The Sydney Journal of Interdisciplinary Engineering
SJIE 1(4) X–X (2025) https://doi.org/XXXX/XXXX

Focused Review of Recent Modelling Strategies in Power-to-X Systems for Renewable Energy Storage in Smart Grids

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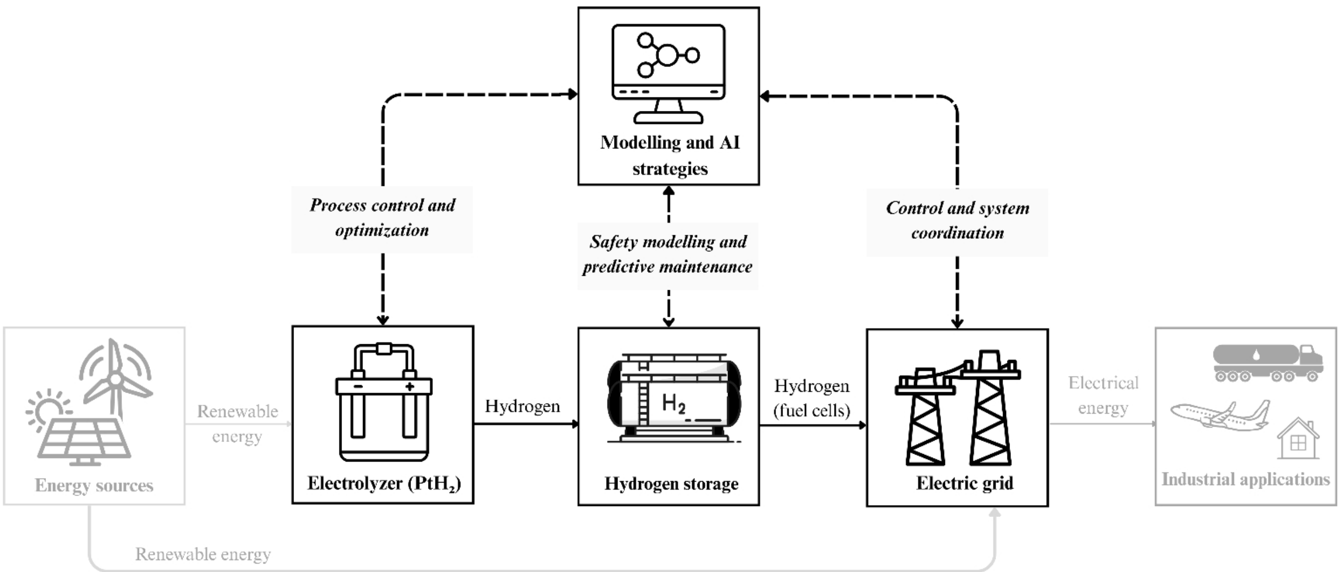
Received xxxxxx
Accepted for publication xxxxxx
Published xxxxxx

Graphical Abstract



Abstract

The variability of renewable energy sources presents a major challenge for maintaining power system stability and long-duration energy storage. Power-to-Hydrogen (PtH_2) systems provide a viable solution by converting surplus renewable into hydrogen, which can be stored and used across different sectors. This review focuses on focuses on modelling strategies applied to three core PtH_2 processes: hydrogen production via electrolysis, storage, and integration into smart grids. Traditional modelling approaches including computational fluid dynamics (CFD), techno-economic analysis (TEA), process simulation, and linear programming (LP) remain essential for system design but are limited in handling dynamic, real-time operations. In contrast, emerging methods including machine learning (ML), reinforcement learning (RL), surrogate modelling, digital twins, and augmented/virtual reality (AR/VR) platforms offer improved adaptability, predictive control, and operator interaction. However, these tools face limitations related to data availability, computational cost, model interpretability, and integration with existing simulation environments. The review identifies a growing shift toward hybrid modelling frameworks that combine physical accuracy with data-driven adaptability. Future research should focus on building standardised datasets, developing interoperable modelling platforms, expanding the role of real-time visualisation technologies, and must be supported not only by technical innovation but also by evolving policy for scalable and resilient PtH_2-integrated smart grid.

Keywords: Power-to-X (P2X), Power-to-Hydrogen (PtH_2), renewable energy storage, smart-grids, advanced modelling, computer simulations, artificial intelligence, machine learning, AR/VR

1. Introduction

The global energy transition is accelerating the deployment of renewable energy sources such as solar and wind[1]. However, their inherent variability introduces operational challenges to modern power systems, particularly in ensuring consistent supply and grid stability.[1] Energy storage technologies have become central to enabling reliable and flexible renewable integration.[2]

Power-to-Hydrogen (PtH_2) has emerged as a promising long-duration energy storage solution.[3-5] By converting renewable energy into hydrogen via electrolysis, PtH_2 enables energy to be stored in chemical form and later utilised across sectors, including electricity, transport, and industrial applications[5]. Unlike conventional battery storage, hydrogen offers higher storage capacity over longer timescales, making it suitable for seasonal balancing and sector coupling.[6]

Recent research has increasingly focused on modelling strategies that support the deployment of PtH_2 systems. Advanced simulations and AI-augmented tools are now being used to enable dynamic integration with smart grid, optimise conversion efficiency and assess techno-economic viability, and enable dynamic integration with smart grids.[7-8] Despite increased attention, few reviews have synthesized the full modelling stack from electrolyis to grid-scale integration.[7]

This review aims to synthesise emerging modelling approaches applied to PtH_2 systems, with emphasis on processes involving energy conversion, compression and storage, and smart grid integration.

2. Modelling strategies across the PtH_2 system

PtH_2 systems core processes include hydrogen production, storage, and electric grid integration, each requires specialised modelling approaches to optimize performance, cost, and control. This section reviews emerging modelling strategies applied at each stage, with particular emphasis on process-level simulations, safety and reliability, and system coordination models. Comparative summaries and case studies are provided to illustrate how these methods are applied in practice and to highlight their respective advantages and limitations.

2.1 Electrolysis process control and optimization

Hydrogen production via electrolysis is the foundational process in PtH_2 systems. Electrolysis enables the conversion of electrical energy typically from renewable energy sources

Table 1 | Traditional and emerging models used in electrolysis systems control and optimization

Type	Approach	Strengths	Limitations	Tools	Ref.
Traditional	Computational Fluid Dynamics (CFD)	High spatial detail; flow and heat analysis	Computationally expensive	COMSOL, ANSYS	[12,18]
	Process Simulation + Techno-economic assessment (TEA)	System-wide modelling; cost-analysis	Rigid to variable input; limited real-time use	Aspen Plus	[13,19]
	Numerical optimization	Effective for tuning and design refinement	Requires well-defined objectives	MATLAB	[13,20]
	Monte Carlo simulation	Captures uncertainty	Requires many runs; less mechanistic	Python, MATLAB	[14,20]
Emerging	Machine Learning (ML)	Fast and adaptive forecasting	Needs large, quality datasets	TensorFlow	[15,21]
	Reinforcement Learning (RL)	Real-time adaptive control under fluctuating inputs	Complex training and policy validation	OpenAI Gym, Stable Baselines	[15,22]
	Surrogate models	Reduces simulation time; enables real-time control	Accuracy limited to trained domain	GPFlow, surrogateML	[12,15]
	AR/VR + Digital twins	Visual diagnostics and operator training	High development cost	Unity	[16,17]

into chemical energy by splitting water into hydrogen and oxygen[9]. The most common types of water electrolysis technologies include Alkaline Water Electrolysis (AEL), Proton Exchange Membrane Electrolysis (PEM), Solid Oxide Electrolyser Cell (SOEC), Anion Exchange Membrane Electrolysis (AEM).[10] These technologies differ in terms of operating temperature, response time, system complexity, and integration potential with variable power inputs.[10-11] These factors influence the selection and design of appropriate modelling strategies for control and optimization.

Table 1 outlines different modelling approaches applied to electrolysis system control and optimisation. Traditional methods such as CFD are used to analyze thermal gradients, flow behaviour, and gas evolution in electrolyser cells[12]. These models provide high physical accuracy but are computationally intensive and limited to offline analysis. At the system level, process simulation combined with TEA supports performance evaluation and cost estimation under different scenarios.[13] However, these models assume fixed input profiles and are not suited for dynamic control. Numerical optimization is used to refine design and operating parameters but requires well-defined objectives and may converge to local minima.[13] Monte Carlo simulations quantify uncertainties in cost drivers or input variability, though they do not capture time-dependent system dynamics.[14]

To address the limitations of static modelling approaches, recent studies have adopted data-driven methods. ML methods such as Artificial Neural Networks (ANN) was used for predicting stack performance and hydrogen output using operational or simulation data.[15,21] These models improve prediction speed but require large, well-labelled datasets. Reinforcement learning (RL) has also been applied for adaptive electrolyser control under fluctuating power inputs, though it demands complex training environments.[15] Surrogate models, derived from CFD or system simulations, are employed for fast approximation in control applications[12]. These are often integrated into digital twins, which combine physical models with real-time data to support diagnostics and optimisation. Moreover, emerging AR and digital twin platforms provide visual interfaces for system monitoring and operator support. While still limited in deployment, these tools have shown potential for training and real-time fault identification.[16]

A recent study[12] integrated CFD and AI and ML-based modeling for enhanced alkaline water electrolysis cell performance for hydrogen production. CFD was coupled with an ANN surrogate model to predict current density in an alkaline electrolyser, reducing simulation time by over 90% while maintaining accuracy demonstrating the advantage of combining physical and data-driven methodologies.

Traditional models remain essential for system design and validation, while emerging approaches improve adaptability and control. Integrating both supports more efficient and robust electrolysis under variable operating conditions.

2.2 Hydrogen storage safety and reliability

Hydrogen storage refers to the containment of hydrogen following its production, through electrolysis, for later use in

Table 2 | Traditional and emerging models used in PtH_2 hydrogen storage safety and reliability

Type	Approach	Strengths	Limitations	Tools	Ref.
Traditional	Finite Element Modelling (FEM)	Structural stress, fatigue, and failure analysis	High setup time, not real-time	ANSYS, Abaqus	[27]
	CFD	Thermal gradient and gas flow simulation	Computationally intensive	COMSOL Multiphysics	[27,28]
	Thermodynamic modelling	Pressure–temperature relationships	Oversimplifies dynamic system behaviour	MATLAB	[29]
Emerging	ML (SVM, ANN)	Fault and anomaly detection	Data quality and availability	MATLAB, Scikit-learn	[23,30]
	Digital twins	Integrated real-time monitoring and simulation	Complex integration, early-stage adoption	Unity, TensorFlow	[31]
	IoT-based monitoring and predictive analytics	Real-time condition tracking and decision support	Sensor dependency; integration complexity	IoT sensors, predictive algorithms	[32]

energy conversion, industrial processes, or transport.[23] Hydrogen produced via electrolysis is commonly stored as compressed gas in tanks or vessels.[24,26] These systems operate under conditions involving high pressure, temperature gradients, and cyclic loading, which introduce risks related to leakage, structural fatigue, and material degradation. While modelling of electrolysis systems often prioritises process optimisation, modelling of storage primarily addresses structural integrity, safety, and system reliability.[23] Predictive modelling supports the identification of failure modes and degradation trends, informing maintenance schedules and system design. As such, current modelling approaches for [illegible] behaviour and enabling condition-based monitoring under variable operating conditions.[25]

Table 2 summarises traditional and emerging modelling approaches applied to hydrogen storage, with a focus on safety, structural reliability, and predictive maintenance. Traditional techniques such as FEM, CFD, and thermodynamic analysis are widely used to assess stress distribution, fatigue, thermal behaviour, and pressure–temperature relationships in storage systems.[27-29] FEM provides detailed insight into structural integrity under cyclic loading, while CFD enables thermal and flow field simulation. Although physically robust, these models are computationally intensive and are not well suited to dynamic or real-time applications. Thermodynamic models offer simplified assessments but may fail to capture transient behaviour under variable conditions. On the other hand, emerging approaches integrate data-driven and system-level methods to improve adaptability and fault prediction. ML algorithms, including support vector machines (SVM) and ANN, have been used for anomaly detection, failure classification, and degradation forecasting from operational sensor data.[23,30] Digital twins extend these capabilities by linking virtual models with live input data to enable real-time condition monitoring and diagnostics. Moreover, IoT-based platforms further support storage reliability by enabling continuous sensor-driven tracking and data-informed decision support. While these methods offer greater responsiveness, they depend on stable data infrastructure and integration with physical systems.[32]

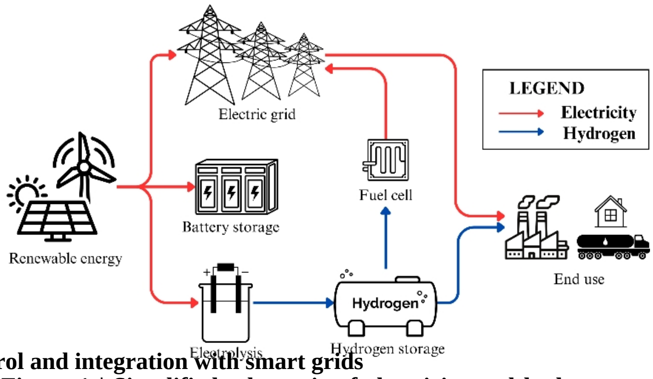


Figure 1 | Simplified schematic of electricity and hydrogen [illegible] is directed to the grid, battery storage, or electrolysis. The hydrogen produced is stored and later used in end-use applications or reconverted to electricity via fuel cells, which are reintegrated into the electric grid during peak demand periods. *Figure by*

Table 3 | Traditional and emerging models used for hydrogen storage control and integration with smart grids

Type	Approach	Strengths	Limitations	Tools	Ref.
Traditional	Rule-based dispatch and scheduling	Easy setup for fixed hydrogen dispatch routines	Cannot adapt to real-time or dynamic events	Excel-based	[41]
	MILP and LP optimization	Generates optimal hydrogen operation schedules with grid inputs	Rigid; not responsive to live grid or market shifts	Solver, Python	[42]
	Deterministic grid simulation	Models grid impact of hydrogen reconversion accurately	Limited for fast, multi-energy coordination	MATLAB	[43]
Emerging	Deep RL	Adapts hydrogen control to real-time grid conditions	Needs large training data and careful tuning	Custom RL framework	[44,45]
	Digital twins	Aligns physical and virtual hydrogen systems for control monitoring	High setup cost; integration remains complex	MATLAB, LabView	[46]
	AR/VR for system visualisation and operator training	Enhances operator awareness for dispatch and fault scenarios	Not embedded in real-time control; interface dependent	Custom VR platforms	[47,48]

An example of integrating traditional and emerging methods is presented by El-Amin et al.[37], who combined CFD-generated hydrogen dispersion data with machine learning models, specifically Random Forest and SVM, to predict concentration profiles in turbulent buoyant jets. The framework reduced computational load while maintaining prediction accuracy, enabling real-time inference for leak detection and storage safety. The system demonstrated predictive capabilities that enhanced operational safety and informed timely maintenance decisions.

The integration of traditional modelling with AI-based approaches enhances the safety and reliability of hydrogen storage systems within PtH_2 operations, offering a pathway toward more resilient and intelligent infrastructure.

2.3 Smart grid control and coordination

The integration of hydrogen storage into smart grids important in accommodating the increasing penetration of intermittent renewable energy sources.[39] Hydrogen storage systems such as PtH_2 technologies, which converts excess renewable electricity into storable hydrogen are essential element for grid balancing and providing long-duration seasonal energy storage, offering capabilities for bulk storage and practically infinite energy storage capacity.[10] However, these hydrogen systems, comprising components like electrolyzers, storage tanks, and fuel cells, are inherently complex to operate.[39] Figure 1 provides a conceptual overview of the typical energy flow in PtH_2-integrated smart grid systems and rather than representing a linear process, the diagram aims to foreground the complex, multi-pathway nature of energy conversion, storage, and utilisation in a hydrogen-augmented energy system.[40]

The complexity of the process coupled with the challenges of integrating variable renewable generation makes modelling techniques indispensable[6]. Accurate and dynamic modelling is essential to characterize efficiency, analyse dynamic behaviour, perform complex optimizations, capture real-world complexities, and manage real-time energy flows.[7,13]. This necessitates advanced control and coordination strategies for optimal operation.[39] Modelling serves as a tool to support the design and evaluation of these control and coordination systems[13] and addressing these challenges effectively requires the application of both traditional and emerging methods.[7,16]

Table 3 summarizes representative traditional and emerging modelling approaches applied in the coordination and control of hydrogen storage systems within smart grid environments. These models vary in computational complexity, real-time adaptability, and integration capacity.

Conventional modelling approaches such as rule-based scheduling, mixed-integer linear programming (MILP) and linear programming (LP), and deterministic grid simulation have historically formed the basis of hydrogen dispatch and grid interaction modelling.[41-43] These techniques are deterministic in structure and generally assume perfect foresight, static grid inputs, and isolated sub-system control. For example, MILP has been used to compute optimal hydrogen operation plans based on pre-defined load forecasts and tariff structures, but lacks responsiveness under real-time fluctuations or market variability.[42] Similarly, deterministic simulation models accurately compute hydrogen reconversion impacts on power system stability and power flow (e.g., voltage deviations), yet are limited in resolving multi-energy coordination or stochastic influences.[43] Furthermore, rule-based dispatch, often implemented in Excel-based methods which provides operational simplicity but cannot adapt to dynamic system feedback or uncertainty.[41] These methods are computationally efficient for system sizing and offline planning but insufficient for online scheduling or integrated sector coupling.

To address these constraints, data-driven and adaptive control methods have been increasingly adopted. Deep RL enable model-free learning of control strategies through interaction with dynamic environments.[44,45] These methods have been shown to optimise hydrogen system dispatch under variable renewable input, demand response signals, and multi-layer objectives (e.g., thermal, electrical, storage). However, effective deployment requires large-scale training data, hyperparameter tuning, and convergence stability management, as seen in the development of actor–critic architectures and dual-network stabilisation.[45] Digital twin frameworks integrates physical system models with real-time sensor data, predictive analytics, and control feedback mechanisms.[46] These systems simulate, monitor, and optimise hydrogen production, storage, and fuel cell systems simultaneously. Although promising, their implementation is constrained by high setup costs, model–data synchronisation issues, and computational overhead—especially in real-time grid-connected applications.[46] On the other hand, AR/VR technologies offer additional operational value by supporting operator situational awareness, particularly during dispatch decision-making and fault management.[47] Platforms such as Verciti provide immersive visualisations of hydrogen operations and enhance safety training for decentralised system operators.[48]

Traditional methods provide guarantees in optimization and deterministic planning, but fail to handle uncertainty, dynamic control, or sector integration. In contrast, AI-driven and hybrid frameworks support adaptable, real-time scheduling but require extensive training, are less interpretable, and lack standardisation for industrial deployment.[41-48] Hybrid models are gaining traction for balancing computational efficiency with physical consistency.[6,44] Recent applications illustrate how traditional modelling can be operationalised through interactive digital environments. For example, Folgado et al.[49] developed a digital twin of a proton exchange membrane (PEM) electrolyser embedded within a MATLAB-based graphical user interface, deployed in a photovoltaic-powered smart grid. The digital twin is based on a deterministic equivalent electrical model and communicates with a PLC via Modbus TCP/IP in real time. This setup enables operators to monitor hydrogen production metrics, assess deviations between simulated and measured performance, and support control decisions. The study highlights how traditional physics-based models can be integrated into real-time, user-interactive systems improving the coordination between hydrogen systems and smart grid operation.

Modelling strategies are shifting from deterministic formulations toward adaptive, interactive frameworks. Case studies such as Folgado et al.[49] demonstrate how equation-based electrolyser models can be embedded in digital twin systems for real-time monitoring within smart microgrids. Future modelling platforms must integrate real-time control logic, data feedback, and intuitive human interfaces to enable scalable hydrogen storage coordination in complex energy systems.

3. Challenges and Future Perspective

Emerging modelling and AI-based approaches offer significant advantages over traditional methods in PtH_2 systems but remains constrained by several technical and operational challenges. These limitations currently hinder the scalability, real-time deployment, and integration of advanced tools within smart grid environments.

The strong dependence on high-quality data is a primary limitation. ML and RL models require large volumes of well-labelled, high-frequency datasets to train predictive or control agents. In PtH_2 applications, this type of data is often unavailable due to limited sensor coverage, proprietary system architectures, or inconsistencies in temporal resolution. As a result, data-driven models risk overfitting or underperforming in real-world settings, particularly when transferred between systems with differing configurations.[44,45]

Another challenge lies in the computational complexity and training overhead of these models. RL, surrogate model development, and real-time digital twins require significant computing resources for convergence and deployment. For example, actor–critic RL algorithms and physics-informed neural networks (PINNs) demand extended training cycles and often rely on specialised hardware. These resource demands limit the feasibility of deploying such models in real-time, safety-critical environments like hydrogen storage and dispatch control.[45,46]

Model transparency and interpretability also present a barrier to adoption. While AI-based models are effective at pattern recognition and dynamic optimisation, their internal decision logic is often non-transparent. This "black-box" nature makes it difficult for operators and engineers to understand, validate, or troubleshoot behaviour during abnormal conditions. In PtH_2 systems, which involve high pressures, thermal gradients, and interdependent components, lack of interpretability can reduce stakeholder trust and pose regulatory challenges.[44]

The integration of AI with traditional physics-based models is another challenge. Hybrid systems that couple data-driven modules with deterministic simulations promise the best of both domains, but remain difficult to implement. Challenges include synchronising time scales, reconciling different data formats, and managing error propagation between subsystems. Few frameworks exist to seamlessly integrate CFD, process simulation, and RL agents within a unified control or optimisation environment.[12,49]

Additionally, operator readiness and system maturity limit the deployment of immersive technologies such as AR/VR and digital twins. These platforms are increasingly used for simulation and training, but rarely serve in active control environments. Visualisation tools and human-in-the-loop interfaces hold promise for enhancing fault awareness and decision support, yet their development is fragmented and lacks standardisation for PtH_2-specific applications.[47,48]

Future research must focus on bridging these limitations. First, hybrid models that embed physical laws into learning architectures could improve adaptability without sacrificing interpretability.[6] Second, developing open-source, interoperable frameworks for co-simulation would facilitate integration between AI and physics-based tools. Third, investment in high-resolution, standardised datasets from operational PtH_2 systems will be essential to unlock the full potential of machine learning. Fourth, AR/VR platforms and digital twins should be developed with greater emphasis on system interoperability and real-time responsiveness, making them viable for not just training but also active supervision. Lastly, regulatory frameworks must evolve in parallel with modelling innovations. For example, Australia's National Hydrogen Strategy and Guarantee of Origin Scheme are advancing hydrogen certification, dedicated AI governance remains underdeveloped.[53-55] Future modelling research should align with emerging standards for transparency, auditability, and validation.

Emerging modelling technologies can evolve from experimental tools into operational enablers for real-time, adaptive, and resilient PtH_2 smart grid coordination by addressing these challenges.

3. Conclusion

This review examined modelling strategies for PtH_2 systems, focusing on three core processes: production, storage, and grid integration, as a response to renewable energy intermittency. While traditional methods remain essential for system design and optimisation, they lack the adaptability required for real-time coordination and multi-vector control. Emerging strategies offer greater responsiveness but are constrained by data requirements, computational demands, limited interpretability, and challenges in integration with existing physical models.

Future researches should prioritise hybrid frameworks that combine physical accuracy with data-driven adaptability by combining traditional with emerging modelling and AI-based strategies across the PtH_2-integrated smart grid system. Moreover, future researches should focus on building standardised datasets, developing interoperable modelling platforms and expanding the role of real-time visualisation technologies. Lastly, modelling must be supported not only by technical innovation but also by regulatory frameworks to promote transparency, auditability, and certification for enabling safe, scalable PtH_2 deployment within smart grid.

Acknowledgements

The author acknowledges The University of Sydney for institutional support provided through the CHNG5603 – Advanced Industrial Modelling and Analysis unit. The author also extends gratitude to Dr. Gobinath Rajarathnam, unit coordinator and lecturer, and Dr. Aoni Xu, co-lecturer, for their guidance throughout the development of this review.

Canva was used for visual editing and layout incorporating elements from free-license image resources. Generative AI tools were used under the author's supervision solely for manuscript editing and language refinement. All content was critically reviewed to ensure technical accuracy.

This research did not receive any external funding.

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