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PROJECT SULPHURREAL: DEVELOPMENT OF DIGITAL TWIN OF THERMOCHEMICAL CYCLE FOR SOLID SULPHUR PRODUCTION FOR LONG-TERM STORAGE OF SOLAR ENERGY

Summary

To advance the sustainable production of solar electricity, the SULPHURREAL project is developing an innovative thermochemical cycle that stores solar thermal energy in solid sulphur, enabling the generation of renewable and dispatchable power. Key processes, including sulphuric acid splitting, sulphur dioxide disproportionation and sulphur combustion, will be demonstrated at lab scale and integrated into an industrial-scale system design. To enable the computational modelling of the whole process, overcoming limitations of traditional chemical engineering tools, a hybrid digital twin is being developed to model and optimize the cycle, combining physics-based and machine learning approaches. Initial results show highly accurate and computationally efficient simulations of a main section of the process, covering the use of solar heat to split sulphuric acid into sulphuric dioxide. Future work will expand the digital twin framework to the full cycle, supporting flexible and real-time system optimization, with potential for integrating future process data.

Keywords: Digital twin, machine learning, sulphur, solar fuel, concentrated solar energy, energy storage

1. Introduction

Sulphur (S) is one of the most abundant elements on Earth and plays a key role in the chemical and fertilizer industries, while its oxidized form, sulphuric acid (H_2SO_4), is one of the most traded chemicals worldwide. A promising concept for using solar energy to produce S from H_2SO_4 for dispatchable renewable power generation was proposed by Wong et al. (2015), leveraging on sulphur's storability and high energy density.

Building on this idea, the European project SULPHURREAL (2023–26) aims to demonstrate and validate a breakthrough approach for the carbon-free conversion of solar thermal energy into elemental solid sulphur, a fuel which can be stored long-term and later combusted in a power cycle to produce on-demand renewable electricity. This novel cycle relies on solar heat and non-critical raw materials (CRM) typically produced as industrial by-products, aligning with circular economy principles and international climate ambitions.

The project focuses on developing the individual processes required for this concept and demonstrating them at a lab scale. The three key components – (i) the sulphuric acid splitting (SAS) reactor; (ii) the sulphur dioxide disproportionation (SDD) reactor; and (iii) a high-power sulphur burner – will be validated under realistic conditions and are expected to reach technology readiness level (TRL) 4. In parallel, a full industrial-scale facility will be designed and simulated, supporting the evaluation of the feasibility and integration of all processes within a unified and compatible system architecture.

Due to the intermittent nature of solar energy, simulating the process under various operating conditions (e.g., typical meteorological year, varying feedstock composition) using conventional chemical engineering software is challenging and computationally expensive. To overcome this, a hybrid digital twin (DT) framework is being developed, combining physics-based and data-driven models. This approach aims to improve process control and reduce operational risks by proactively monitoring key parameters throughout the entire cycle, enabling accurate performance prediction and real-time system optimization.

Therefore, this study presents an overview of the SULPHURREAL cycle and outlines the development and implementation of the hybrid DT approach.

2. Process overview

The SULPHURREAL cycle relies on five main chemical reactions, as presented in Table 1. First, high-temperature heat is used in the SAS reactor to dissociate H_2SO_4 into water (H_2O), sulphur dioxide (SO_2), and oxygen (O_2). This happens through two combined reactions (1a-b): the first produces steam and sulphur trioxide (SO_3), while the second splits SO_3 into SO_2 and O_2 using a high-temperature catalytic reactor (650–1000 °C), both driven by the heat from a solar power tower system – similar to thermochemical hydrogen production methods like the sulphur-iodine and hybrid sulphur (HyS) cycles. Then, SO_2 is converted into elemental S and H_2SO_4 inside the SDD reactor (reaction 2). Then, the S can be burned in air to produce heat and SO_2 (reaction 3). The main product of the cycle is not a chemical, but the high-temperature heat (over 1200 °C) from burning sulphur, which is useful for efficient power generation. The SO_2 is recycled back into S and H_2SO_4 by existing industrial processes (reactions 4-5), forming a closed loop as depicted in Figure 1.

Tab. 1: Main reactions relevant for the solid sulphur storage and power generation in the SULPHURREAL cycle

Reaction			T (°C)	ΔH (kJ mol^{-1})
Sulphuric acid splitting	1a 1b	$3\ H_2SO_4(aq) \rightarrow 3\ H_2O(g) + 3\ SO_3(g)$ $3\ SO_3(g) \rightarrow 3/2\ O_2\ (g) + 3\ SO_2(g)$	450–500 650–1000	826
Disproportionation	2	$3\ SO_2(g) + 2\ H_2O(l) \rightarrow 2\ H_2SO_4(aq) + S(s)$	50–200	-254
Sulphur combustion	3	$S(l) + O_2(g) \rightarrow SO_2(g)$	500–1500	-297
Contact process	4	$SO_2(g) + 1/2\ O_2\ (g) \rightarrow SO_3(g)$	–	-99
Absorption	5	$SO_3(g) + H_2O(g) \rightarrow H_2SO_4(aq)$	–	-176

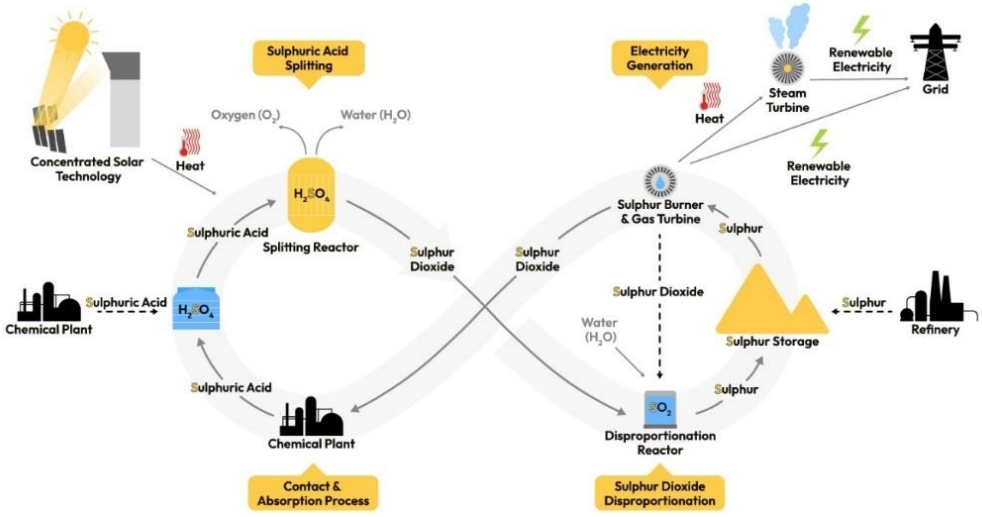

Fig. 1: Simplified scheme of SULPHURREAL cycle

S and H_2SO_4 can be stored cheaply and safely using existing technologies, making such a system practical and sustainable. While we focus on a cyclic design, the process is flexible and can also run in an open loop configuration, for producing or using S-based materials e.g., from refineries and other chemical plants.

3. Digital twin development

Digital twins (DTs) in chemical engineering enable real-time monitoring, optimization, and prediction by serving as virtual replicas of physical systems (Pal et al., 2025). Existing DT solutions typically rely either on physics-based models, grounded in scientific principles, or on data-driven approaches that use machine learning (ML) trained on historical and real-time data (Kang et al., 2021; Sitapure et al., 2023; Parente and Swaminathan, 2024). Hybrid DTs combine both strategies, integrating first-principles simulations with AI-driven insights for greater accuracy and adaptability (Kasilingam et al., 2024).

Here, we propose a hybrid DT approach for simulating and optimizing the SULPHURREAL cycle. Our method uses data from Aspen Plus simulations and physics-based models to train ML models. Due to the high computational cost and convergence challenges of comprehensively simulating the entire cycle, we propose two complementary model training approaches:

- **Full-plant model:** This approach treats the whole plant as a single system and trains a model to predict key outputs (e.g., sulphur production, power generation, utility consumption) from core inputs such as direct normal irradiance, H_2SO_4 flow rate, concentration, pressure, and temperature. Although based on a smaller dataset, it captures overall system behaviour and allows the evaluation of plant-wide performance.
- **Modular block model:** Here, the cycle is divided into sequential process blocks (e.g., acid decomposition, gas separation, sulphur combustion). A separate ML model is trained for each block, enabling detailed analysis of individual process steps. Intermediate variables can be manually adjusted for flexible scenario testing and targeted optimization.

The modular block model offers greater flexibility and detail, while the full-plant model provides more realistic system-wide results. Therefore, the former is validated against the latter to ensure coherence and feasibility across the full cycle. Finally, the trained model is accessible in a user-friendly interface, enabling instantaneous parameter adjustments and outcome prediction.

4. First results and outlook

At this stage of the project, synthetic data for both the full-plant and modular block models were successfully generated, focusing on the DT of Block 1 – H_2SO_4 splitting – as a proof-of-concept. In such part of the process H_2SO_4 is converted mainly into SO_2 using solar heat, via reactions 1a-b in Table 1. Using Aspen, we created a dataset by iterating through all input combinations, generating a number of records at the order of 1×10^6, containing combinations of input variables, while registering output parameters such as energy demand, feed composition, mass flow rate and thermodynamic state.

A linear model with second-order interactions was trained on the dataset for Block 1, achieving nearly zero prediction error due to the process's linear nature. This approach performed several orders of magnitude faster than conventional Aspen simulations and is accessible through a user-friendly web analytics platform. Currently at the proof-of-concept stage, the digital twin (DT) demonstrates strong potential as a surrogate for time-consuming simulations, enabling faster experimentation and optimization. For the more complex, non-linear blocks – corresponding to the remaining parts of the SULPHURREAL cycle currently being modelled – a CatBoost ensemble model was trained. In addition, advanced deep learning methods, such as feedforward neural networks (FNNs), long short-term memory networks (LSTMs) for sequential dependencies, and graph neural networks (GNNs), are being considered to further enhance predictive performance.

Future work will expand to more blocks and increase the complexity of the process modelling, ultimately covering all of the processes in the SULPHURREAL cycle. Since real data generation within our project is limited to lab-scale testing of key components, the development of this methodology is a crucial step for creating digital twins for complex solar-driven chemical processes. In the future, this model could be trained not only on synthetic data but also on real measured data, enhancing the plant's operational efficiency and reliability while providing valuable services for process monitoring, prediction, and control.

5. References

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