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Dynamic Analysis of the Solid-Gas Thermochemical Heat Transformers for Industrial Heat Recovery

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***Abstract* –** A significant portion of the energy supplied to the industries is dissipated as low, medium, or high-grade waste heat. In the sake of improved energy efficiency and sustainability in the industrial sectors, significant recovery and heat upgrading measures for these waste heat streams are needed. Thermochemical heat transformers (THTs) have emerged as a promising sort of technological solutions for upgrading waste heat streams in industry. Among various types of THTs, solid-gas (SG) species reacting type provides significant advantages, including a higher temperature lift, greater heat storage capacity, and scalability. This study presents a dynamic model of an innovative SG-THT technology under development for waste heat upgrading for process heating applications in the range of 200-300℃, using $SrBr_2.H_2O$ as the working pair due to its stable chemical properties and high energy density. The system is programmed in Modelica and dynamically simulated to track its chemical reactions within the hydration and dehydration reactors. The results indicate the maximum temperature lift of the system to be 84.59℃ under the considered realistic operational conditions at an overall thermal energy efficiency of 66.65%. The results indicate that the proposed SG-THT system can show a satisfactory performance in transient conditions such as fluctuating off-design loads, start-up, and shutdown demonstrating its capability for making a potential role in the industrial sector decarbonization. This dynamic simulation provides important information for designing the system more effectively to reach better efficiency levels, reducing capital and operational costs, and cope better with use case dynamics.

***Keywords*:** Solid-gas thermochemical heat transformer, Industrial waste heat, Heat upgrading, Process heating.

1. Introduction

Industries are among the largest energy end-users across all sectors [1]. So, there is a huge demand of energy, especially as heat in different temperature levels, to drive the industrial processes, which is mainly supplied by fossil fuels. Unfortunately, a big portion of the called energy by industries is wasted as low-, medium, and even sometimes high-temperature heat. Therefore, an immediate solution towards enhancing the sustainability of the industrial sector- and thereby the entire global energy systems- can be waste heat recovery from the industrial processes to reduce environmental pollution. Due to the low quality of energy in low-grade waste heat streams as well as the mismatch of the demand and available temperature in medium and high temperature waste streams, efficient technologies are needed to upgrade their temperature after recovery. THTs have been introduced as a promising class of technologies for heat recovery and temperature lifting in industries [2]. Among different types of these, SG-THTs offer significant advantages such as high energy density and scalability.

Recently, various theoretical and experimental studies have been conducted on SG-THT systems. Li et al. [3] proposed a solar-based SG-THT system for domestic hot water production and evaluated its performance in terms of energy, exergy, economy, and environmental aspects. The results showed that the proposed system with strontium bromide hexahydrate ($SrBr_2.6H_2O$) salt can be an attractive option. The energy efficiency, exergy and CO_2 emission rates for this system were reported to be 76.3%, 89.2% and 0.115 kg/kWh, respectively. Malleswararao et al. [4] proposed several configurations for waste heat recovery of high temperature heat pumps. They used a K_2CO_3 salt-based SG-THT system for heat recovery and demonstrated that a specific configuration of this system can lead to an optimal arrangement, reaching an overall system efficiency of 85.3% at 145℃. The SG-THT system was also capable of lifting the temperature of the recovered heat to the temperature range of 120–165℃. Michel et al. [5] conducted an experimental study on a $CaCl_2$ salt-based SG-THT system, showing the specific power of 341 W/kg and temperature lift of 60℃ for this system, respectively. Stengler et al. [6] experimentally and numerically investigated a $SrBr_2$ salt-based SG-THT system with a capacity of 1 kW. This study focused on the performance of the reactors, and they concluded that this system is capable to store and upgrade heat at a quite high efficiency. They also showed that an efficient reactor design may enhance the heat transfer between the heat transfer fluid (HTF) and the salt, and thereby the system's overall performance. Stengler et al. [7] continued their studies by showing that strontium bromide monohydrate ($SrBr_2.H_2O$) salt was able to increase temperature by 100℃ and this working pair maintained its stability after 34 charging/discharging cycles. Michel et al. [8] conducted a dynamic study on the SG-THT system and investigated the effects of different working pairs. This study was based on the chemical reaction carried out in reactors and their results show that $SrBr_2$ and $CaCl_2$ salt-based working pairs have better performance and temperature lifting than others.

Most studies have focused on theoretical and experimental modeling of chemical reactors, while those addressing system-level design have not been dynamically investigated. Therefore, in the present study, the dynamic performance of a SG-THT system with $SrBr_2.H_2O$ has been investigated. $SrBr_2.H_2O$ has significant advantages such as stable chemical properties and high energy density. The dynamic modelling and simulation here is used to investigate the progress of the chemical reaction and the system performance over time. This model shows the temperature changes of the salt, as well as the outgoing HTF during the hydration and dehydration processes. The amount of recovered heat, and the upgraded heat for reuse depend on the temperature of the salt and the HTF, which are the most significant parameters in this system. Another parameter is the working pressures of the SG-THT, which affect the progress of the chemical reaction in the system. The system overall description, the mathematical model of the THT, and the simulation results along with their interpretations come in the following sections.

2. System Description

The overall schematic of the proposed SG-THT system is shown in Fig. 1.

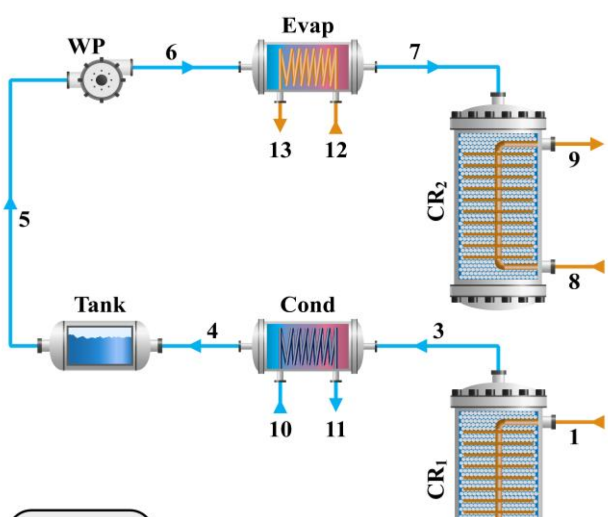

Fig. 1: Schematic overview of the proposed SG-THT system

The proposed system works as a batch process. This system generally consists of two main processes: hydration and dehydration. In the first phase, the oil flow carries industrial waste heat to the proposed system (states 1 and 12), and after heat recovering in the next step, it gets out of the system (states 2 and 13). The dehydration process in the CR_1 reactor is considered an endothermic process. In this process, water molecules in the monohydrate salt are evaporated by receiving waste heat. The released steam enters the Tank as a saturated liquid after passing through the condenser (states 3 and 4). Next, the WP pumps the stored water in Tank up to the high pressure of the system (states 5 and 6). The high-pressure water changes phase to steam after passing through the evaporator and enters the CR_2 reactor (stage 7), and the hydration process begins in the following. This process is known as an exothermic process which produces significant heat. The generated heat is transferred to the thermal oil for industry use (states 8 and 9).

3. Dynamic Modelling

The reversible thermochemical reaction for the strontium bromide monohydrate is as follows [6]:

$$SrBr_2.H_2O(s) \rightleftharpoons SrBr_2(s) + H_2O(g) + \Delta H_R \tag{1}$$

where, the ΔH_R indicates the enthalpy of the reaction.
The reaction rate ($\frac{dX}{dt}$) and the pressure-dependent reaction temperature for the dehydration process are obtained from the following empirical equations proposed by Ref. [6]:

$$\frac{dX}{dt} = (1.38 \cdot 10^6) \cdot exp\left\{\frac{-75.7 \cdot 10^3}{R \cdot T}\right\} \cdot (1 - X) \cdot \left(1 - \frac{P_{Cond}}{P}\right)^{0.25} \tag{3}$$

$$log\left(\frac{P}{P_{Ref}}\right) = 14.69 - \frac{6.41 \cdot 10^3}{T} \tag{4}$$

for the hydration process, these are formulated as follows [6]:

$$\frac{dX}{dt} = (3.04 \cdot 10^{-5}) \cdot (1 - X) \cdot \left(T_{@P_{Evap}} - T\right)^{1.79} \tag{5}$$

$$log\left(\frac{P}{P_{Ref}}\right) = 8.18 - \frac{3.19 \cdot 10^3}{T} \tag{6}$$

here, R indicates the universal gas constant, P and T are equilibrium pressure and temperature, respectively. $T_{@P_{Evap}}$ is the saturation temperature at the evaporator pressure and P_{Cond} represents the condenser pressure. The first law of thermodynamics is used to model the system for each control volume. The mass and energy balance for a control volume under dynamic conditions will be as:

$$\frac{dm}{dt} = \dot{m}_{In} - \dot{m}_{Out} \tag{7}$$

$$\frac{dH}{dt} = \dot{Q} - \dot{W} + \sum(\dot{m} \cdot h)_{In} - \sum(\dot{m} \cdot h)_{Out} \tag{8}$$

where, m, $\dot{m}$, $\dot{Q}$ and $\dot{W}$ represent mass, mass flow rate, heat rate and power, respectively. The overall thermal efficiency of the SG-THT system in the heat upgrading mission can be calculated via dividing the upgraded heat by the recovered waste heat:

$$\eta_{Th} = \frac{\int \dot{Q}_{Hyd}\, dt}{\int \dot{Q}_{Deh}\, dt + \int \dot{Q}_{Evap}\, dt} \tag{9}$$

The design parameters and operating conditions of SG-THT system are presented in Table 1. It should be noted that the sensible heat of the steam outflow from the dehydration reactor before entering the condenser is considered to be negligible and is therefore not included in this analysis. In reality, this heat accounts for approximately 4–5% of the total energy output of the system and could potentially be utilized. However, since the temperature of the stream is somewhat that could only be used for secondary purposes such as district heating supply, it is kept out of the scope of this study's design.

Table 1: Design and operational conditions of the proposed system.

Parameter	Variable	Value	Unit
Ambient pressure	P_{Amb}	101.325	kPa
Ambient temperature	T_{Amb}	20	℃
Condenser pressure	P_{Cond}	4.0	kPa
Evaporator pressure	P_{Evap}	350.0	kPa
Initial dehydration temperature	$T_{Deh,init}$	200.0	℃
Initial hydration temperature	$T_{Hyd,init}$	260.0	℃
Reaction enthalpy	ΔH_R	71.98	kJ/mol
Reference pressure	P_{Ref}	1.0	kPa
Universal gas constant	R	8.314	$kJ/mol \cdot K$
Upgrade heat stream mass flow rate	$\dot{m}_8$	0.2052	kg/s
Waste heat stream mass flow rate	$\dot{m}_1$	0.44	kg/s

4. Results and Discussion

The SG-THT system is dynamically modelled in Modelica based on the design conditions and the first laws of thermodynamics presented in the previous section. The simulation results are presented and discussed in this section.

4.1. Verification of Modelling

The results obtained from the dynamic model of the SG-THT system have been compared with the experimental results of Ref. [6] to evaluate the accuracy of the developed model.

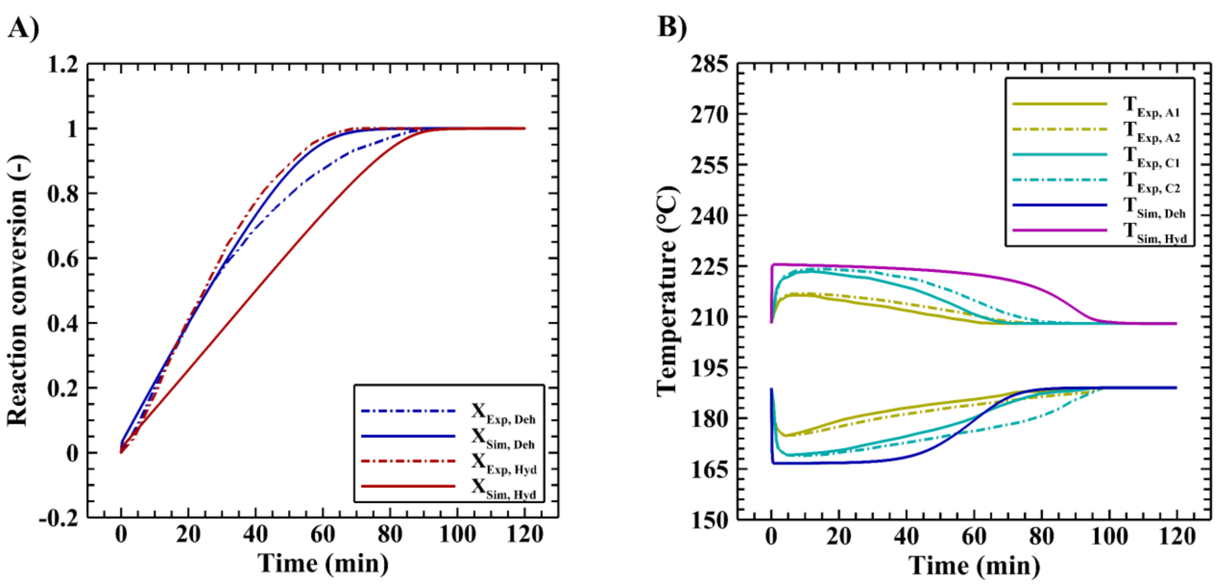

Fig. 2: Experimental and simulated results of dehydration and hydration processes of strontium bromide monohydrate salt: A) The changes in reaction conversion with respect to time, B) The changes in salt temperature with respect to time.

In the reference study, i.e. Ref. [6], the laboratory setup consists of a packed bed chemical reactor containing 5.059 kg of $SrBr_2.H_2O$. The starting temperatures of the dehydration and hydration reactions are 189℃ and 208℃, respectively. As shown in Fig. 2, the modelling results follow the experimental results well; however, a time difference is evident in both processes, which can be due to the simplifications made in the modelling of the SG-THT system, known as the lumped model.

4.2. Thermodynamic Analysis Results

The proposed SG-THT system is designed for heat recovery and temperature elevation for reuse. This system can boost the temperature of industrial waste heat up to 284.59℃ within approximately 132 minutes. The Clausius-Clapeyron diagram of the proposed system is shown in Fig. 3.

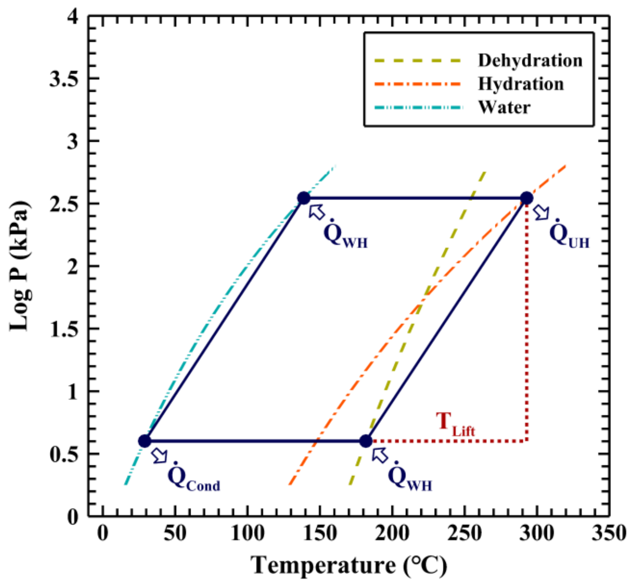

Fig. 3: The Clausius-Clapeyron diagram of the proposed SG-THT system.

The Clausius-Clapeyron diagram includes the liquid-vapor (L-V) and solid-gas (S-G) equilibrium lines. The S-G lines are drawn based on Eqs. 4 and 6 for the hydration and dehydration processes. Initially, the H_2O molecules in the monohydrate salt change phase from solid to gas by absorbing 82.00 MJ of heat in the S-G region. Then, they release 46.37 MJ of heat in the L-V region while converting from gas to liquid. Subsequently, liquid water transitions to the gas phase by absorbing 45.86 MJ of heat in the L-V region and then transitions from gas to solid by releasing 85.22 MJ of heat in the S-G region. The temperature of the released heat in the S-G region ranges from 260℃ to 284.59℃. Frequent phase transitions reduce the system's dependence on electrical energy. The power consumption of the pump for increasing the pressure from 4 kPa to 350 kPa is negligible. Based on the thermodynamic analysis of the proposed system, thermal efficiency has been determined to be 66.65%, indicating effective heat recovery and temperature upgrading.

The overall performance of the SG-THT system is directly affected by the chemical reactions in the hydration and dehydration reactors. The temperature of the salt and the amount of absorbed or released heat depend on the reaction conversion and vary over time. To better understand the reactors' dynamic behavior, the variations in these three parameters are presented in Figs. 4-6. The dehydration reaction begins with the absorption of heat from HTF, which leads to a rapid decrease in the temperature of salt. Upon completion of the reaction, the temperature of the salt returns to its original value. In contrast, the hydration reaction begins with steam entering the reactor, and the temperature of the salt first increases and then gradually decreases as the reaction progresses. The time it takes for the salt temperature to rise or fall at the end of the process is slightly longer than the reaction time, because at the end of the reaction, the salt retains some sensible heat, causing a slight time difference between the two stages.

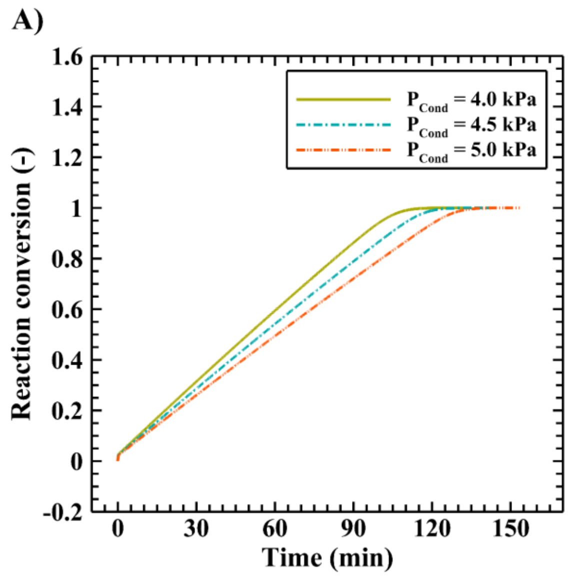

Fig. 4: Changes in reaction conversion over time and the effect of pressure on it: A) Dehydration process, B) Hydration process.

The duration of the reaction is directly dependent on the heat transfer rate to/from the reactor. Therefore, the mass flow rate of the HTF is adjusted so that both processes are completed in the same period. Also, the thermal power of the system is a function of the HTF outlet temperature and follows similar trends of salt temperature changes. According to Fig. 6, the maximum heat absorption and release rates in the dehydration and hydration processes are 13.48 and 14.35 kW, respectively.

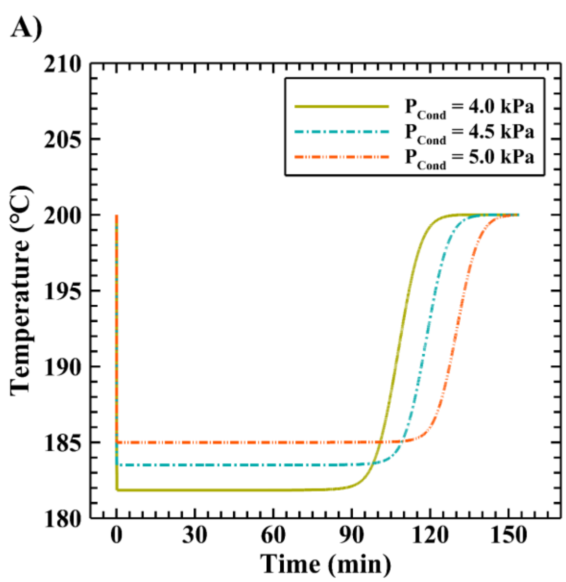

Fig. 5: Changes in salt temperature over time and the effect of pressure on it: A) Dehydration process, B) Hydration process.

Other key factors in system performance are condenser and evaporator pressures. The minimum temperature of the salt in the dehydration process and its maximum temperature in the hydration process are directly dependent on the pressure-dependent reaction temperature (i.e., the condenser and evaporator pressures, respectively). Therefore, changing the pressure can improve the heat recovery ability and the temperature lift. According to Figs. 4-6, increasing pressure causes an increase in the duration of the dehydration reaction and reduces the system's ability to recover heat. In contrast, the hydration process exhibits a different behaviour, such that with increasing pressure, the reaction time decreases and the system's ability to increase temperature increases.

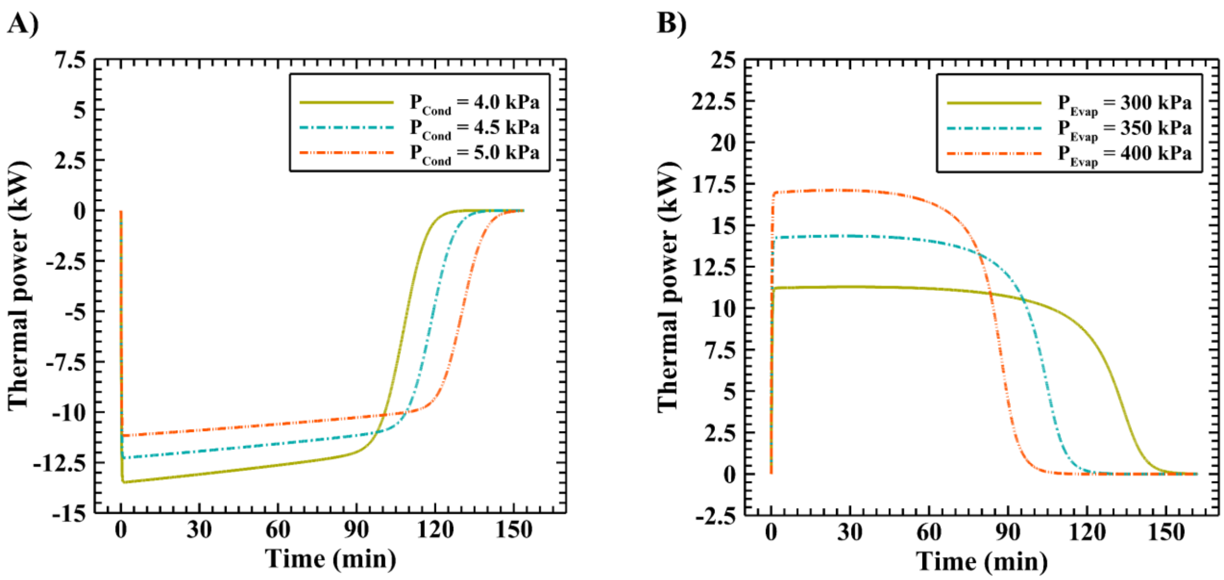

Fig. 6: Changes in thermal power over time and the effect of pressure on it: A) Dehydration process, B) Hydration process.

5. Conclusion

This study investigated the dynamic performance of a novel SG-THT system under development by TechUPGRADE consortium [9] for upgrading industrial waste heat temperature for direct reuse in industrial process heating applications. The specific configuration of TechUPGRADE being investigated here can lift the temperature of waste heat streams up to 284.59℃ depending on the conditions considered for the dehydration and hydration processes. Thermodynamic analyses indicates that a setup of the THT using 250 kg of $SrBr_2.H_2O$ is capable of supplying 23.67 kWh of upgraded heat at the overall thermal efficiency of 66.65%. System performance analysis shows that HTF mass flow rate in hydration and dehydration processes, condenser pressure, and evaporator pressure have significant impacts on the efficiency of the system. Therefore, determining their optimal values is essential to reach higher efficiency levels. The findings further show that detailed dynamic modeling of the system is essential for gaining a deep understanding of its operation in real-life conditions and its behavior under transient and partial load conditions. This knowledge is crucial for designing a highly effective THT system for real-world industries.

Nomenclature

Nomenclature		*SG-THT*	Solid-Gas THT
h	Specific enthalpy (kJ/kg)	*Sim*	Simulated
H	Enthalpy (kJ)	*THT*	Thermochemical heat transformer
m	Mass (kg)	*UH*	Upgrade heat
$\dot{m}$	Mass flow rate (kg/s)	*WH*	Waste heat
P	Pressure (kPa)	*WP*	Water pump
$\dot{Q}$	Rate of heat transfer (kW)		
R	Universal gas constant (J/mol.K)	**Subscripts**	
T	Temperature (K)	*Deh*	Dehydration

$\dot{W}$	Power (kW)	*Hyd*	Hydration
X	Reaction conversion (-)	*In*	Input
		Out	Output
Abbreviations		*R*	Reaction
Cond	Condenser	*Ref*	Reference
CR	Chemical reactor	*Th*	Thermal
Evap	Evaporator		
Exp	Experimental	**Greek symbol**	
HTF	Heat transfer fluid	η	Efficiency

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