

**Sami S**

*Cardiff University  
School of Engineering*

**Qadrdan M**

*Cardiff University  
School of Engineering*

**Zhou Y**

*Cardiff University  
School of Engineering*

**Wu J**

*Cardiff University  
School of Engineering*

SUSTAINABLE ENERGY

# Modelling and Simulation of a Hydrogen-Based Energy Storage System

In this study, a mathematical model of a Hydrogen-based Energy Storage System (HESS) was developed. The HESS includes sub-models of a Polymer Electrolyte Membrane (PEM) water electrolyser stack, a PEM fuel cell stack, hydrogen storage tanks, a compressor and AC/DC converters. For validation, simulation results were compared to results reported in the literature. The model of the HESS can be used for power systems dynamic simulation studies, such as providing ancillary services to the power system operator.

*Keywords:*

*Hydrogen-based Energy Storage System, Proton Exchange Membrane electrolyser model, dynamic models.*

*Corresponding author:*

*SamiS1@cardiff.ac.uk*



S. Sami, Y. Zhou, M. Qadrdan, and J. Wu, 'Modelling and Simulation of a Hydrogen-Based Energy Storage System', *Proceedings of the Cardiff University Engineering Research Conference 2023*, Cardiff, UK, pp. 135-139.

[doi.org/10.18573/conf1.ae](https://doi.org/10.18573/conf1.ae)

## INTRODUCTION

Hydrogen has the potential to contribute to tackling the climate change and reducing CO<sub>2</sub> emissions in power systems. A Hydrogen-based Energy Storage System (HES) is a long-term storage solution to decarbonise power systems as the excess electricity from renewables can be stored for later use in the form of hydrogen.

In this study, models of the HES components were developed and verified against experimental data from the literature [1]. The HES model can be used for dynamic simulation studies, where the HES, for example, is providing frequency support services to the power system operator. As shown in Fig. 1, the HES consists of a Polymer Electrolyte Membrane or Proton Exchange Membrane (PEM) electrolyser stack, low-pressure and high-pressure hydrogen storage tanks, a two-stage hydrogen compressor and a PEM fuel cell stack. The modelling of the HES accessories, such as gases purification systems, pressure regulators and flow regulators, is beyond the scope of this study.

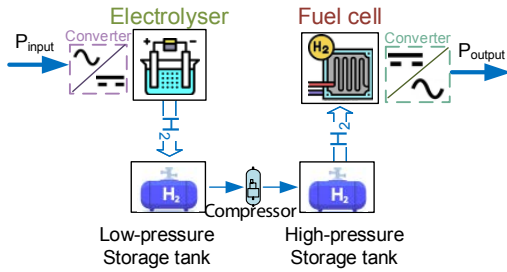


Fig. 1. The developed model of HES.

## MODELLING OF HES COMPONENTS

Electrolyser and fuel cells stacks are the key parts of HESs. This study focused on the modelling of the electrolyser as exactly the reverse electrochemical processes are occurring in the PEM fuel cells.

### Modelling of a PEM electrolyser stack

A mathematical model of the PEM electrolyser is developed based on [1-3]. Information listed in [1, 3] were based on HES projects in the USA and Germany. The dynamic model consists of three parts or sub-models, i.e. an electrochemical, hydrogen production and thermal sub-models. It is assumed that pressure effects and pressure drops are neglected, the temperature is uniform in the electrolyser stack and all cells have identical thermal behaviour [1]. Figure 2 shows the block diagram of the three sub-models of the developed electrolyser model. The dynamic behaviour of the thermal part impacts the other parts through the change in the temperature.

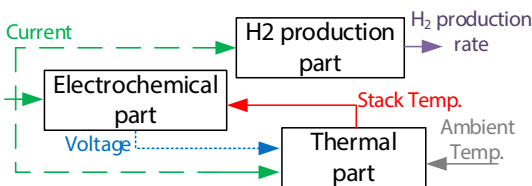


Fig. 2. The block diagram of interaction between the electrolyser sub-models.

### Electrochemical part

The electrochemical part represents the current-voltage characteristics of the electrolyser cell. The mathematical description of the electrolyser cell voltage is given in equation (1) [1, 2]:

$$V_{cell} = V_{OC} + V_{act} + V_{ohm} + V_{diff} \quad (1)$$

where  $V_{OC}$  is the open-circuit voltage (V),  $V_{act}$  is the activation overpotentials at the anode and cathode ( $V_{act}$ ),  $V_{ohm}$  is ohmic overpotential ( $V_{act}$ ),  $V_{diff}$  is the diffusion or concentration overpotential (V).

Nernst equation is used to compute the open-circuit voltage for water electrolysis [2]:

$$V_{OC} = E_{rev} + \frac{RT}{zF} \left[ \ln \left( \frac{p_{H_2} \sqrt{p_{O_2}}}{a_{H_2O}} \right) \right] \quad (2)$$

where  $E_{rev}$  is the reversible electrolyser cell voltage (V),  $R$  is the universal ideal gas constant (J/mol K),  $T$  is the electrolyser stack temperature (K),  $p_{O_2}$  and  $p_{H_2}$  are the partial pressures of oxygen and hydrogen (Pa),  $a_{H_2O}$  is the water activity between electrode and membrane,  $z$  is the number of moving electrons and  $F$  is Faraday's constant (A sec/mol).

The reversible voltage equals 1.229 V at standard temperature and pressure conditions. At other temperatures, it can be determined by [2]:

$$E_{rev} = 1.229 - 0.9 \times 10^{-3} (T - 298) \quad (3)$$

The activation overpotential or overvoltage describes the speed of the reactions taking place at the electrode surface. As electrons are transferred to or from the electrodes, part of the applied voltage is lost [2]. Different representations of the activation overpotential were found in literature, and Tafel correlation was adopted in this research [1]:

$$V_{act} = \frac{RT}{\alpha_{act} z F} \left[ \ln \left( \frac{i}{i_0} \right) \right] \quad (4)$$

where  $\alpha_{act}$  is the charge transfer coefficient,  $i_0$  in (A/m<sup>2</sup>) is exchange current density and  $i$  in (A/m<sup>2</sup>) is the electrolyser stack current density, which is calculated by [1]:

$$i = \frac{I}{A_{cell}} \quad (5)$$

where  $I$  in (A) is the electrolyser stack current and  $A_{cell}$  in (m<sup>2</sup>) is the electrolyser cell active area. The value of the charge transfer coefficient and the exchange current density were extracted from experimental data using non-linear regression analysis because the materials of the catalyst were unknown [1]. Additionally, the kinetics of the hydrogen reactions at the cathode occur faster than the kinetics of the oxygen reactions at the anode, and hence the activation overpotentials at the cathode are neglected [1].

The ohmic overvoltages or overpotentials are caused by the ohmic resistance of the bipolar plates, electrolytes and surfaces of the electrodes [1, 2]. Since the membrane resistance is about 10 times bigger than other resistances, other resistances are neglected in this research [1]. This study adopts the empirical correlations proposed by [4]:

$$V_{ohm} = \frac{t_m i}{\sigma_m} \quad (6)$$

where  $t_m$  in (m) is the membrane thickness and  $\sigma_m$  in (S/m) is the membrane conductivity.  $\sigma_m$  is a function of the protonic exchange, which in turn is a function of the temperature:

$$\sigma_m = (0.005139\lambda_m - 0.00326)e^{\left[1268\left(\frac{1}{303} - \frac{1}{T}\right)\right]} \quad (7)$$

where  $\lambda_m$  is the average membrane water content. It is considered that the membrane is completely saturated with water, and hence a value of 17 represents good hydration [1].

The diffusion or concentration overpotential or overvoltage occurs due to the mass transfer process that changes the concentration of the reactants at the surfaces of the electrodes [1, 2]. The diffusion overpotential can be described by [1]:

$$V_{diff} = \frac{RT}{\beta 2F} \left[ \ln \left( 1 + \frac{i}{i_{lim}} \right) \right] \quad (8)$$

where  $\beta$  is an empirical coefficient and  $i_{lim}$  in (A/m<sup>2</sup>) is called limit current density. Both values were extracted from experimental data using non-linear regression techniques [1].

#### Hydrogen production part

The production rate of the hydrogen is directly proportional to the transfer rate of electrons at the electrodes, according to Faraday's law [1-3]. For an electrolyser of ( $n$ ) cells connected in series, the hydrogen production rate ( $\dot{n}_{H_2}$ ) in (mol/s) is expressed by:

$$\dot{n}_{H_2} = \eta_F \frac{nI}{2F} \quad (9)$$

where  $\eta_F$  is Faraday's efficiency. Faraday's efficiency is the ratio of the actual to theoretical maximum amount of hydrogen produced by the electrolyser. This efficiency is often called current efficiency as it is caused by parasitic current losses along the gas ducts in the cell block [5]. Faraday's efficiency empirical expression is [1]:

$$\eta_F = -0.0922 + 0.0091I + 0.00003I^2 - 0.0000003I^3 \quad (10)$$

#### Thermal part

An equivalent thermal parameters model is used to simulate the overall thermal energy balance in the electrolyser cells stack [3]. An electrical analogy is used to represent the potential of heat storage in the electrolyser cells by a capacitance and heat transfer resistance from the cells to the surrounding. The rate of internal thermal energy generated (i.e.  $\dot{Q}_{gen}$  in W) in the electrolyser due to inefficiencies is partly stored in the surrounding mass (i.e.  $\dot{Q}_{store}$  in W). Part of the generated thermal energy is lost or transferred to the ambient (i.e.  $\dot{Q}_{loss}$  in W). A water-based auxiliary cooling system is assumed, which is responsible for transferring another part of the generated thermal energy to maintain the stack temperature stable (i.e.  $\dot{Q}_{cool}$  in W). The overall thermal energy balance is represented by:

$$\dot{Q}_{store} = \dot{Q}_{gen} - \dot{Q}_{loss} - \dot{Q}_{cool} \quad (11)$$

$$\dot{Q}_{store} = C_{th} \frac{dT}{dt} \quad (12)$$

$$\dot{Q}_{gen} = n(V_{cell} - V_{th})I \quad (13)$$

$$\dot{Q}_{loss} = \frac{T - T_a}{R_{th}} \quad (14)$$

$$\dot{Q}_{cool} = C_{cw}(T_{cw,i} - T_{cw,o}) = UA_{HX}LMTD \quad (15)$$

where  $C_{th}$  is the heat capacity of the electrolyser stack (J/°C),  $T_a$  is the ambient temperature (°C),  $R_{th}$  is the equivalent thermal resistance (°C/W),  $V_{th}$  is the thermoneutral voltage,

$C_{cw}$  is the heat capacity of the water used for cooling per second (W/°C),  $T_{cw,i}$  is the inlet temperature of the cooling water (°C),  $T_{cw,o}$  is the outlet temperature of the cooling water (°C),  $UA_{HX}$  is the effective heat exchange coefficient for the cooling process, which is the product of the heat transfer coefficient by the exposed surface area (W/°C), LMTD is the Logarithmic Mean Temperature Difference between the cold and hot feeds at each end of the auxiliary cooling system (°C).

The capacity and resistance can be estimated experimentally using heating curves and they are related to the rated power of the electrolyser [1]. Based on values found in the literature [1], an average value of (3 J/°C W) for the capacity and (0.09 °C/W) for the resistance were considered [1]. Hence, for a 6 kW PEM electrolyser, 21 kJ/°C of thermal capacity and 0.09 °C/W of thermal resistance were considered.

The effective heat transfer coefficient can be calculated in terms of the electrolyser current, an empirical expression that considers the heat transfer by heat conduction and convection is used [3]:

$$UA_{HX} = a_{cond} + I b_{conv} \quad (16)$$

where  $a_{cond}$  is the conductive heat exchange coefficient (W/°C) and  $b_{conv}$  is the convective heat exchange coefficient (W/°C A). The LMTD is calculated by:

$$LMTD = \frac{(T_{cell} - T_{cw,i}) - (T_{cell} - T_{cw,o})}{\ln \left( \frac{T_{cell} - T_{cw,i}}{T_{cell} - T_{cw,o}} \right)} \quad (17)$$

If the LMTD is assumed to be of a constant temperature, the outlet temperature of the cooling water is:

$$T_{cw,o} = T_{cw,i} + (T_{cell} - T_{cw,i}) \left[ 1 - e^{-\frac{UA_{HX}}{C_{cw}}} \right] \quad (18)$$

It was assumed that the water-based auxiliary cooling system is identical to the system reported in the literature [3, 6]. Hence, the same model parameters were used. Table 1 list the values used for all parameters of the electrolyser.

#### Modelling of hydrogen storage tanks

Two tanks were assumed to store the produced hydrogen. Figure 3 shows the block diagram of both tanks and the hydrogen compressor.

##### Low and high-pressure storage tanks

It was assumed that the temperature of the stored hydrogen in both tanks is kept constant, i.e. equal to the electrolyser temperature during the production of the hydrogen, using cooling and heating processes. However, the cooling and heating processes are out of this research scope. The Beattie-Bridgeman equation was used to describe the relationship between values of the pressure, volume and temperature in both storage tanks, as follows [7]:

$$p_{tank} = \frac{\dot{n}_{H_2}^2 RT}{V_{tank}^2} \left[ 1 - \frac{c \dot{n}_{H_2}}{V_{tank} T^3} \right] \left[ \frac{V_{tank}}{\dot{n}_{H_2}} + B_0 \left( 1 - \frac{b \dot{n}_{H_2}}{V_{tank}} \right) \right] - \frac{A_0 \left( 1 - \frac{a \dot{n}_{H_2}}{V_{tank}} \right) \dot{n}_{H_2}^2}{V_{tank}^2} \quad (19)$$

where  $p_{tank}$  in (atm) is hydrogen pressure in the tank,  $V_{tank}$  in (litre) is the volume of the tank and  $a$ ,  $b$ ,  $c$ ,  $A_0$ ,  $B_0$  are constants, for hydrogen gas they are (-0.00506 litre/mol, -0.04359 litre/mol, 504 litre·K<sup>3</sup>/mol, 0.1975 atm litre<sup>2</sup>/mol<sup>2</sup>, 0.02096 litre/mol respectively).

The ideal gas law [5] was used to estimate the amount of hydrogen stored in both tanks:

$$n_{H_2} = \frac{p_{\text{tank}} V_{\text{tank}}}{RT} \quad (20)$$

where  $n_{H_2}$  in (mol) is the total amount of gas,  $p_{\text{tank}}$  is in Pa,  $V_{\text{tank}}$  is in  $m^3$ ,  $T$  is in K and  $R$  is in  $kPa \cdot m^3 / kmol \cdot K$  [8]. For the volume of  $25 m^3$ , the buffer or low-pressure tank can hold approximately  $245 Nm^3$  (10.91 kmol), i.e. when the pressure is 13 bar and the temperature is  $85^\circ C$  (i.e. close to the electrolyser temperature at the rated power of 6 kW). While the volume of the high-pressure tank of  $26 m^3$  can hold approximately  $2349 Nm^3$  (104.8 kmol), i.e. when the pressure is 120 bar and the temperature is  $85^\circ C$ .

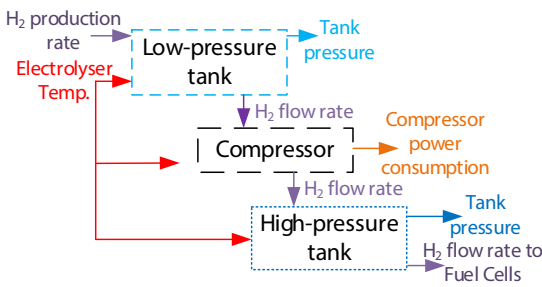


Fig. 3. The block diagram of the interaction between storage tanks and the compressor models.

**Table 1.** The values of parameters of the electrolyser.

$E_{\text{rev}}$ (at standard conditions)	1.229 V	$R_{\text{th}}$	$0.09^\circ C/W$
$R$	$8.3145 J / mol K$	$i_{\text{lim}}$	$1401 A/m^2$
$V_{\text{th}}$ (at standard conditions)	1482 V	$F$	$96485 A \text{ sec} / mol$
$z$	2	$C_{\text{th}}$	$21 kJ/^\circ C$
$\alpha_{H_2O}$	1	$T_a$	$20^\circ C$
$\alpha_{\text{act}}$	0.5316	$\beta$	0.315
$i_0$	$0.0004576 A/m$	$C_{\text{cw}}$	$697.67 W/^\circ C$
$t_m$	$0.00003306 m$	$b_{\text{conv}}$	$0.02 W / (^\circ C \cdot A)$
$\lambda_m$	17	$T_{\text{cw}_i}$	$14.5^\circ C$

Table 1. The values of parameters of the electrolyser.

#### Hydrogen compressor

A model of a two-stage polytropic compressor reported in [5] was adopted. The work done by the compressor ( $P_{\text{compressor}}$ ) in (W) is [5]:

$$P_{\text{compressor}} = \frac{\eta_{H_2} (P_{\text{stage 1}} + P_{\text{stage 2}})}{\eta_{\text{compressor}}} \quad (21)$$

$$P_{\text{stage 1}} = \frac{k_{\text{plt}} R T}{k_{\text{plt}} - 1} \left[ 1 - \left( \frac{p_x}{P_{\text{stage 1}}} \right)^{\left( \frac{k_{\text{plt}} - 1}{k_{\text{plt}}} \right)} \right] \quad (22)$$

$$P_{\text{stage 2}} = \frac{k_{\text{plt}} R T}{k_{\text{plt}} - 1} \left[ 1 - \left( \frac{P_{\text{stage 2}}}{p_x} \right)^{\left( \frac{k_{\text{plt}} - 1}{k_{\text{plt}}} \right)} \right] \quad (23)$$

$$p_x = \sqrt{P_{\text{stage 1}} + P_{\text{stage 2}}} \quad (24)$$

where  $\eta_{\text{compressor}}$  is the compressor efficiency (equal 63% [9]),  $k_{\text{plt}}$  is the polytropic coefficient (equal 1.4),  $p_x$  in (Pa) is the intermediate stage pressure,  $P_{\text{stage 1}}$  in (Pa) is the first stage pressure (i.e. 1300 kPa (equal 13 bar)) and  $P_{\text{stage 2}}$  in (Pa) is the second stage pressure (i.e. 12000 kPa (equal 120 bar)).

A compressor controller was modelled based on [5]. The compressor follows a simple controlling approach: it is switched ON when the pressure in the buffer tank rises above 10 bar and switched OFF when the buffer tank pressure drops below 6 bar. The compressor works with a constant hydrogen flow rate of  $5 Nm^3/h$ . The compressed hydrogen is stored in the high-pressure tank, as shown in Fig. 3.

#### Fuel cells stack model

The dynamic model of a fuel cell stack available in Simulink/Matlab® library was adopted in this study.

#### Modelling of AC/DC converters

Since both stacks of electrolyser cells and fuel cells are operating using the DC voltage, AC to DC converters are required. A simplified model of AC/DC converters developed in [10] was used.

## SIMULATION RESULTS AND VALIDATION

The model of electrolyser was validated by comparison with experimental results from the literature and Root Mean Square Error (RMSE) was used to indicate the difference between the results. The data reported in [1] were presented in graphic form, and hence extracted data accuracy from these publications might be affected slightly. Regarding the validation of models of storage tanks and the compressor, the different experimental conditions in [5, 7] prevented the direct comparison of the results. The validation of the PEM electrolyser model was carried out by comparing polarization and hydrogen production curves against experimental data from a project in the USA [1]. Figure 4 shows the hydrogen production rate of the electrolyser, and the RMSE value is  $0.0044 Nm^3/h$ . Figure 5 depicts the V-I characterisation (polarisation) curve of the electrolyser, and the RMSE value is  $0.027 V$ .

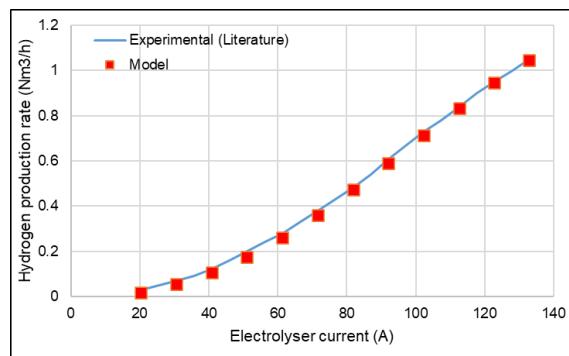


Fig. 4. The hydrogen production rate of the electrolyser.

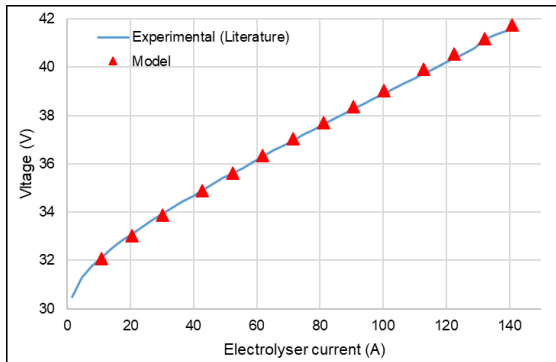


Fig. 5. The polarisation curve of the electrolyser.

## CONCLUSIONS

Models of the components of a HESS, i.e. an electrolyser, hydrogen storage tanks and hydrogen compressor were developed, simulated and validated based on data reported in the literature. The model of the HESS can be used for dynamic simulation studies of power systems.

### Acknowledgements

This work has been carried out in the framework of the European Union's Horizon 2020 research and innovation program under grant agreement No 957852 (Virtual Power Plant for Interoperable and Smart isLANDS'- VPP4ISLANDS). The work was also supported by FLEXIS, i.e. a project part-funded by the European Regional Development Fund (ERDF) through the Welsh Government (WEFO case number 80836).

### Conflicts of interest

The authors declare no conflict of interest.

## REFERENCES

- [1] P. Fragiaco and M. Genovese, 'Modeling and energy demand analysis of a scalable green hydrogen production system', *International Journal of Hydrogen Energy*, vol. 44, no. 57, pp. 30237–30255, Nov. 2019. doi.org/10.1016/j.ijhydene.2019.09.186
- [2] Z. Abidin, C. J. Webb, and E. MacA. Gray, 'Modelling and simulation of a proton exchange membrane (PEM) electrolyser cell', *International Journal of Hydrogen Energy*, vol. 40, no. 39, pp. 13243–13257, Oct. 2015. doi.org/10.1016/j.ijhydene.2015.07.129
- [3] Ø. Ulleberg, 'Modeling of advanced alkaline electrolyzers: a system simulation approach', *International Journal of Hydrogen Energy*, vol. 28, no. 1, pp. 21–33, Jan. 2003. doi.org/10.1016/S0360-3199(02)00033-2
- [4] T. E. Springer, T. A. Zawodzinski, and S. Gottesfeld, 'Polymer Electrolyte Fuel Cell Model', *Journal of the Electrochemical Society*, vol. 138, no. 8, pp. 2334–2342, Aug. 1991. doi.org/10.1149/1.2085971
- [5] Ø. Ulleberg, 'Stand-Alone Power Systems for The Future: Optimal Design, Operation and Control of Solar-Hydrogen Energy Systems', PhD, Norges teknisk-naturvitenskapelige universitet, Norway, 1999.
- [6] M.H. Nehrir, C. Wang, *Modeling and Control of Fuel Cells: Distributed Generation Applications*, John Wiley & Sons, USA, 2009. doi.org/10.1109/9780470443569
- [7] C. Wang, 'Modeling and Control of Hybrid Wind/ Photovoltaic/Fuel Cell Distributed Generation Systems', PhD, Montana State University, USA, 2006.
- [8] Y.A. Cengel, M.A. Boles, *Thermodynamics: an Engineering Approach*, McGraw-hill, USA, 9<sup>th</sup> ed, 2018.
- [9] T. Zhou and B. Francois, 'Modeling and control design of hydrogen production process for an active hydrogen/wind hybrid power system', *International Journal of Hydrogen Energy*, vol. 34, no. 1, pp. 21–30, Jan. 2009. doi.org/10.1016/j.ijhydene.2008.10.030
- [10] S. Sami, 'Virtual Energy Storage for Frequency and Voltage Control', PhD, Cardiff University, UK, 2017.

*Proceedings of the Cardiff University Engineering Research Conference 2023* is an open access publication from Cardiff University Press, which means that all content is available without charge to the user or his/her institution. You are allowed to read, download, copy, distribute, print, search, or link to the full texts of the articles in this publication without asking prior permission from the publisher or the author.

Original copyright remains with the contributing authors and a citation should be made when all or any part of this publication is quoted, used or referred to in another work.

E. Spezi and M. Bray (eds.) 2024. *Proceedings of the Cardiff University Engineering Research Conference 2023*. Cardiff: Cardiff University Press.  
[doi.org/10.18573/conf1](https://doi.org/10.18573/conf1)

*Cardiff University Engineering Research Conference 2023* was organised by the School of Engineering and held from 12 to 14 July 2023 at Cardiff University.

The work presented in these proceedings has been peer reviewed and approved by the conference organisers and associated scientific committee to ensure high academic standards have been met.

First published 2024

Cardiff University Press  
Cardiff University, PO Box 430  
1st Floor, 30-36 Newport Road  
Cardiff CF24 0DE

[cardiffuniversitypress.org](https://cardiffuniversitypress.org)

Editorial design and layout by  
Academic Visual Communication

ISBN: 978-1-9116-5349-3 (PDF)



This work is licensed under the Creative Commons Attribution - NoCommercial - NoDeriv 4.0 International licence.

This license enables reusers to copy and distribute the material in any medium or format in unadapted form only, for noncommercial purposes only, and only so long as attribution is given to the creator.

<https://creativecommons.org/licenses/by-nc-nd/4.0/>