Highly efficient and low cost photovoltaic-electrolysis (PVE) system to generate hydrogen by harvesting the full spectrum of sunlight

MID-TERM ACTIVITY REPORT & Lessons Learn Report

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SUMMARY

Photovoltaic electrolysis (PVE) is a promising approach to produce renewable hydrogen (H_2) for export from sunlight and water. However, the barriers of PVE uptake, including expensive precious-metal electrodes, external heat sources and low stability make adoption impractical. This project aims to enable enhanced conversion efficiency of renewable primary energy (solar) to hydrogen by developing a low-cost, highly efficient, integrated PVE system to harvest the electricity and heat produced by a concentrator photovoltaic (CPV) receiver which will power an alkaline water electrolyser. The heat harnessed will be transferred to the electrolyser (made of earth-abundant electro/photo-catalysts) to lower the reversible potential of water splitting, increase the reaction kinetics and decrease the system resistance which will lead to an enhanced catalytic performance. The solar UV light will also be harnessed to activate the semiconductor co-catalysts, which will increase the current density, lower the overpotentials and deliver additional improvements to the performance of the PVE system. Figure 1 summarize how the project works. The expected project outcome is the development of a new low-cost PVE system with a genuine solar-to-hydrogen (STH) efficiency >30% and proven stability (> 1000 h).

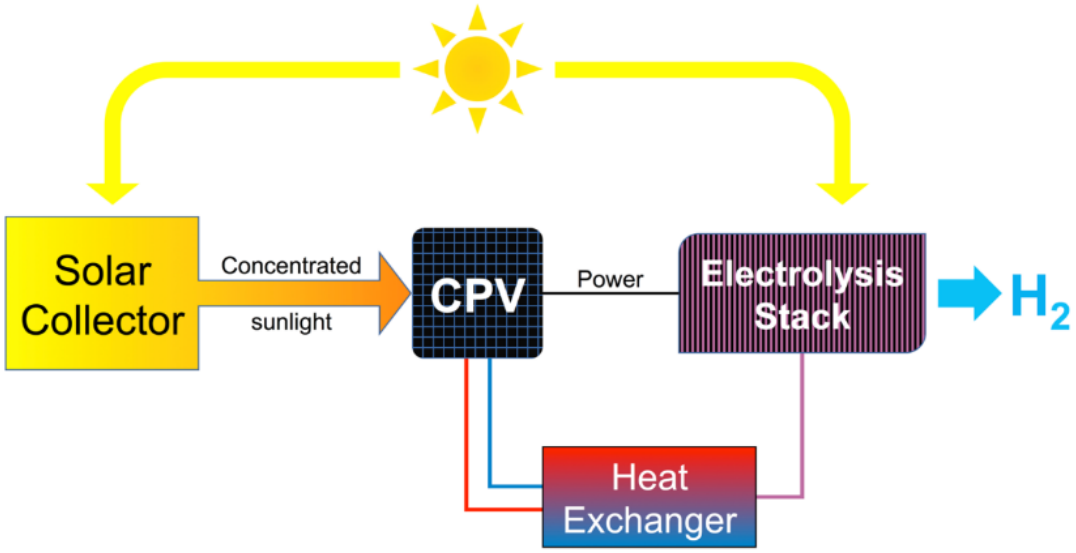

Figure 1. Schematic diagram summarizing the project

SCOPE

This project uses an innovative approach to develop a low-cost, highly efficient, integrated PVE system to harvest the whole spectrum of sunlight as the sole source of electricity, heat and light, which then will power an alkaline water electrolyser to convert renewable primary energy (solar) to hydrogen. Raygen's Concentrator Photo Voltaic (CPV) which has been successfully demonstrated as the world's highest 'central receiver' system with system efficiency at 27% (@250kWe) for electrical out-put and a combined efficiency for heat and power of over 75%; and novel electrocatalyst composites from UNSW will be utilised to achieve this outcome. Thus, the scope of the project includes:

1. Development of active and stable catalyst materials and evaluation of its performance for Hydrogen generation via Oxygen Evaluation Reaction (OER), Hydrogen Evaluation Reaction (HER) and water splitting;

2. Design, construction and optimisation of water electrolyser cell assembly and evaluate its performance using developed catalyst;
3. Design and fabrication of an integrated 20W lab-scale PVE system prototype with an overall Solar To Hydrogen conversion (STH) efficiency >30%;
4. Optimisation and scale up of the PVE technology through experiments and process modelling to achieve 100W scale;
5. Techno-economic analysis of the PVE system so as to provide an overall cost/performance model for establishment of a business model and roadmap to a commercial product.

UPDATE ON PROGRESS

The project commenced on 1 August 2018, and at this mid-term point, some important outcomes which have been achieved are:

1. Development and evaluation of activities of catalyst materials for Oxygen Evolution Reaction (OER) and Hydrogen Evolution Reaction (HER).
    a. A novel electrode for oxygen evolution reaction (OER) has been fabricated. The electrode is only comprised of earth abundant elements (Nickel (Ni) and Iron (Fe)), and displays an extremely high OER catalytic activity in alkaline media, which even outperforms the precious metal based benchmarks, such as iridium oxide.
    b. A novel strategy has been employed to reduce the amount of precious metals (such as platinum) used in catalysts for hydrogen evolution reaction (HER) meanwhile retain the high catalytic activity. By exploiting the interactions between metal clusters and isolated metal atoms, a series of new HER catalysts have been developed. With only 0.5 wt% of precious metals (Platinum (Pt) or Ruthenium (Ru)), these catalysts exhibit superior catalytic activity to the platinum on carbon benchmark that contains 20 wt% of Pt.
    c. The effects of temperature on affecting the OER and HER performances have been studied. Increasing the reaction temperature will benefit the OER to a great extent, resulting in reduced onset potentials and enlarged current densities at any given potentials. By contrast, HER is not obviously affected by the change of reaction temperatures.
2. Demonstration of concentrator photovoltaic (CPV) solar cell heatsink and electrolyser heat exchanger has been developed and tested.
3. Design, construct and optimise water electrolyser cell assembly and evaluate its performance:
    a. A customised alkaline electrolyser for water splitting has been fabricated, employing the OER electrode and HER catalysts developed in this project. When operated in 6 M Potassium Hydroxide (KOH) at 80^{o}C, the cell is capable of delivering a current density of 300 mA/cm^2 at an applied cell voltage of 1.5 V.
    b. Electrolyser modelling and design optimisation through Computational Fluid Dynamics (CFD) modelling:
    A three-dimensional transient CFD model is developed for alkaline water electrolysis process for process understanding and optimisation and then improving hydrogen production. This model offers a cost-effective way to evaluate electrolyser's design and performance under different operating conditions and structure configurations; Based on this model, massive numerical simulations will be conducted for testing innovative designs and new materials and then improve hydrogen production.
    c. Numerical study of the effects of bubbles behaviours on electrolyser's performance.
    A three-dimensional transient model of single serpentine flow channel is successfully developed and used to understand the bubbles behaviours in the flow channel, including bubbles growth, bubbles coalescence and breakup, and transition of flow regimes.

KEY HIGHLIGHTS AND DIFFICULTIES EXPERIENCED

The key highlights and challenges experienced will be summarized and presented in the form of Lessons Learnt report.

Lessons Learnt

Lessons Learnt Report: Scaled manufacturing of large area oxygen electrodes

Project name: Highly efficient and low cost photovoltaic-electrolysis (PVE) system to generate hydrogen by harvesting the full spectrum of sunlight

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Water electrolyser
State/Territory:	NSW

Key learning

Scaled manufacturing allows us to enlarge the surface area of the oxygen electrodes prepared in the laboratory from ~ 1 cm^2 to 25 cm^2, meanwhile maintaining their apparent catalytic activity.

Implications for future projects

The method enables the production of large-scale, cost-effective oxygen electrodes for industrial scale alkaline water electrolysis for hydrogen production.

Knowledge gap

Although there are many high-performance oxygen electrodes reported in literature, they are only effective with a small surface area (< 1cm^2), which has hindered their application in practical water electrolysers, and calls for innovative preparation methods.

Background

Objectives or project requirements
The objective of this project is to fabricate large area oxygen electrodes with high apparent catalytic activity.

Process undertaken

A novel hydrothermal manufacturing process is designed to prepare oxygen electrodes with large surface area. This process allows the deposition of large amount of active species (such as nickel and iron) on the surface of current collectors (like nickel foam) with high uniformity and strong adhesion. So far, a series of electrodes has been prepared using this method ranging from 1 cm^2 to 25 cm^2. All of them exhibit similar, good catalytic performances.

Lessons Learnt Report: Lowering the precious metal content for hydrogen evolution

Project name: Highly efficient and low cost photovoltaic-electrolysis (PVE) system to generate hydrogen by harvesting the full spectrum of sunlight

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Water electrolyser
State/Territory:	NSW

Key learning

A series of novel catalysts with extremely low precious metal content (< 0.5 wt% of Ruthenium and Platinum) has been designed and developed in this project. These catalysts exhibit similar or even higher hydrogen evolution activity than the benchmark platinum catalysts supported on carbon (Platinum/Carbon (Pt/C), 20 wt% of Pt).

Implications for future projects

These catalysts can be used in commercial water electrolysers, lowering the material cost meanwhile maintain the high level of activity.

Knowledge gap

Precious metal free catalysts for hydrogen evolution has been the focus of research for the past few years, while few of them can compete with the Pt/C in terms of intrinsic activity. Novel preparation methods are required to obtain catalysts materials with low material cost and high catalytic activity to replace the expensive Pt/C.

Background

Objectives or project requirements
The objective of this project is to fabricate cost-effective and active catalysts for the cathodic hydrogen evolution reaction.

Process undertaken
Novel strategies are employed to control the structure of Pt and Ru at the atomic level, and to reduce the usage of precious metals including transition metal doping. By precisely controlling the number of atoms in a cluster, we are able to tune the catalytic performance of the catalyst materials obtained. The optimised catalyst only has precious metal (Pt or Ru) loading of 0.5 wt%, and when subjected to identical measuring conditions, they exhibit a 40-time increase in terms of turnover frequency (TOF) over the Pt/C benchmark catalyst.

Lessons Learnt Report: Electrolyser design and optimisation through CFD modelling

Project name: Highly efficient and low cost photovoltaic-electrolysis (PVE) system to generate hydrogen by harvesting the full spectrum of sunlight

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Hydrogen R&D project
State/Territory:	NSW

Key learning
A mathematical model is developed to describe the internal state and predict performance of electrolyser by coupling computational fluid dynamics (CFD) approach and electrochemical theory. In this part, the alkaline water electrolyser, especially the electrochemical reactions related heat and mass transfer phenomena, can be described in detail using numerical models. The combination of experiments and numerical modelling greatly contribute to the development of alkaline water electrolyser.

Challenges
The numerical studies of electrolysis in the open literature only focus on flow. A new advanced model is required to be developed and validated when the electrochemical reactions are considered. It is scientifically challenging and need joint effort of CFD and electrochemical theory.
The electrolyser model is computationally expensive. In order to address this issue, the code requires to be modified to allow the large-scale computing on supercomputers – National Computation Infrastructure (NCI).

Implication for future projects
The model provides a pathway to cost-effectively design novel electrolyser and optimise operating conditions of electrolyser for improving its efficiency in terms of yield and energy consumption, particularly the structure of specific components of electrolysers, by means of conducting massive but cost- and time-effective numerical tests. Also, the newly developed materials and innovative reactor designs from the team members will be tested and optimised for the enhancement of system efficiency.

Knowledge gap
The interaction between numerical and experimental tests may be improved. The CFD simulations generated have been used for process understanding successfully and should be further applied to process optimisation.

Background
Objectives or project requirements
The objective of this project is to develop a robust and efficient numerical electrolyser model, which is employed to support the practical alkaline electrolyser efficiency improvement.

Process undertaken
To demonstrate the progress of the numerical model development and the capability of this model, the following part briefly illustrates some typical in-electrolyser phenomena in terms of the flow and species transfer during electrolysis. The subsequent large-scale computing and the summarised results will be reported in the near future.
A 2D transient lab-scale electrolyser model is developed, in which the function of membrane is introduced, and it controls the hydroxide transfer in the electrolyte flow. Figure 2 shows the flow regime, and the

species transfer occurred on both sides of membrane, where the only hydroxide goes through membrane and approaches to the electrode. The implement of membrane function bridges the last gap of comprehensive modelling electrolyser. Figure 3 (a) shows the internal structure of a typical electrolyser, which is modelled by the above-mentioned method and more components are introduced. Figure 3 (c and d) shows the preliminary simulation results of the hydrogen and oxygen molar fraction distribution in the serpentine electrolyte flow channel. Such simulation results directly reflect the performance of electrolyser. Consequently, the effects of material properties' variation, i.e., electrode and catalyst, and the operating conditions, such as electrolyte temperature and concentration, can be examined and evaluated flexibly.

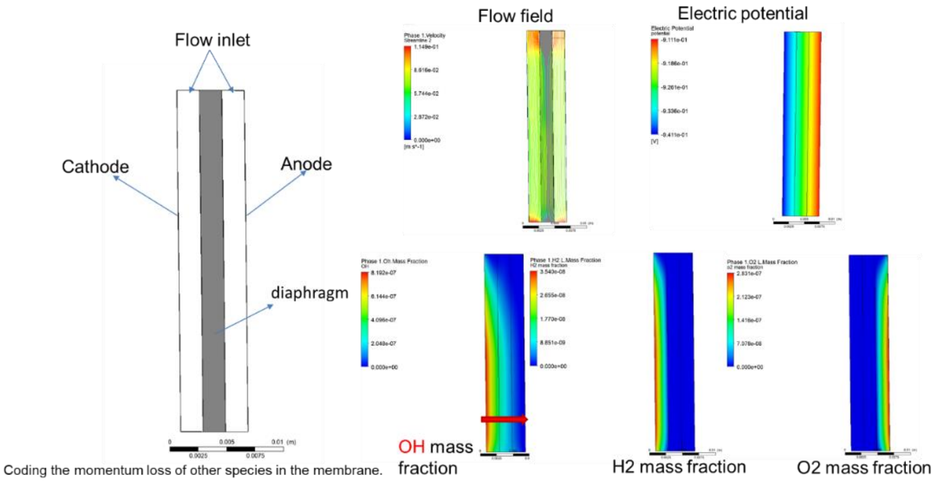

Figure 2 Simulation results under assumed operating conditions: flow regime and the species transfer occurred on both sides of membrane

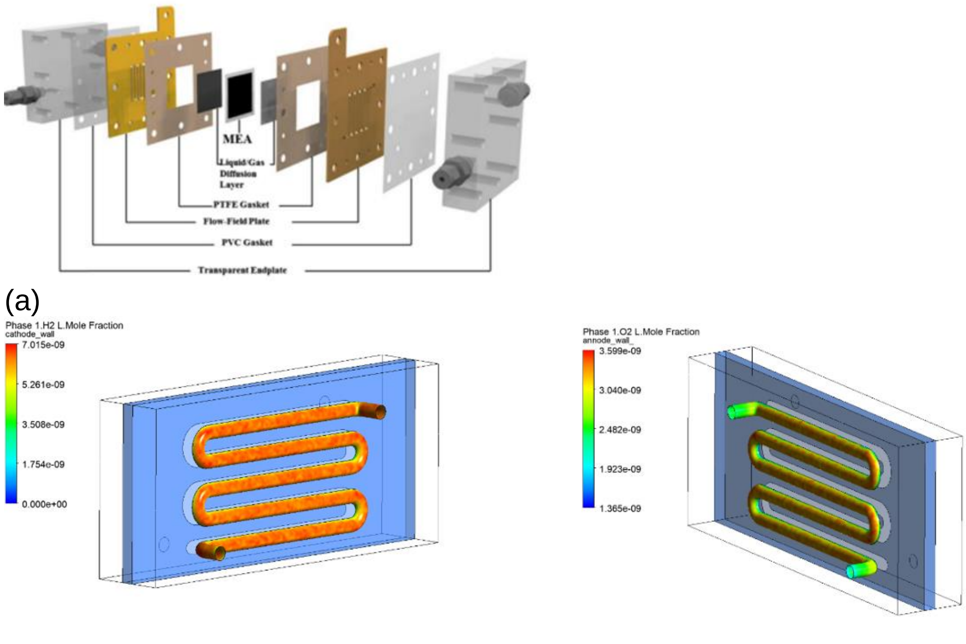

Figure 3 (a) Snapshot of the structural configuration of a typical electrolyser; (b) Simulated molar fraction of hydrogen in electrode channel; (c) Simulated molar fraction of oxygen in electrode channel

Lessons Learnt Report: Design, development and testing of lab-scale CPV solar cell-heat exchanger

Project name: Highly efficient and low cost photovoltaic-electrolysis (PVE) system to generate hydrogen by harvesting the full spectrum of sunlight

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Hydrogen R&D project
State/Territory:	NSW

Key Highlights

Development and testing of a first iteration concentrator photovoltaic (CPV) solar cell heatsink and electrolyser heat exchanger.

Achieved CPV system efficiency of 38% using a 1-cm^2 triple-junction CPV cell, including concentration optics and improved thermal contact between the CPV cell and heatsink.

Challenges

Compared to commercial scale, parasitic losses are relatively large for a lab scale system. The design of a next iteration lab scale heat transfer system with higher performance and lower parasitic loss requires detailed characterisation using high accuracy temperature, flow and pressure sensors. This is currently underway.

Implication for future projects

RayGen's experience designing, building and operating commercial scale CPV systems has shown that parasitic losses can be substantially reduced, so are not as big an issue as suggested by lab scale systems.

RayGen already has a highly developed CPV cell mounting approach, including excellent thermal contact between the CPV cells and heatsink to maintain the cells at a suitable operating temperature as well as provide useful by-product heat.

Knowledge gap

Demonstrate and quantify efficient heat transfer and minimal parasitics in a lab scale PVE system.

Determine what is the best method to transfer heat into the electrolyser cell stack

Background

Objectives or project requirements

To demonstrate enhanced performance of PVE (photovoltaic electrolysis) by the integration of a cogenerating PV system and an electrolyser with an enhanced catalyst. The performance of the electrolyser/catalyst is enhanced using by-product heat from the PV system to elevate its temperature, increasing hydrogen output at a given (low) voltage. This in turn reduces the amount of electricity required per kg of H_2 produced (Fig. 4) and the subsequent cost of renewable hydrogen. To effectively achieve this, the heat must be transferred from the PV system to the electrolyser with minimum parasitic losses.

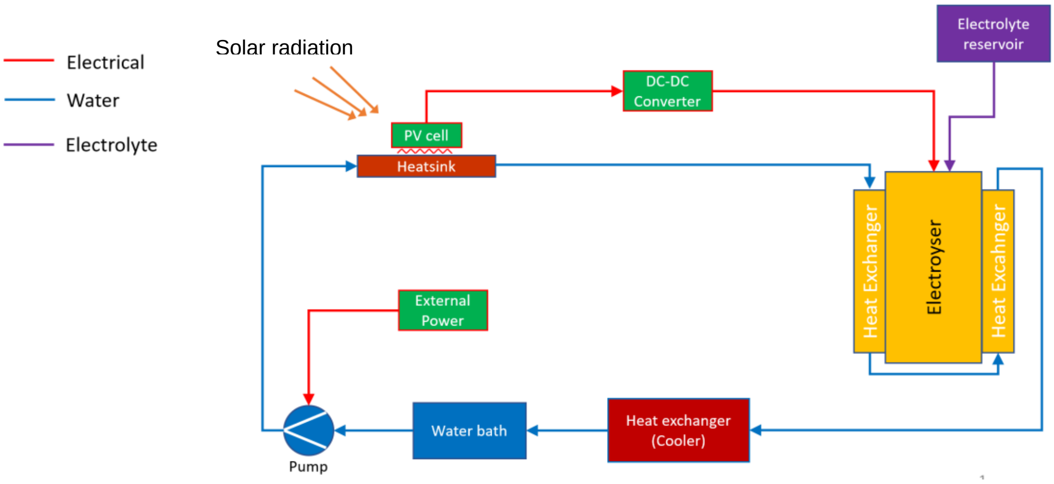

Fig. 4 Schematic layout of PV-powered electrolysis (PVE) including the use of by-product heat.

Process undertaken

Lab scale demonstration of PVE, targeting 30% solar-to-hydrogen efficiency.

COMMERCIALISATION PROSPECTS

In this project, novel catalyst materials are developed for both the anodic oxygen evolution reaction and cathodic hydrogen evolution reaction. These catalysts are low in material costs, while their activities are superior to their precious metal-based benchmarks (e.g. Iridium Oxide (IrO_x) for OER and Pt/C for HER). Besides that, novel and scalable manufacturing processes are employed in this project to produce electrodes with large surface area that can meet the commercial requirements. It is believed that water electrolysers assembled based on the electrodes developed in this project will lead to lower capital expenditures and higher energy efficiency, thereby leading to lower levelized costs for hydrogen to meet the target set by the Australian government in the National Hydrogen Strategy.

A commercial scale version of RayGen's co-generation technology has been demonstrated over many years, producing electricity and cheap useful by-product heat (Fig. 5). This system is suited to running commercial scale electrolyser systems at the temperatures of interest (70-90°C). A full scale test bed therefore already exists at RayGen in Australia to perform a side-by-side comparison of a commercial scale off-the-shelf alkaline electrolyser with one using the newly developed catalysts and by-product heat. The changes required of the existing RayGen system are relatively minor, and provided the new catalysts can be scaled up and swapped into the alkaline electrolyser, relative PVE performance boosts and reduced $/kg H2 of 20-30% are anticipated.

Figure 5. RayGen PV Ultra solar energy system. The output is 0.5 MW of electricity and 1 MW of by-product heat.

SUMMARY OF KNOWLEDGE SHARING ACTIVITES COMPLETED

Knowledge sharing activities on the project outcomes in addition to the Lessons Learnt report provided below include:

- Plenary/Keynote lectures by CI Amal at different international conferences including AMN9, New Zealand, February 2019, ICMAT 2019, Singapore, July 2019, ISECSM 2019, Brisbane, August 2019, ICONN 2020, February 2020.

- CI Amal also presented a breakfast seminar organised by NSW Chief Scientist and Engineer Office in February 2020.
- CI Lu attended the following conferences in 2019 and presented the work on OER and HER catalyst: 1st International Conference on Clean Technologies for a Blue Planet, and 18th Asian Pacific Confederation of Chemical Engineering Congress and workshops held in Shanghai Jiaotong University and Zhejiang University
- CI Amal is a member of the Conference Committee for the 4th Energy Futures (EF4) Conference. The conference was due to be held in Sydney on 27-29 May 2020. At this stage, due to COVID-19, the conference has been tentatively postponed to February 2021. EF4 includes Themes of Renewable Hydrogen and Energy Conversion amongst others. The website can be found at www.ausenergyfuture.com
- A paper titled '*Uncovering Atomic-Scale Stability and Reactivity in Engineered Zinc Oxide Electrocatalysts for Controllable Syngas Production'* recently published on Advanced Energy Materials, vol 10, 28, article 2001381: https://onlinelibrary.wiley.com/doi/full/10.1002/aenm.202001381