATION ELECTRIC ENERGY ABSORPTION** The method comprises the following steps S1, **a dynamic model of the high-temperature solid oxide electrolytic cell with fluctuating renewable energy source electric power as a unique energy source is constructed based on the electrochemistry and heat transfer mechanism**; S2, constructing a dynamic model of each auxiliary machine part of the high-temperature solid oxide electrolytic hydrogen production system, and simulating the electrolytic hydrogen production process; S3, performing double-input double-output transfer function model identification on the mechanism model of the high-temperature solid oxide water electrolysis hydrogen production system; and S4, **performing model predictive control (MPC) design based on the established identification model.** The stability of the hydrogen production system is thus improved. **Status** Under examination	 9 renewable energy DC power, 13 electrolytic cell

ELOXY1-16	**CN117210834 (A)** **Jun 10th 2022** **UNIV SICHUAN [CN]** **Dec 12th 2023** **Electrochemical conversion of dienes to DICAs using CO_2 includes nickel cathode and carbon, including meshed glassy carbon, anode plus use of renewable electricity is specified but not a flow cell** **From 3.1.1**	**METHOD FOR PROMOTING CO2 TO SYNTHESIZE DICARBOXYLIC ACID COMPOUND BASED ON ELECTROCHEMISTRY** The invention discloses **a method for promoting CO_2 to synthesize dicarboxylic acid compounds based on electrochemistry, and belongs to the technical field of organic synthesis.** The method mainly comprises the following steps that a substrate, alkali and an additive are added into a reaction container, then a solvent is added in the CO_2 atmosphere, an electrolytic reaction is conducted at the temperature of 20-50 DEG C, after the reaction is finished, a product is separated and purified, and the dicarboxylic acid compounds are obtained. The method has the characteristics of mild reaction conditions, simplicity and convenience in operation, cheap and easily available raw materials, excellent selectivity and high atom economy. **The preparation method disclosed by the invention is wide in applicability, various substrates such as non-conjugated dienes, 1, 3-butadiene derivatives and heterocyclic aromatic hydrocarbons can be efficiently subjected to dicarboxylation reaction, and accurate construction of various novel diacid monomers is rapidly realized.** **Status** Under examination **Comment** – Proposes the use of renewable electric energy to power the electrochemical cell. Also proposes the possibility of using meshed glassy carbon for the anode.	 FIG.1 is a reaction mechanism diagram of the present invention.

ELOXY1-31	CN115618616 (A) Oct 24th 2022 YUNNAN POWER GRID CO LTD Jan 17th 2023	**METHOD FOR CONSTRUCTING HYBRID ENERGY STORAGE RELIABILITY EVALUATION MODEL OF SOURCE, NETWORK AND LOAD RESOURCES** The invention discloses a method for constructing a hybrid energy storage reliability evaluation model of source, network and load resources, which comprises the following steps of: modeling a pumped storage power station and electrochemical energy storage **on the basis of establishing a wind power and photovoltaic power generation model**; **establishing different demand response models** for the industrial load and the commercial and residential load; **analyzing a mathematical formula of the energy storage system, and modeling flexible resources of a source, a network and a load**; and integrating all the models to construct a new energy storage system, and performing reliability evaluation on the energy storage system. **Status** Under examination	

ELOXY1-08	**CN116479446 (A)** **Oct 27th 2022** **UNIV LISHUI [CN]** **Jul 25th 2023**	**GREEN SYNTHESIS METHOD OF ELECTROCHEMICAL CATALYSIS SULFONYLATION ISOXAZOLE DERIVATIVE** According to the method, beta, gamma-unsaturated ketoxime and p-toluene sulfonyl hydrazide are used as initial raw materials, **under the condition that C (+)/C (-) is used as an electrode, the current is I = 10mA, the room temperature reaction is performed for 4 hours, the oxidative sulfonylation reaction of an alkenyl oxime substrate can be smoothly realized, and the sulfonylated isoxazole derivative is obtained**. The method comprises the following steps: carrying out single electron oxidation on a p-toluene sulfonyl hydrazide anode to generate sulfuryl free radicals, then carrying out free radical addition on alkenyl oxime to generate benzyl free radicals, and further carrying out a benzyl free radical oxidation reaction and an intramolecular nucleophilic cyclization reaction on the anode to generate a sulfonylated isoxazole product. Compared with the traditional synthesis scheme, **the sulfuryl group can be introduced into the skeleton of the isoxazole ring under the electrochemical condition only by adding the inorganic electrolyte as a conductive medium and without adding metal and additional oxidizing agent under the mild condition**; and the constructed aryl alkyl sulfone compound widely exists in medical and bioactive products and materials, and has important biological and synthetic research values. **Status** Under examination	**No particularly informative figure available**

ELOXY1-09	**CN115613060 (A)** **Nov 11th 2022** **UNIV ZHEJIANG TECHNOLOGY [CN]** **Jan 17th 2023**	**METHOD FOR SYNTHESIZING C-3 PHOSPHORYLATED 2H-INDAZOLE COMPOUND THROUGH DIRECT ELECTROCHEMICAL OXIDATION** The invention relates to **a method for synthesizing a C-3 phosphorylated 2H-indazole compound through direct electrochemical oxidation**, and the C-3 phosphorylated 2H-indazole compound. The method comprises the following steps: by taking a 2H-indazole compound as shown in a structural formula (II) and a trialkyl phosphite compound as shown in the structural formula (II) as reaction substrates, **carrying out electrolytic reaction by adopting a two-electrode system**, and after the reaction is finished, carrying out separation treatment to obtain the C-3 phosphorylated 2H-indazole compound as shown in the structural formula (I). The method has the main beneficial effects that **(1) clean electric energy is used as an oxidizing agent, so that the environmental cost is reduced;** (2) the universality of a reaction substrate is good; (3) reaction conditions are mild; and (4) a class of novel C-3 phosphorylated 2H-indazole compounds are provided, and a basis is provided for screening of new drugs. **Status** Under examination	**No particularly informative figure available**

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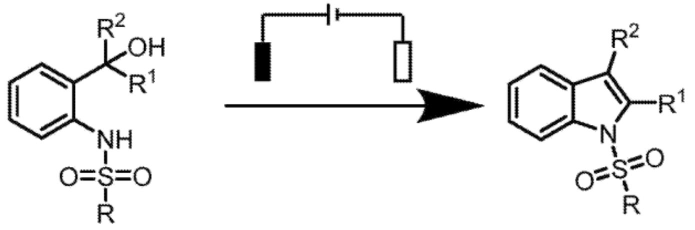
ELOXY1-11	**CN115807233 (A)** **Dec 12th 2022** **UNIV SOUTHWEST [CN]** **Mar 17th 2023**	**METHOD FOR ELECTROCHEMICAL SYNTHESIS OF SUBSTITUTED INDOLE FROM GAMMA-HYDROXYLAMINE** The method comprises the following steps: mixing a substrate, an organic additive, an electrolyte and a solvent to obtain a homogeneous solution, adding the homogeneous solution into **an electrochemical reaction device with a carbon cloth anode and a platinum cathode**, and synthesizing the substituted indole through an electro-catalysis one-step method. **The synthesis of substituted indole by gamma-hydroxylamine is combined with an organic electrocatalysis technology, and the oxidation-reduction reaction is realized by using clean electric energy, so that the use of an oxidation or reduction reagent is avoided.** The electrochemical indole synthesis strategy has excellent functional group, water and air tolerance. Compared with the prior art, the synthesis method disclosed by the invention is efficient and economical, free of metal residues in products, short in reaction time, simple and easily available in raw materials and high in yield; the application of the material in the field of biomedical materials is more competitive. **Status** Under examination	 1 2 FIG. 1 is the reaction equation of the present invention synthetic substituted indole compound.

ELOXY1-12	**CN115799484 (A)** **Dec 29th 2022** **UNIV GUILIN TECHNOLOGY [CN]** **Mar 14th 2023**	**ELECTROCHEMICAL METHOD FOR PREPARING N-ARYL SULFIMIDE COMPOUND** An electrochemical method for preparing an N-aryl sulfimide compound comprises the following steps: **in an air atmosphere, adding a sulfoximine compound and alpha-ketonic acid into a reactor according to a molar ratio of 1: 2**, adding an electrolyte tetrabutylammonium tetrafluoroborate and a catalyst nickel bromide, and then adding an acetone solution; stirring the mixture by using a magnetic stirring device to dissolve the mixture, **inserting two electrodes, electrifying for 3h at 6mA by using a graphite electrode as a positive electrode and a platinum sheet electrode as a negative electrode**, after the reaction is finished, evaporating to remove the solvent under reduced pressure to obtain a crude product, and purifying by column chromatography to obtain the N-aryl sulfonimide compound. Compared with the traditional synthesis method, the method has the advantages that the reaction condition is mild, and the reaction can be smoothly carried out at room temperature; the operation is simple, and all operations can be carried out in an open system; **the reaction uses current as an oxidation method, so that the pollution of a chemical oxidant is avoided**; the raw materials are easy to obtain, the functional group compatibility is good, and the substrate application range is wide. **Status** Under examination	**No particularly informative figure available**

ELOXY1-32	**CN116305819 (A)** **Jan 20th 2023** **UNIV TSINGHUA ELECTRIC POWER SCIENT RES INST [CN]** **STATE GRID ZHEJIANG ELECTRIC POWER CO LTD [CN]** **Jun 23rd 2023**	**ELECTRIC POWER AND ELECTRIC QUANTITY BALANCE SCENE CONSTRUCTION METHOD FOR HIGH-PROPORTION RENEWABLE ENERGY SOURCES** The invention belongs to the field of electric power system supply and demand relation balance, and aims at: **solving the problem of electric power and electric quantity balance of a high-proportion renewable energy source system and minimizing the total investment and operation cost of a multi-energy electric power system**; and establishing a planning-operation double-layer optimization configuration model, and **carrying out collaborative optimization on the light field area, the heat storage capacity, the power generation capacity and the electrochemical energy storage capacity of the photo-thermal power station.** An original problem is decomposed into a planning layer and an operation layer, and the planning layer and the operation layer are finally integrated into a mixed integer linear programming model for solving. **Status** Under examination	**No particularly informative figure provided**

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ELOXY1-33	**CN116497380 (A)** **May 8th 2023** **CHINA THREE GORGES CORP [CN]** **Jul 25th 2023**	**METHOD AND DEVICE FOR DETERMINING OPERATION MODE OF MICRO-GRID SYSTEM CONTAINING ELECTROCHEMICAL ENERGY STORAGE** The method comprises the steps: obtaining the load demand variation of a power utilization end and the load demand of the power utilization end, and when the load demand is greater than the total output power of a renewable energy unit, determining the operation mode of the renewable energy unit; determining a residual load demand exceeding the total output power of the renewable energy unit, and based on the residual load demand, determining the carbon emission during power output based on the non-renewable energy unit and the external power grid in the micro-grid system, and based on the load demand of the power consumption end, the load demand variation of the power consumption end and the residual load demand, determining the carbon emission during power output based on the non-renewable energy unit and the external power grid; and **determining the total cost when the output power of the micro-grid system meets the load demand of the power utilization end, and determining the micro-grid system operation mode meeting the user demand according to the carbon emission and the total cost**, so as to reduce the influence on the environment in the operation process while reducing the operation cost of the micro-grid system. **Status** Under examination	**No particularly informative figure available**

Summary of the SotA regarding KER6 – Strategy for integrating EOPs with RES, incorporating modelling and simulation tools

Although **ELOXY1-27** was published well outside the chosen date range, it is included here as it discloses an early example of the application of modelling and simulation to the regulation of energy networks.

Each of **ELOXY1-29** through **ELOXY1-33** discloses an example of the application of modelling and simulation to the regulation of hybrid energy networks in which a combination of renewable energy sources [RESs] of electricity are combined with alternative energy sources (usually the national grid) to provide a balanced electricity supply to electrochemical processes.

Each of **ELOXY1-08, ELOXY1-09**, **ELOXY1-11, ELOXY1-12** and **ELOXY1-16** from **Section 3.1.1** discloses the use of renewable sources of electricity (also known in China as ‘clean electricity’ and ‘new energy’) to power electrochemical systems for the oxidation of organic chemicals.

Overall summary – Although several publications were found that disclose the modelling of energy systems that include RESs for powering of electrochemical systems and several were found that disclose the application of RES-derived electricity to the electrochemical oxidation of organic chemicals, no patent or patent application was discovered that discloses both.

3.2. Overall summary of the SotA for each KER

Below are collated the overall summaries from **Section 3.1.1** through **Section 3.1.6** regarding the SotA for each **KER**.

KER1 – Metal-free EOPs for conversion of cycloalkanes, cycloalkenes and TOFA to oxo-functionalisation products

From **Table 3.1.1.1**, it is clear that each of the 16 publications listed in **Table 3.1.1** discloses one or more inventions that show some degree of overlap with the electrochemical oxidation process [EOP] technology developments that the partners plan to make during the **ELOXYCHEM** project. However, none discloses all of them. In particular the use of cycloalkanes, cycloalkenes and TOFA as substrates for EOPs was not found to be disclosed in any publication.

KER2 – Methodology for the scale-up of EOP chemical production from pilot to commercial scales

Whilst publications were identified that disclose means for scaling up electrochemical processes e.g. **WO2023161695 (A1)** that discloses scale-up of an electrochemical process for making nanocrystalline carbons to the level of mass-production, no patents or patent applications were found that disclose the scale-up of electrochemical oxidation processes [EOPs].

KER3 – EOP platform system for lab to demo and pilot scale process development

Whilst publications were identified that disclose electrochemical technology platforms e.g. **EP3453064 (B1)** that discloses an advanced electrode technology platform for electrochemical reduction of CO_x species, no patents or patent applications were found that disclose such a platform for electrochemical oxidation processes [EOPs].

KER4 – ML methodology to optimise operating conditions for enhanced EOP performance

No publications were found that disclose the application of machine learning to the optimisation of electrochemical oxidation processes or the devices/reactors/cells in which they are carried out.

KER5 – AI-based control and monitoring software for EOPs based on a Digital Twin

Numerous publications were found that disclose the application of artificial intelligence, especially neural networks of different types to data from non-destructive monitoring of electrochemical systems (especially lithium ion batteries) and/or to the creation of digital twins of such systems. However, no publication was found that specifically discloses the application of AI to electrochemical oxidation processes for the conversion of organic substrates to high added-value chemicals and/or the creation of DTs thereof for EOP optimisation.

KER6 – Strategy for integrating EOPs with RES, incorporating modelling and simulation tools

Although several publications were found that disclose the modelling of energy systems that include RESs for powering of electrochemical systems and several were found that disclose the application of RES-derived electricity to the electrochemical oxidation of organic chemicals, no patent or patent application was discovered that discloses both.

3.3 Summary of the SotA for the proposed ELOXYCHEM KERs

Reviewing the overall summaries for each KER collated above, it is obvious that the partners in the ELOXYCHEM project are currently working at the very cutting edge of technology in each of the relevant technology sectors.

Nevertheless, each patent search provides only a snap-shot of the SotA on the day on which it was undertaken. Therefore, it will be essential for the partners to continue to monitor competitor patenting and commercial activity throughout the remainder of the project and beyond (see **Section 6** below for suggestions as to how this might be achieved).

4. Summary of the current SotA vs Freedom to Operate

As recorded at **Section 1.3** of this report, one of the principal objectives of this **1st Iteration T-FA** is to'…confirm continued Freedom to Operate [FTO] with planned technology developments.'. In this section the criteria for patentability are first addressed before the partners' FTO with the anticipated project results is examined.

4.1 Patentability of the ELOXYCHEM project results

The three main criteria for an invention to attract patent protection are that it must be **novel over the prior art**, it must be **capable of industrial applicability**, and, most importantly, it must **involve an inventive step**, that is, the inventor must have made an unprecedented leap of imagination to create it that is non-obvious to 'one skilled in the art' in their particular technology sector or in related sectors. The examiner of any patent application will look to its Claims to see if these three criteria are met. Then, so long as it is not excluded from patentability by legislation in the local jurisdiction, it may be granted as a patent.

Should the partners in the **ELOXYCHEM** project contemplate making patent applications for any of their inventions in the project, they must ensure that those inventions meet the three criteria listed above before doing so. This will require them (or their patent attorneys) to undertake a patentability search, that is to search the patent databases for prior art that might prevent them from getting a patent. The prior art can be found in, *inter alia*, scientific publications, in blogs on the internet, in patent applications that were not or might not be granted and in granted patents. Should they find that their invention meets the three criteria, they may then choose to submit a patent application for it.

4.2 FTO with the ELOXYCHEM project results

Should they be lucky enough to be eventually awarded a patent for their invention(s), the partners should then have freedom to operate [FTO] with it (them) on markets in that jurisdiction and in any other where a patent is granted[4].

As far as FTO with the actual **ELOXYCHEM** project results is concerned, this cannot be judged as it appears that none of the processes/products is completed and, therefore, their potential for patentability and/or infringing third party IPRs cannot be properly assessed at this time.

What can be said is that of the relevant patents or patent applications found during the searches for this **1st Iteration T-FA**, listed in **Table 3.1.1** through **Table 3.1.6**, 78% of them are from Chinese enterprises and are for Chinese national patents or national utility model patents only. This means that, so long as they do not attempt to launch any related product on Chinese markets, the partners cannot infringe the IPRs in the inventions disclosed in those publications. However, the teachings of all of them now form part of the prior art and must be taken into account should the partners decide to seek patent protection for their own inventions arising during the **ELOXYCHEM** project.

That said, there appears to be very little overlap between published EOP systems powered from renewable energy sources and the proposed technology developments in the **ELOXYCHEM** project meaning that the partners may well be able to get patent protection for their own inventions made during the project and eventually enjoy FTO with them.

N.B. As pointed out in **Section 3.3** above, it will be essential for the partners to continue to monitor competitor patenting and commercial activity throughout the remainder of the project and beyond (see **Section 6** below for suggestions as to how this might be achieved).

5. Competitors

5.1 Potential competitors identified in searches for this T-FA

[4] Note that there may be reasons why they do not have FTO with their granted patent, for example, it might be challenged in the courts by a competitor and subsequently revoked.

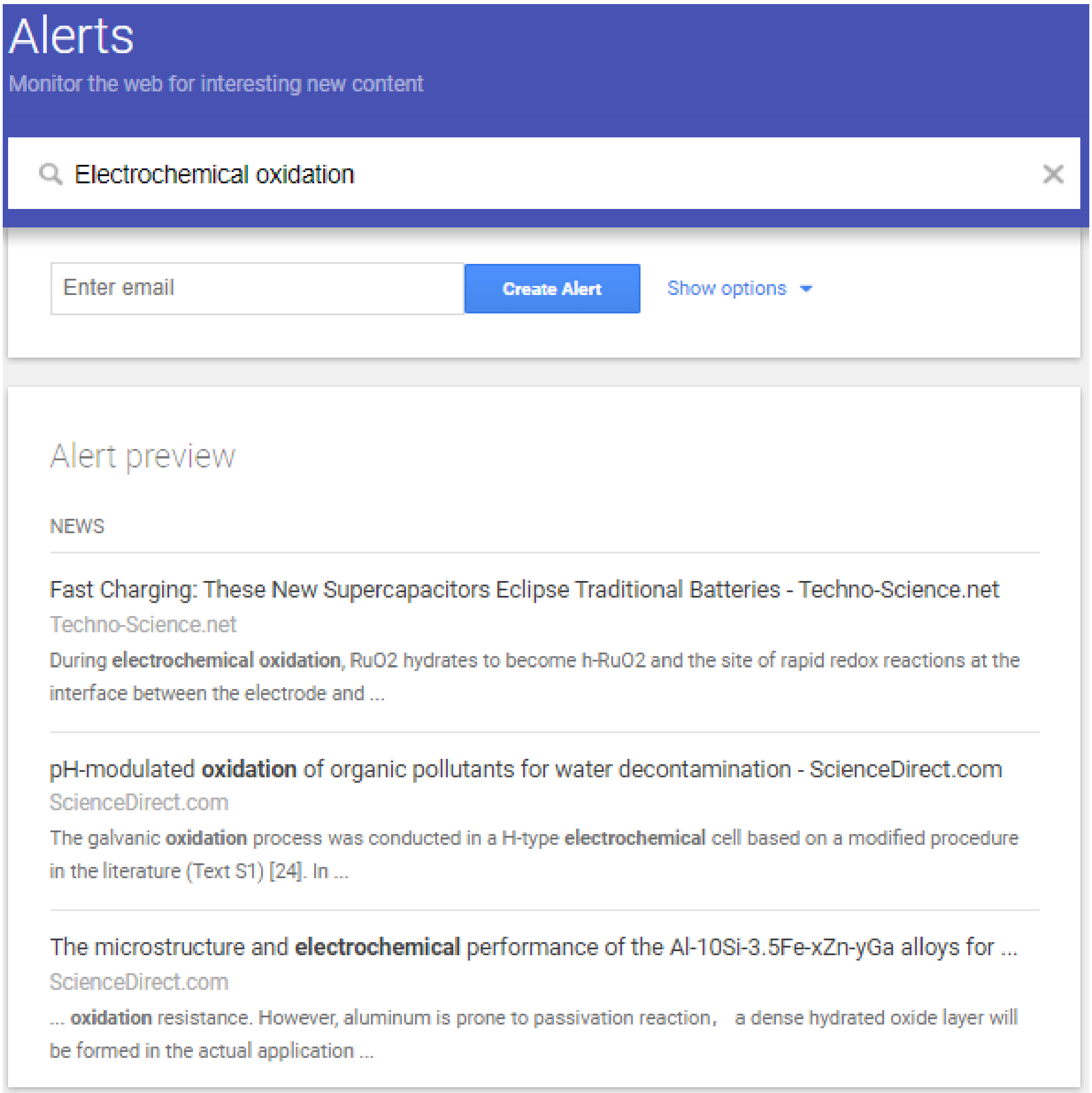
As noted in **Section 4.2** above, 78% of the publications listed in the tables at **Section 3.1** are from Chinese enterprises. Of these, **UNIV GUILIN TECHNOLOGY** has published the most that are relevant to the technology developments anticipated in the **ELOXYCHEM** project: **ELOXY1-04**, **ELOXY1-05**, **ELOXY1**-12 and **ELOXY1-19.** This may mark them out as potential competitors and it may be worthwhile to maintain a watching brief on them and their published patent applications.

From the conclusions in **Section 3.3** and in **Section 4**, it seems that there is a global lack of competitors offering EOP systems for the conversion of cycloalkanes, cycloalkenes and TOFA into high added value chemicals that are powered from RESs. However, as pointed out in **Section 3.3** above, it will be essential for the partners to continue to monitor competitor patenting and commercial activity throughout the remainder of the project and beyond (see **Section 6** below for suggestions as to how this might be achieved).

6. Monitoring developments in ELOXYCHEM technologies

6.1 Setting of ELOXYCHEM technology alerts

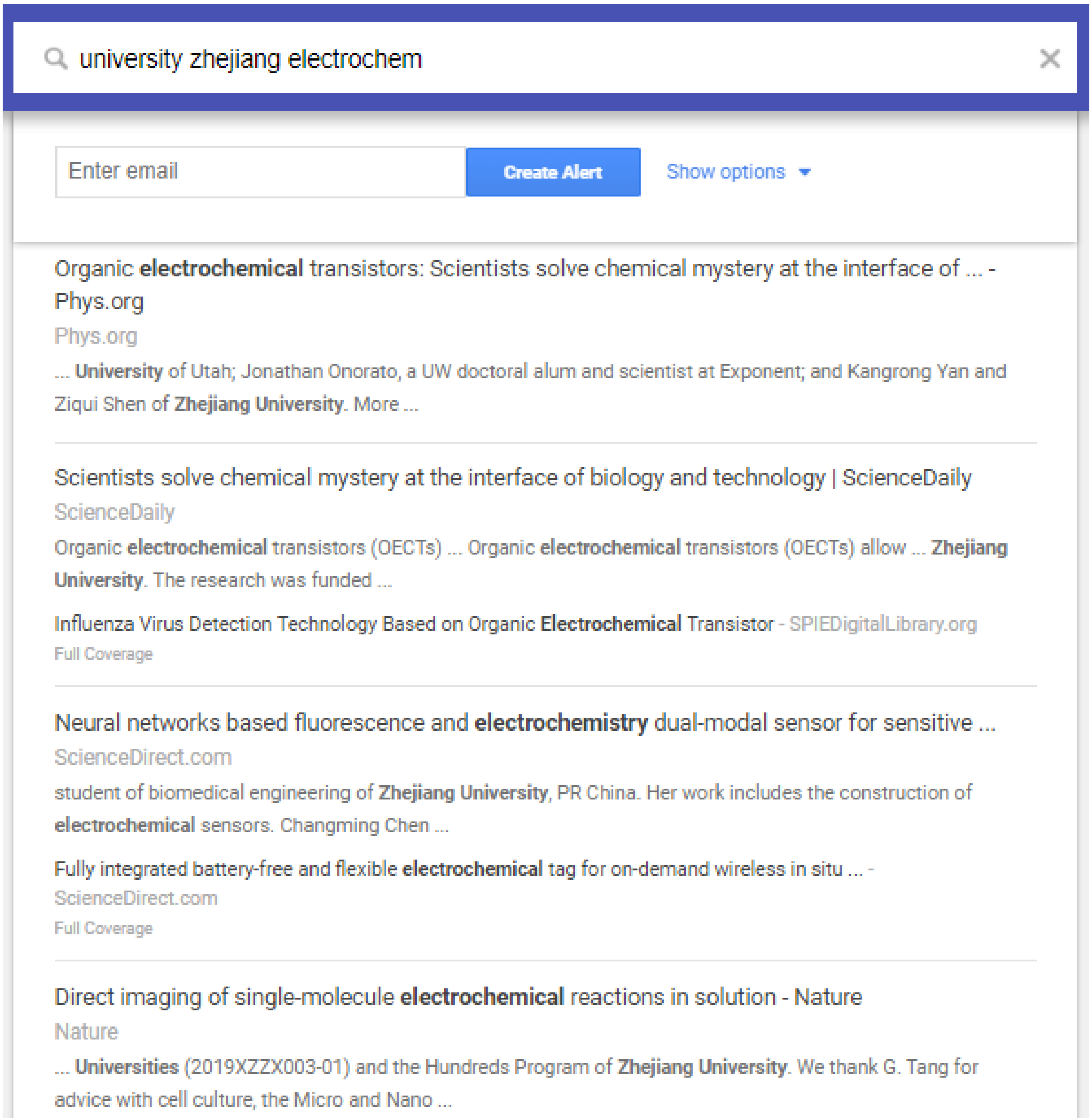
To monitor developments in the ELOXYCHEM technology arena, alerts can be set up with, for example, using the same key words and phrases used in the patent searches above:



6.2 Monitoring potential competitors identified during this T-FA

The same can be done with the names of potential competitors such as **UNIV ZHEJIANG TECHNOLOGY** identified as such in **Section 5.1** above.

Putting 'university zhejiang electrochem' as key words into Google Alerts brings up the results shown overleaf.



e-mails containing such results can be sent to an address of choice at intervals of choice e.g. daily, weekly, monthly.

6.2 Second and third Iterations of ELOXYCHEM T-FA

Two further iterations of **T-FA** will be undertaken, one towards the middle of the project and one close to its end. The middle iteration will not only enable an update of the SotA in each of those technologies but will also enable an assessment of the progress in the project developments versus the benchmark provided in this report.

The third and final iteration will allow an assessment of the partners' freedom to operate [FTO] with their, hopefully completed, technology developments. In addition, the analysis will enable an assessment of the value of the partners' foreground intellectual property [FGIP] and how that may be exploited using the **RAPID** strategy outlined in the Grant Agreement (PDF pp150-151).

7. Conclusions

The conclusions from this **report** are clearly laid out in **Section 3** and **Section 4** above and summarised there and in the **Executive Summary**:

In summary, this **1st Iteration T-FA** report has provided a timely update of the SotA in technology sectors relevant to the six anticipated **K**ey **E**xploitable **R**esults [**KER**s] of the project, whilst simultaneously providing an indication of the patentability of the projects results and the partners' freedom to operate [FTO] with those results now and in future.

This report will be followed by reports on two further iterations of **T-FA** – one towards the middle of the project and one towards the end of the project.

ANNEX 1: Patent **Status** and utility models explained

A1.1 Patent **Status**

When patent applications are published, the examiner provides a report that goes along with the publication. The report usually comments on the Novelty of the invention(s) disclosed, whether or not they required an Inventive Step for their realisation and whether or not they are capable of Industrial Applicability.

Failure to meet any of the three criteria results in the application being rejected. This can then be followed by one or more re-applications, usually with amended claims.

Eventually, an application is:

- ✓ published as a granted patent;
- ✓ abandoned by the applicants in any jurisdiction where no further re-applications are permitted; or
- ✓ revised and resubmitted as a new application in the same or other jurisdiction.

When a PCT patent application is made through the agency of the World Intellectual Property Office [WIPO], the examiner first publishes what is called a 'Written Opinion of the International Search Authority' like this one taken from **ELOXY1-29** of this report:

> **Status**
>
> Written Opinion of the International Search Authority*
>
> Novelty: Claims 3-5, 10-20: YES; The rest: NO
>
> Inventive Step: Claims 4-5, 12-20: YES; The rest: NO
>
> Industrial Applicability: Claims 1-20: YES

Later, the same information is published as the 'International Preliminary Report on Patentability' Ch.1.

WIPO does not grant patents! Instead, it acts as a clearing house for simultaneous launch of patent applications across multiple global jurisdictions, e.g. the UK, China, Japan, the USA, Europe, Canada, Australia, etc., etc., where the applications are examined by the competent authorities in those jurisdictions. They decide the fate of that application in their jurisdiction. When that fate has not yet been determined, the WOISA or the IPRP – whichever is more recent, is included in this **T-FA** report so that readers can gain some insight into the likely fate of the application.

In the case of very recent applications to some patent offices, there may be no data available on the current fate of the application for some months after its publication. Where this was discovered in the patent searches for this report, the application is simply marked as 'Data not available' or 'Under examination' or 'Under review'.

A1.2 Utility models

These are minor patents that can be awarded in some countries for inventions that are technical in nature but would not normally attract full patent protection.

They are often awarded for a shorter period than a full patent in the same jurisdiction. For example, a utility model in China will attract ten years protection rather than the full 20 years a granted Chinese patent would attract.

END