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Basic design principles and specifications for a novel thermochemical heat storage and upgrading solution

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Abstract:

Thermochemical energy systems in various specifications are showing very promising to become important elements of the future sustainable energy matrix. These may come for various applications from large-scale heat storage, to heat-to-power (and vice versa) conversion, waste heat recovery and so on. STOREDGE thermochemical heat storage/transformer offers a cost-effective pathway for utilizing medium-temperature industrial waste heat for a wide range of industrial applications. While material screening and development for this concept is still underway, low-cost calcium hydroxide ($Ca(OH)_2$) in structured forms is a great primary option for temperature upgrading via the reversible $Ca(OH)_2 \rightleftharpoons CaO + H_2O$ reaction, owing to its high energy density, environmental compatibility, and abundance. Calcium hydroxide is dehydrated during the charging mode by absorbing waste heat in the form of chemical bonds, and the stored energy is released during the discharging mode.

In this study, a kW-scale design of this thermochemical system is presented. The proposed system involves moving bed reactors, heat exchangers, a condenser, an evaporator, and auxiliary components such as pumps and storage tanks. The system development requires precise consideration of the first and second laws of thermodynamics and optimal integration of components. For simplification, this initial design step is presented based on a steady-state operation assumption. Although this brings inaccuracies in component sizing, process design, and performance assessments compared to a detailed dynamic model of the system (next steps of this research), it gives valuable insights into the expected technical and economic key performance indicators of the technology.

Keywords:

Thermochemical heat storage; decomposition of calcium hydroxide; system-level; heat upgrading.

1. Introduction

According to International Energy Agency (IEA), the industrial sector uses 37% of global energy in 2022. Increase in industrial energy demand leads to increase in greenhouse emission, which is alone responsible for releasing 9.0 Gt of CO_2 in the European Union (EU). This solely accounts for 25% of global energy CO_2 emissions. Along with power industry, they lead to 70% EU's greenhouse emission. This is not aligned with the net-zero emission (NZE) by 2050 target. To come along with NZE, total direct emissions due to industry must decline by approximately 25% to 2030.

At the same time, more than 65% of industrial process energy demand is used for process heating of different sectors (e.g., iron&steel, chemical, food, pulp and paper, textile, and automotive industries, non-metallic mineral, etc.). Today, 50% of the industrial heat demand occurs at low and medium temperature (<200°C). Deploying renewable power/heat (e.g., solar, wind) is one of the solutions to provide necessary heat for industry. Industrial heat pumps are promising integration of renewable power to generate process heat at low/medium temperature [1]. For example, Zuberi et al. [2] reported potential of deploying industrial heat pump systems in different sectors through bottom-up approach. They projected that this technology may provide 36% of the global energy demand with 71% reduction in CO_2 emission in 2050. Alternatively, heat transformers can be employed to the industry to convert renewable heat to process heat. For example, Mahmoudinezhad et al. [3] presented molten salt driven energy conversion system for sustainable process heat for factory demanding saturated steam at 10 bar. The system produces steam at temperature of 180°C with levelized cost of heat 67€/MWh. Bellos et al. [4] developed a solar-driven heat transformer system to convert solar heat into industrial heating. The LiBr/water working pair was used to thermochemical heat absorption. The system produced 37 MWh industrial heat with energy and exergy efficiency of 21% and 5.8%, respectively with levelized cost of heat at 0.07 €/kWh. They system was able to reduce annually 8504 kg CO_2-eq emission.

In addition to industrial heat demand at low temperature, around 50% of process heat has emerged at high temperatures (>500°C), i.e. metal processing requires very high-temperature processes (600-1500 °C) [5], which is provided dominantly by fossil fuels. Industrial heat pumps are not effective to be deployed in the industry for supplying process heat at that temperature level. One possibility is to use hydrogen, biofuels, or electro-fuels which could be generated from renewables [6,7] and used in a gas turbine or a fuel cell-based system to provide industrial heat and power. Due to several difficulties at every step of the process (generation, transportation, storage, and use), the actual cost of hydrogen becomes too large (3 – 7.5 $/kg) [8]. Therefore, biogas/biofuels and CO_2-electrofuels have gained more attention compared to hydrogen. Pastore et al. [9] projected that electrofuels may meet more than 50% demand of industrial heat by 2050 in the low-biomass availability scenario. Moreover, they reported that use of biogas has become larger than electrofuels in the scenario of high biomass availability. However, biogenic feedstocks gasification continues to face several technical challenges (e.g., gas cleaning, feedstock variability, irregular feedstocks flow, etc.) [10]. An integration of renewable energy to generate process heat might not match the real-time demand of the industries due to unavoidable fluctuating output of renewable technologies.

On the other hand, there is significant potential for waste heat to be stored or upgraded for use in process heating. Papapetrou et al. [11] calculated potential of waste heat by different sectors, temperatures, and countries in EU in 2015. Based on this, the iron and steel industry generates more than 160 TWh per year, more than 50% of which is accounted for by high temperatures (>500 °C). Thermochemical heat storage and upgrading technology potentially enables effective utilization of available waste heat for sustainable and cost-effective high-temperature heat generation. Thermochemical systems would give very high energy density (0.5-1 kWh/kg), while they are still at the research and development stage [12,13].

In this study, within the framework of a recent EU funded project STOREDGE (https://storedge-project.eu/), we introduce basic design principles and specifications for a novel thermochemical heat storage and upgrading solution for the process heat generation. The study aims to demonstrate the basic system design and performance for available waste heat storage and upgrade to the process heat.

2. Technology description

2.1. Manuscript preparation process

As described in Fig. 1, thermochemical heat storage and upgrade systems work with reaction pairs. One reaction is endothermic to absorb heat (charging mode), while the reverse reaction is exothermic to release heat (discharging mode). In the discharging mode, the system can upgrade the stored heat to a higher temperature level to provide high-temperature heat for direct process heating.

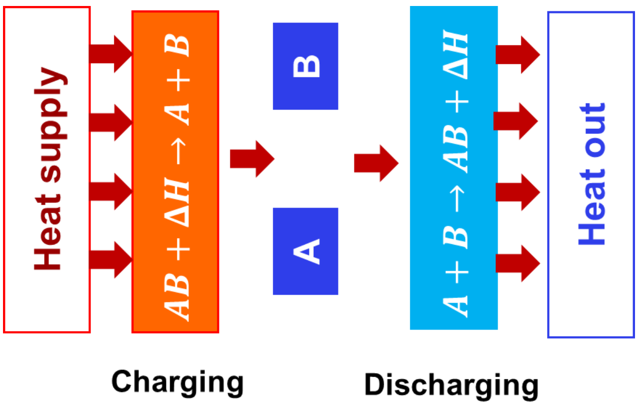

Figure. 1. *A description of thermochemical heat storage concept*

There are various candidate materials for the system (e.g. carbonates, metal hydroxides, hydrides, etc.) [14]. All materials come with trade-offs. For example, although carbonates are cheap and can be operated at high temperatures, they have low cyclability due to high agglomeration. Hydrides provide high energy density but suffer from high cost of materials. Metal hydroxides are cheap and non-toxic, which makes them a priority over other candidates. In this study, we present the capability of calcium hydroxide, $Ca(OH)_2$, material for the reaction pair. In the charging mode, decomposing of $Ca(OH)_2$ takes place (dehydration, Eq. 1), while calcium oxide (CaO) is hydrated in the discharging mode (Eq. 2).

$$Charging: Ca(OH)_2(s) \rightarrow CaO(s) + H_2O(g)\ ;\ \Delta h = -104.4\ kJ/mol \quad (1)$$

$$Discharging: CaO\ (s) + H_2O\ (g) \rightarrow\ Ca(OH)_2\ (s);\ \Delta h = 104.4\ kJ/mol\ (2)$$

3. System description

As illustrated in Fig. 2, the proposed system involves two separate reactors (for dehydration and hydration), a condenser, an evaporator, the heat exchangers, and a pump. In the dehydration reactor, the heat transfer fluid (HTF) gives its heat to the bed of the reactor in which the decomposition of $Ca(OH)_2$ takes place (see Eq. 1). As a result of this reaction, CaO and steam are generated. CaO is conveyed to the other reactor, while steam is sent to the heat exchanger for the precooling before condensation. In the precooler, the temperature of steam decreases to just above the condensation temperature. Steam is then condensed in condenser at the pressure of dehydration reactor. Condensed liquid water is stored for later use in the heat-releasing process. When the heat release process is required, the stored liquid water is first sent to the preheater, which increases its temperature just below the evaporation temperature at the hydration reactor pressure. The liquid water then evaporates and is superheated through the evaporator and superheater, preparing it for the hydration process. At the same time, the stored CaO is sent to the reactor. Superheated steam diffuses through the CaO-filled reactor bed, resulting in the generation of $Ca(OH)_2$ and heat (see Eq. 2). The generated $Ca(OH)_2$ is sent back to the reactor for cyclability, whereas the released heat is absorbed by the HTF to be transferred into the industrial purposes.

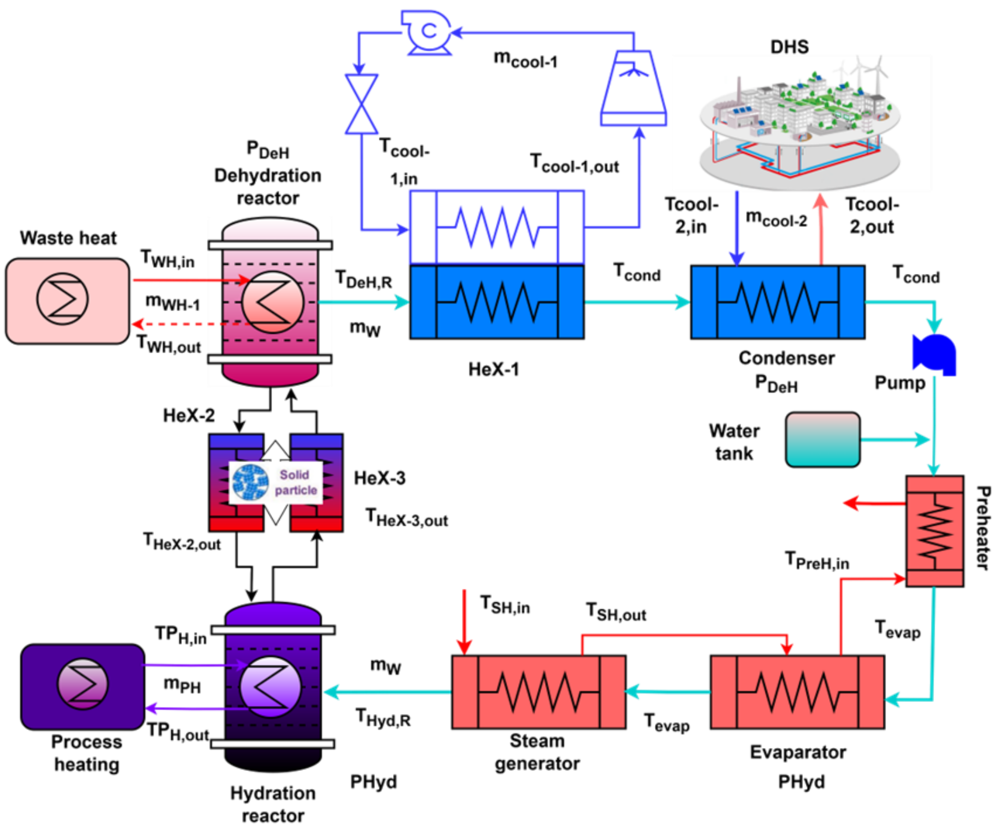

Figure. 2. *A schematic illustration of presented thermochemical heat storage and upgrading system*

4. Method

In this study, a mathematical model estimating basic design specifications and performance of the system is presented. Three physical phenomena are considered for the model: i) thermodynamic balances, ii) chemical kinetics, and iii) thermal-fluid equations. The equilibrium can be expressed in terms of temperature (T_{eq}) and pressure of steam (p), as given in Eq. 3. Based on this, the equilibrium is shown in Fig. 3.

$$\ln\left(\frac{p}{10^5}\right) = -\frac{12845}{T_{eq}} + 16.508 \qquad (3)$$

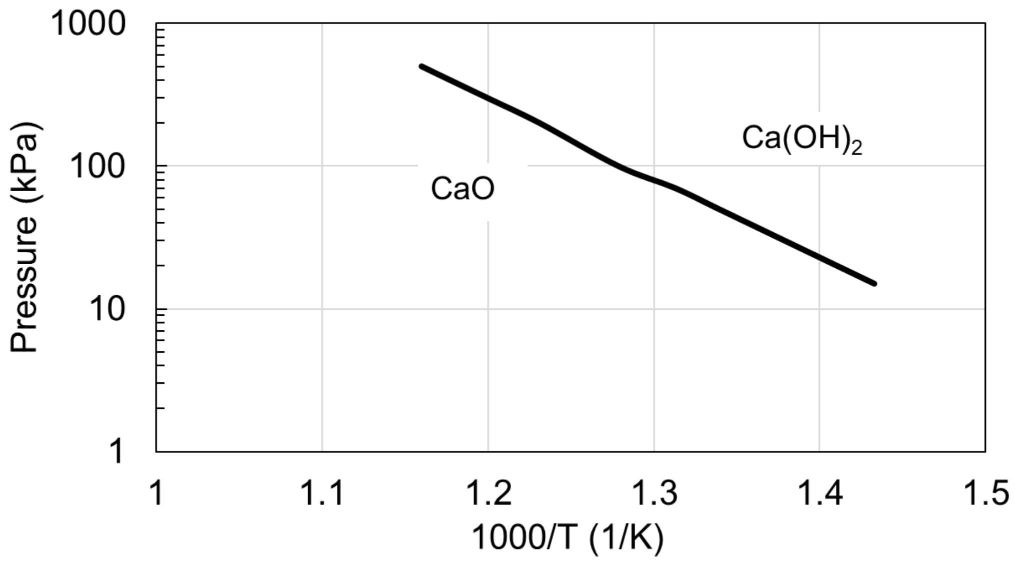

Figure. 3. *Thermodynamic equilibrium of* $Ca(OH)_2 \leftrightarrow CaO + H_2O$

The chemical kinetic equation is used to define the reaction rate of dehydration ($\left(\frac{dX}{dt}\right)_{DeH}$, Eq. 4) and hydration ($\left(\frac{dX}{dt}\right)_{Hyd}$, Eq. 5):

$$\left(\frac{dX}{dt}\right)_{DeH} = A_{DeH} \cdot \exp\left(-\frac{Ea_{DeH}}{RT}\right) \cdot (1-X) \cdot \left(\frac{T}{T_{eq}} - 1\right) \qquad (4)$$

$$\left(\frac{dX}{dt}\right)_{Hyd} = A_{hyd} \cdot \exp\left(-\frac{Ea_{Hyd}}{RT}\right)\left(y_{H_2O} - y_{eq}\right)^3 (1-X)^{2/3} \qquad (5)$$

where A_{DeH} and A_{hyd} are pre-exponential factors of dehydration and hydration reactions, respectively. Ea_{DeH} and Ea_{Hyd} are activation energies for dehydration and hydration reactions, respectively. R is universal gas constant. T is temperature. T_{eq} is equilibrium temperature. X is the conversion ratio. y_{H_2O} is the molar fraction of steam, whereas y_{eq} represents equilibrium molar fraction of steam at equilibrium pressure. The kinetic parameters can be found in the study of Schaube et al. [15]. Generated water mass flow rate ($\dot{m}_W$) can be found by using the following equation:

$$\dot{m}_W = \left(\frac{dX}{dt}\right)_{DeH} \cdot m_{Ca(OH)_2} \qquad (6)$$

Thermochemical heat rate of the reactors ($\dot{Q}_{DeH}$ for dehydration and $\dot{Q}_{Hyd}$ for hydration) can be found as follows:

$$\dot{Q}_{DeH} = \left(\frac{dX}{dt}\right)_{DeH} \cdot m_{Ca(OH)_2} \cdot \Delta H_{rxn} = UA_{DeH} \cdot \Delta T_{WH} \qquad (7)$$

$$\dot{Q}_{Hyd} = \left(\frac{dX}{dt}\right)_{Hyd} \cdot m_{CaO} \cdot \Delta H_{rxn} = UA_{Hyd} \cdot \Delta T_{PH} \qquad (8)$$

where $m_{Ca(OH)_2}$ and m_{CaO} are mass of material inside of the reactor, respectively. ΔH_{rxn} is enthalpy of reaction. The heat rate for dehydration is taken up by HTF, that goes around the reactor without contacting the particles inside of the reactors (in-direct). UA_{DeH} and UA_{Hyd} are a design specification that describes the heat exchange between the waste and process heat streams and the reactors, calculated using the logarithmic mean temperature difference (LMTD, ΔT_{WH}, ΔT_{PH}) between them. More specifically, U and A represent overall heat transfer coefficient and heat transfer area, respectively.

The heat transfer during condenser ($\dot{Q}_{cond}$) and evaporator ($\dot{Q}_{evap}$) are calculated by Eq. 9 and Eq. 10, respectively.

$$\dot{Q}_{cond} = -\dot{m}_W \cdot h_{fg}\big|_{P_{DeH}=P_{cond}} \qquad (9)$$

$$\dot{Q}_{evap} = \dot{m}_W \cdot h_{fg}\big|_{P_{hyd}=P_{evap}} \qquad (10)$$

where $h_{fg}\big|_{P_{DeH}=P_{cond}}$ and $h_{fg}\big|_{P_{hyd}=P_{evap}}$ represent latent heat of vaporization for condensation and evaporation, respectively at the elevated pressures.

In this system, the performance is defined as the useful heat released by the system relative to the thermal energy input for dehydration and evaporation, as given in Eq. 11.

$$\eta = \frac{\dot{Q}_{Hyd}}{\dot{Q}_{DeH} + \dot{Q}_{evap}} \qquad (11)$$

In this study, five different cases are examined to evaluate system performance, as presented in Table 1. The technical interpretation of these cases is illustrated in Fig. 4. From Case 1 to Case 5, the pressure difference between the dehydration and hydration reactors increases, enabling the system to lift the temperature. Consequently, the system shifts from heat storage operation in Case 1 toward waste-heat upgrading in Case 5.

Table 1. *Cases considered in this study for the system performance investigation*

Cases	Dehydration pressure	Hydration pressure
1	100 kPa	100 kPa
2	70 kPa	200 kPa
3	50 kPa	300 kPa
4	30 kPa	400 kPa
5	15 kPa	500 kPa

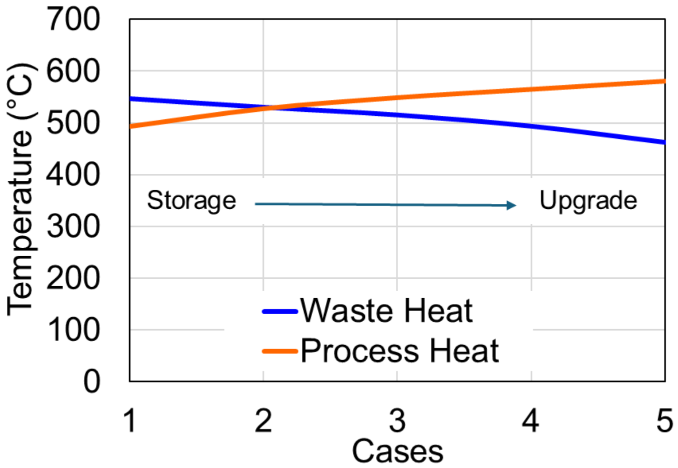

Figure. 4. *Technical interpretation of five different cases given in Table 1*

5. Results and Discussion

In Fig. 5a, the heat duties are displayed for different cases. From Case-1 to Case-5, the heat duty decreases gradually from 130 kW to 15 kW. This can be explained by the reduction in pressure of dehydration from 100 kPa in Case-1 to 15 kPa in Case-5, while hydration pressure increases from 100 kPa in Case-1 to 500 kPa in Case-2. The decrease in pressure leads to a reduction in temperature, which lowers the kinetic rate of steam generation in the dehydration reactor. The steam generation, as a result of decomposition of $Ca(OH)_2$, is displayed in Fig. 5b. The steam generation rate decreases from 0.022 kg/s to 0.018 kg/s from Case-1 to Case-5. The reduced steam production then limits the hydration rate and consequently reduces the overall heat duty available for the system. This technically limits amount of heat supplying from waste heat source.

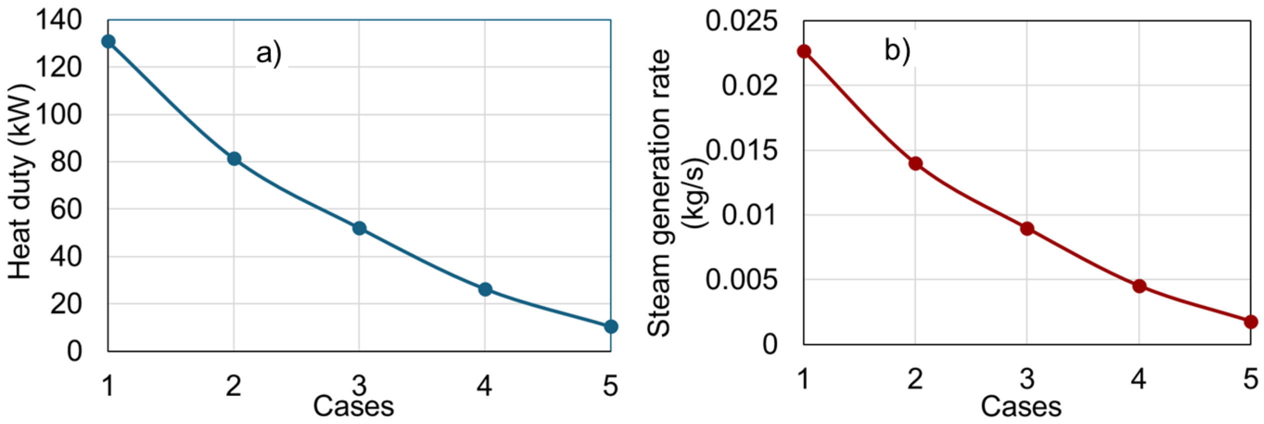

Figure. 5. *Main results from the system-level assessment a) heat duty of the reactor and b) steam generation rate*

Decrease in heat rate in Fig. 5 limits design of heat exchanger employed in the reactors. *UA* combines measure of the exchanger's ability to transfer heat, allowing comparision of different heat-exchanger concepts. In Fig. 6, *UA* specifications of the dehydration and hydration reactors are demonstrated for different cases. It is found that UA value of heat exchange in dehydration reactor is found to be 5.25 kW/K, whereas it is found to be 5.2 kW/K for the hydration reactor for Case-1. It then decreases to 0.41 kW/K and 0.4 kW/K for dehydration and hydration reactors, respectively in Case-5.

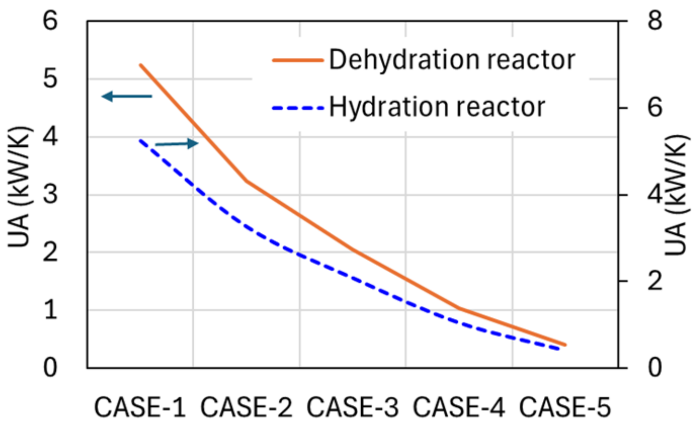

Figure. 6. *UA specification for dehydration and hydration reactors,*

From the point of system design, as given in Table 2, we found temperatures and mass flow rates for each state in the system (displayed in Fig. 2) for specific Case 3. It is worth mentioning that pinch point between HTF outlet and the reactors' temperature is taken 10 °C [16]. It is also assumed that heat from Heat Exchanger-1 and Condenser is taken by district heating system that requires temperatures of 70 °C forward and 30 °C return [17]. For the basic system design without optimal thermal integration, the WH mass flow rate is needed for almost two-times higher than process heat gas flow rate. Moreover, if the WH is also used for steam generator, evaporator, and preheater, its flow rate needs to increase by 50%. However, based on constraints considered, the WH's temperature increases by 10% in this scenario which may be tolerable from the point of system design. Based on findings in Table 2, the heat duty of the components and *UA* designs specifications are estimated and given in Table 3 for Case-3. Based on this, heat duty for the Heat Exchanger-1, the condenser, the evaporator, and the steam generator represent the largest heat duty with values of 7.34 kW, 20.69 kW, 19.42 kW, and 8.54 kW, respectively after the reactors. *UA* values of condenser, evaporator, and steam generator are found to be 0.67 kW/K, 0.97 kW/K, and 0.85 kW/K, respectively, which represent the largest *UA* requirements aside from the dehydration and hydration reactors.

Table 2. *Temperature and mass flow rates in the system for specific Case-3*

State	Temperature (°C)	Mass flow rate (kg/s)
WH in/out	515.6/485.6	1.591
DeHR	558.4	0.008976
Condensation	81.32	0.008976
Cool-1 in/out	20/86.32	0.02647
Cool-2 in/out	30/71.32	0.1197
Evaporation	133.5	0.008976
Evap in/out	168.4/143.5	0.7699
HydR	558.4	0.008976
SH in/out	573/563.4	0.7699
PreH in/out	153.1/138.5	0.1591
PH in/out	518.4/548.4	0.78

Table 3*. Heat duty and design specifications of the components in the system for specific Case 3*

Component	Heat duty (kW)	UA (kW//K)
Dehydration Reactor	52.14	2.085
Hydration reactor	51.41	2.056
Heat exchanger-1	7.341	0.01738
Condenser	20.69	0.6747
Preheater	2.354	0.05841
Evaporator	19.42	0.9758
Steam generator	8.54	0.854

In Fig. 7, system efficiency calculated based on Eq. 11 is investigated for cases. The system efficiency decreases from Case-1 to Case-5. This can be explained that temperature upgrading through difference in kinetics of the reactors requires increasing of the heat demand for evaporator, steam generator, and preheater. Moreover, increase in the pressure difference between two lines (dehydration and hydration lines) increases the pump power demand. We estimated that the system efficiency decreases from 0.64 to 0.61 from Case-1 to Case-5.

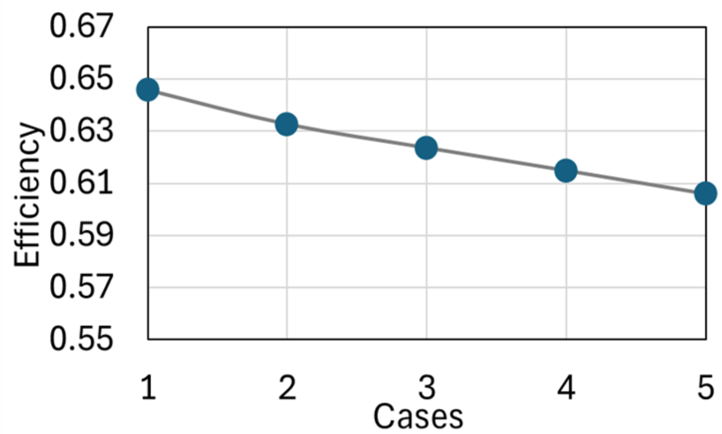

Figure. 7. *The system efficiency for various cases*

6. Conclusions

In this study, we present basic design principles and specifications for a novel thermochemical heat storage and upgrading system. Five different cases are considered that the system shifts from heat storage operation in Case 1 toward waste-heat upgrading in Case 5. It is demonstrated that lower dehydration pressure combined with higher hydration pressure enables heat upgrading, with a resulting in a slight reduction in system efficiency (5%). Decrease in dehydration pressure limits the reaction kinetics, resulting in reduction in steam generation from dehydration reactor. This also limits the performance of the hydration reactor, resulting in lower heat release from the hydration. Therefore, we found lower *UA*, measures of the exchanger's ability to transfer heat, in Case-5 based on the considered conditions. Moreover, for the basic system design without optimal thermal integration, it is found that the required WH mass flow rate is almost two-times higher than process heat gas flow rate needed. If the WH is also used for steam generator, evaporator, and preheater, the flow rate needed increases by 50%. This study provides insights into future economic assessment of the proposed concept. In the next phase, different operational scenarios will be evaluated, including cases where solar heat is stored and subsequently utilized for process heat supply or integrated into power-generation cycles.

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