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Simplified Thermal Analysis of a Concentrated Solar Water-Splitting Photocatalytic System

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Abstract. Photocatalytic water-splitting (PWS) technologies that produce hydrogen are approaching the necessary efficiencies to become a cost competitive alternative to traditional electrolysis. Continuous advancements in the solar-to-hydrogen (STH) efficiencies of PWS materials can be seen globally. This work presents a theoretical investigation into understanding the thermal behavior of a PWS system under concentrated light conditions. Ordinary differential equations (ODEs) were used to theoretically simulate experimental conditions. A python-based code solved the ODEs, the simulated results successfully matched the experimental results reaching an equilibrium temperature of 79 ° C, which is slightly outside the bounds of the experimental range temperature range of 75 ° C ± 3 ° C reported in literature. The implementation of a simplified thermal model enabled initial analysis of this system. The current model provided a useful tool for assessing various conditions and observing system behavior in a timely manner which can feed into future design decisions of PWS systems.

Keywords: Thermal Analysis, Photocatalytic Water-Splitting, Concentrated Photocatalysis, Ordinary Differential Equations (ODE), Thermal Modelling

1. Introduction

Efficient, cost-effective, and scalable photocatalytic water-splitting (PWS) technologies to produce green hydrogen with low or no concomitant carbon emissions could soon become a reality. Near-term green hydrogen production facilities produced via electrolysis of water are being hindered on a global scale. Factors such as the cost or availability of renewable power, skilled labor shortages and the scarcity of rare earth materials have caused an increase in the levelised cost of green hydrogen (LCOH) to rise by 30 – 65% in 2023 [1]. Developing alternative methods for green hydrogen production, such as PWS, can help mitigate risks and accelerate the global decarbonisation journey. These alternatives not only diversify the technological approaches to hydrogen production but also offer potential solutions to some of the challenges faced by electrolysis. For instance, the PWS process can utilise abundant and renewable solar energy, reducing dependence on electricity grids and minimising strains on the electrical infrastructure. Additionally, PWS materials often require fewer rare earth materials, alleviating supply chain constraints and lowering production costs. In parallel with PWS, several other solar-driven hydrogen production technologies are also emerging with promising potential. Notably solar thermochemical [2], photoelectrochemical [3, 4] and catalytic methane decomposition [5] have reached technology readiness levels (TRL) of 3 or higher. By expanding the range of viable green hydrogen production technologies, we can enhance resilience, optimise resource utilisation, and achieve a more robust and sustainable transition to a low-carbon economy.

Recent advances in PWS materials have led to significant improvements in solar-to-hydrogen (STH) efficiencies, with a world-leading 9.2% STH efficiency reported by [6], supporting the approaching commercial competitiveness of PWS to produce cost effective green hydrogen. Several studies have shown that exposing PWS materials to elevated temperatures using concentrated solar conditions has positive effects on hydrogen production yields [3, 7-9]. This is achieved by coupling a concentrated solar radiation technology to a PWS material and can also be referred to as concentrated solar photocatalytic water-splitting (CSPWS). CSPWS systems are being developed by companies such as Sparc Hydrogen, which identifies potential benefits in scaling up the coupling technologies to produce hydrogen with low or no carbon emissions [10]. A CSPWS system has been demonstrated in an outdoor testing experiment by Zhou et al., which achieved reaction temperatures of 75 ° C by utilising a 1.1 m x 1.1 m Fresnel lens producing a concentrated solar light intensity of 160.70 kWm^{-2} on an 8 cm x 8 cm focal plane containing the photocatalyst sample [6]. A theoretical understanding of the thermal dynamics in CSPWS systems can provide deeper insights into the energy transfer with the various reactors components such as the photocatalyst material. This can influence future design choices to manage and maintain desirable temperature conditions in photocatalytic reactors under varying on-sun conditions.

In this work, we develop a thermal model using first-order ordinary differential equations (ODEs) to theoretically simulate the conditions in the outdoor testing demonstration of Zhou et al. [6]. First-order ODEs are an appropriate representation of the CSPWS system as it allows modeling for simple dynamic systems in early stages of development, this elevates time in understanding the dominant thermal characteristics of the system compared to timely and computationally expensive 3D models. In this context, they allow us to accurately describe how temperature within the PWS reactor changes over time in response to varying conditions [8]. Results of the model can be validated with experimental results, and the model can be manipulated to determine how favorable temperature conditions can be met, mitigating the need for costly experimental trial and error.

2. Concept

The CSPWS reaction occurs in a glass chamber, which consists of a small cylinder connected to a larger cylinder for gas collection. In this analysis the model is simplified by focusing on the heat transfer mechanisms occurring in the small cylinder, in addition, the photocatalyst holder has also been removed from the system. The outdoor set up described by Zhou et al. consists of a pyrex glass reactor (glass), demineralised water, InGaN/GaN nanowires supported on silicon wafer photocatalyst (PC) and ordinary A4 printing paper for the insulating layer (ins) [6]. There are two main energy transfer components in the system; thermal transfer and optical transfer both represent the energy transfer in joules per second. Thermal transfer involves the three modes of heat transfer conduction, convection and radiation. The representation of each mode and the reactor component involved is denoted in Equation 1.

$$Q_{i,\ j\text{-}k} \tag{1}$$

Where *i* represents the heat transfer mode: conduction (cond), convection (conv), or radiation (rad) *j* is the reactor component from which the mode is leaving, and *k* is the reactor component interacting with *j.* The optical transfer involves transmission, absorption and reflection. For the purposes of thermal analysis, absorption is the crucial component which affects temperature. The representation of the amount of energy absorbed spectrally is represented in Equation 2,

$$Q \tag{2}$$

Which is represented in J/s. The ODEs for the temperatures of each reactor component can be generally represented in Equation 3 below.

$$dT_c / dt = [(\text{Energy In}) - (\text{Energy Out})] / [m_c * Cp_c] \tag{3}$$

Where *c* is the reactor component, *Energy In* is the energy entering the component in J/s, *Energy Out* is the energy leaving the reactor component in J/s, *m* is the mass of the reactor component in kg and *Cp* is the heat capacity of the component in J/kgK.

The ODEs described in Equation 3 determine the change in temperature for each reactor component. There are 20 different heat transfer modes representing the thermal interactions between the glass, water, photocatalyst and insulation, visualised in Figure 1 below.

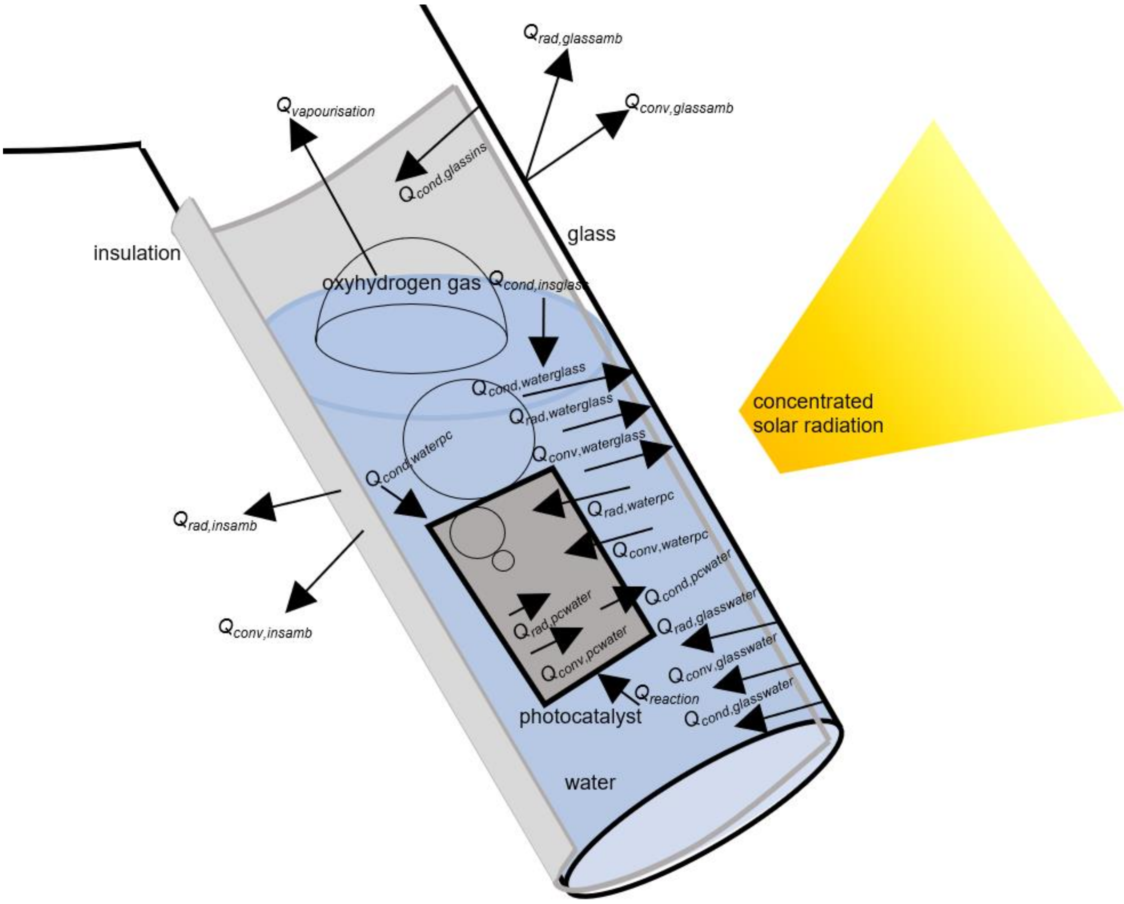

Figure 1. *Diagram of heat transfer mechanisms in the CSPWS demonstration by Zhou et al. [6]*

2.1 Python implementation

Modelling ODEs in Python provides a versatile platform for analysing this complex dynamic system. Python's function scipy.intergrate.solve_ivp allows for efficient and accurate calculations in a timely manner. The Python code was coupled with an open-source library called CoolProp which contains thermophysical properties of fluids for a full range of temperatures and pressures [11]. The code system works by specifying initial conditions and a time span of the system, then the function performs a numerical integration to solve each ODE in respect to time. As each time step is solved the function calls the CoolProp library to update the thermophysical properties of the fluid. This is depicted in Figure 2.

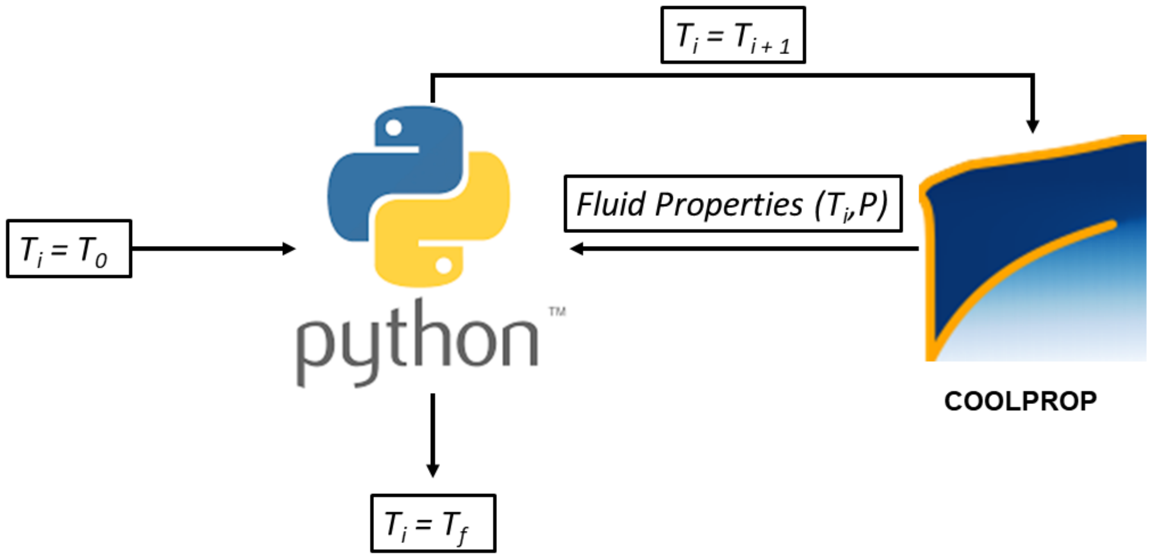

***Figure 2.** Flow chart of the modeling procedure.*

2.2 Validation of results

When the thermal model is inputted with the same outdoor conditions described by Zhou et al. [6], the reaction water reaches an equilibrium temperature of ~79 C, a 5.3% difference from the reported experimental temperature, as seen in Figure 3. The experimental study reported a stable temperature range of 75 C ± 3 C, which is expressed in the experimental region shaded in Figure 3, clearly validating the assumptions in the model. Another interesting aspect is time, the experimental study does not explicitly state the duration required for the reaction water to reach thermal equilibrium. However, the model implies that outdoor testing includes a period for stabilising the temperature before commencing the 140-minute experiment

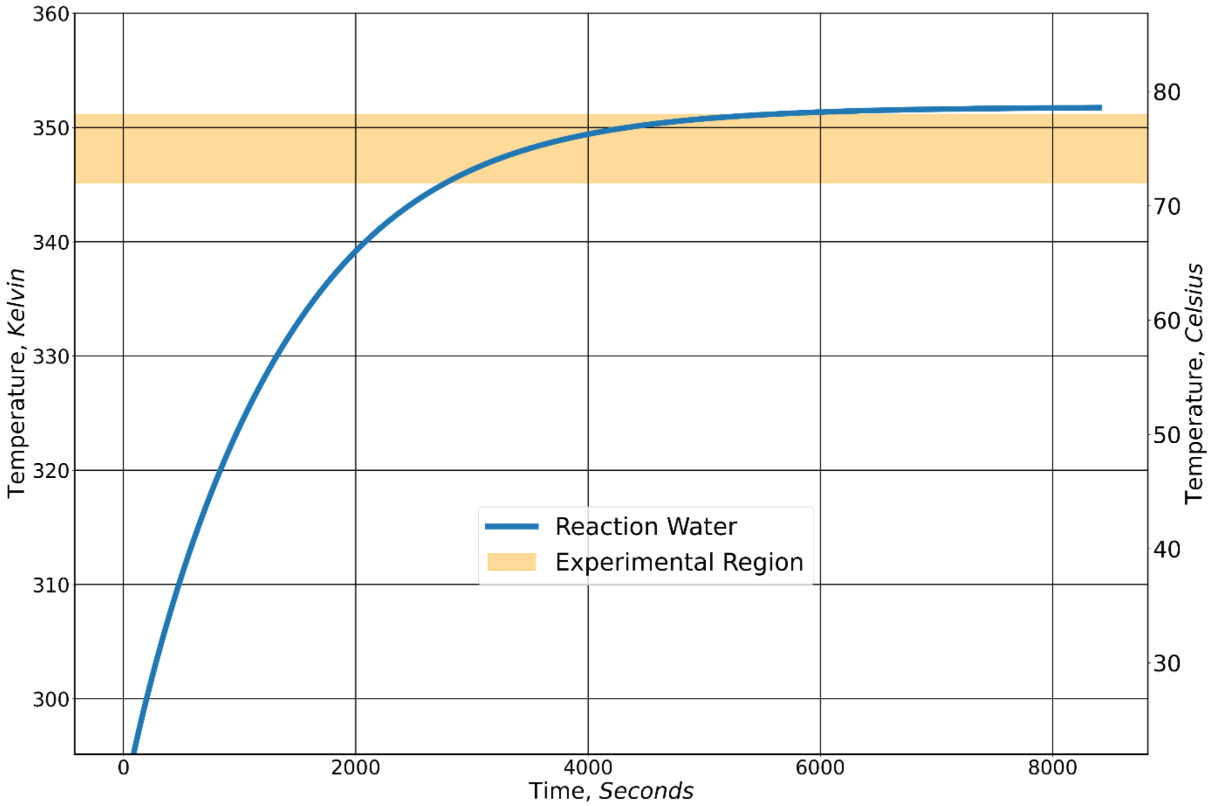

Figure 3. *Simulated temperature of the reactor using the thermal model. Thermal equilibrium is reached after 6000 seconds.*

2.3 Thermal assessment

Analysing the time-dependent behaviour of each heat transfer component enhances the understanding of reactor thermal dynamics. Figure 4 illustrates the heat transfer values for all 20 components described in Equation 3. While most components remain constant throughout the simulation, some exhibit significant changes.

$Q_{cond,pc\text{-}water}$: Initially, the heat conduction between the photocatalyst and the surrounding water is unstable, attributed to a high heat transfer coefficient (~11,733 W/K) due to the photocatalyst's small thickness. This volatility is influenced by the temperature difference between the photocatalyst and the water, which stabilises around 500 seconds into the simulation.

$Q_{cond,glass\text{-}water}$: At the start, heat is transferred from the glass to the water. Over time this reverses, resulting in a negative heat transfer value as the water conducts heat back to the glass. This causes a larger temperature differential between the glass and its environment, leading to increased convective losses, $Q_{conv,\ glass\text{-}amb}$, and contributing to system losses until thermal equilibrium is reached.

The system assumes that the glass has an absorptivity of 0.01%, while the water absorbs approximately 17% of the incoming energy. Initially, the glass heats up, transferring energy to the water (and subsequently to the photocatalyst). Over time, the water absorbs significant thermal energy and eventually heats the surrounding glass, which then loses thermal energy to the environment through convection. Figure 4 also shows that insulation losses to the environment via convection, though present, are relatively minor, demonstrating that insulation effectively helps maintain the system's equilibrium temperature.

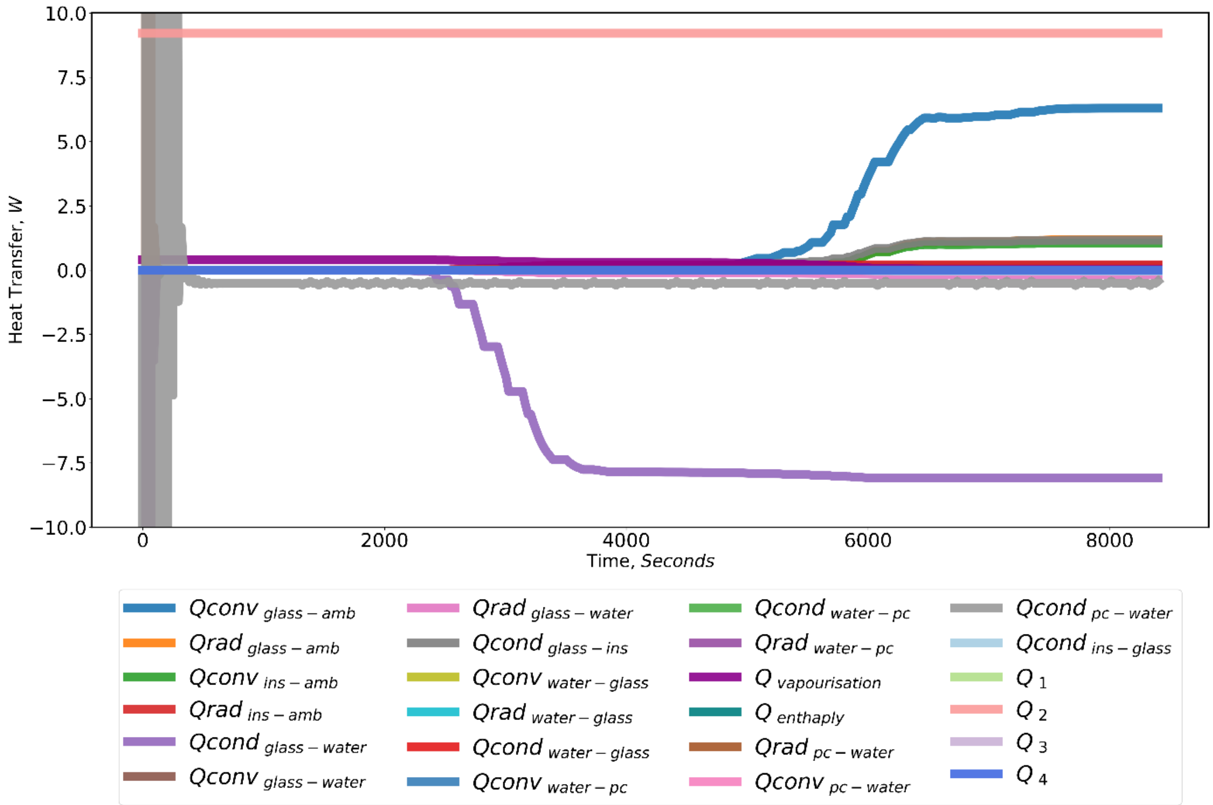

Figure 4. *Simulated thermal behaviour of each heat transfer component over the experimental time of 8400 seconds.*

The net energy flow analysis of the system at equilibrium is illustrated in Figure 5.

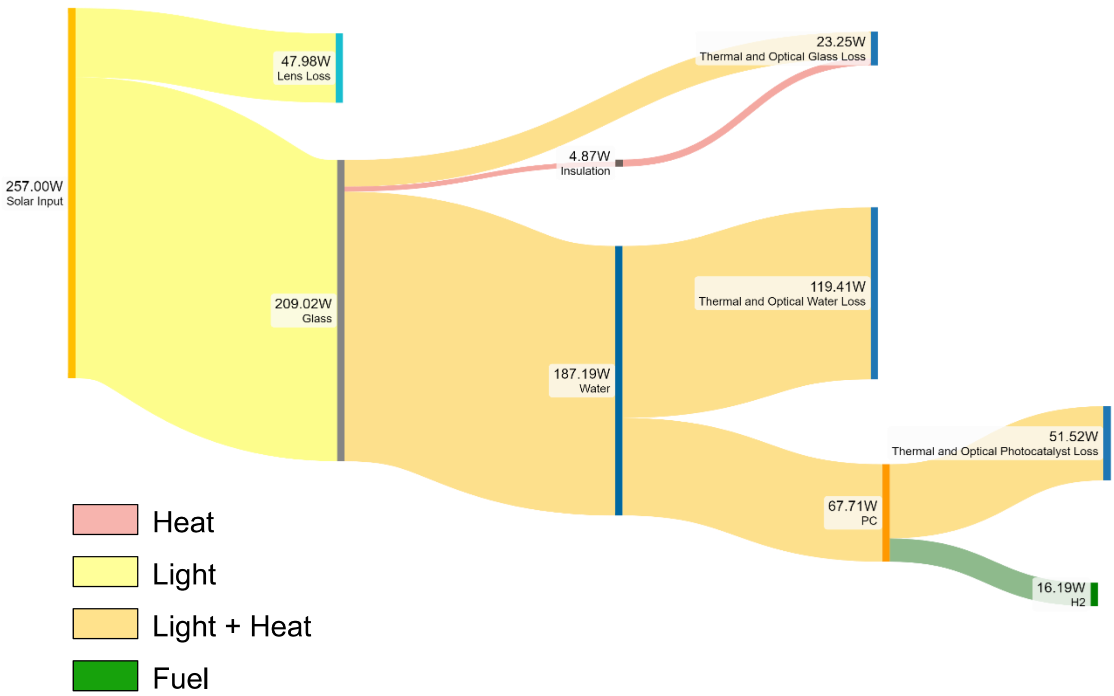

Figure 5. *Sankey diagram illustrating the net energy flows within the CSPWS system, showing the magnitude and routing within each reactor component.*

While the thermal model developed has yielded promising results, it represents only the initial stage of a more sophisticated analysis. This model supports preliminary thermal investigations and facilitates timely decision-making. However, it is important to note that the conditions used were based on educated assumptions derived from literature rather than precise measurements. This initial framework provides a valuable foundation for more comprehensive and refined models and enables convenient analysis, potentially influencing reactor designs and operational conditions.

3. Conclusion

A thermal model was developed using an open-source Python-based coding platform to solve the ODEs governing the system's thermal behaviour. The results demonstrated a close alignment with experimental data, validating the model's accuracy and reliability. Specifically, the model predicted that the reaction water would reach an equilibrium temperature of ~79 °C within 8400 seconds, a mere 5.3% difference from the experimental temperature reported by Zhou et al [6]. This temperature stability falls slightly outside the bounds of the experimental temperature range of 75 °C ± 3 °C. Furthermore, the model revealed that the main contributor of losses of the system are from the thermal losses to the environment and that the insulation layer does help reduce this effect.

Given the simple geometry of a typical photocatalytic systems, a simplified model can be considered sufficient to capture the dominant thermal behaviour of a CSPWS system. This approach facilitates a faster evaluation of system performance, which is valuable in the early stages of design. While a 3D model could offer a more detailed insight into complex regions of heat and mass transfer it was not pursed in this study.

Overall, the thermal model developed presents a promising alternative to costly simulation software and experimental trial and error, offering a robust and accessible tool for preliminary thermal investigations and facilitating timely decision-making. As more accurate data on the system's thermal and optical characteristics become available, the model's complexity and accuracy can be further enhanced, potentially influencing future reactor designs and operational conditions.

Data availability statement

Due to the conditions given by the related project and concerning the cooperation with external partners the authors cannot place the used data in an openly available space.

Author contributions

Anthony E. Pellicone: Conceptualisation, Methodology, Formal analysis, Investigation, Validation, Software, Visualisation, Writing- Original draft preparation. **Patrick C. Tapping**: Software **Woei L. Saw:** Validation, Visualisation, Writing- Reviewing and Editing, Supervision. **Gregory F. Metha:** Validation, Visualisation, Writing- Reviewing and Editing, Supervision.

Competing interests

Intellectual properties related to this work have been licensed to Sparc Hydrogen, a joint venture between Sparc Technologies, Fortescue, and the University of Adelaide. The University of Adelaide has financial interest in Sparc Hydrogen.

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