DOI: 10.15669/pnst.7.267

Progress in Nuclear Science and Technology
Volume 7 (2025) pp. 267-272

ARTICLE

A numerical study on Carnot Battery using chemical heat storage/pump and brayton cycle

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Carnot batteries are promising energy systems for storing surplus electricity generation from renewable energy. Their charge-discharge cycle consists of converting electricity into heat, storing it by means of heat storage technology, and reusing the heat to run a thermal cycle on demand. In this paper, the possibility of using a chemical heat storage/pump in a Carnot battery was investigated. The focus is on the heat output operation involving the exothermic hydration of calcium oxide. In order to find insights for the design of new heat exchangers for packed-bed reactors, a multi-objective optimization approach was used. A numerical model simulating heat transfer with chemical reaction was combined with the energy balance of a Brayton cycle using supercritical carbon dioxide. Starting from a certain configuration, a parametric study determined the optimal half-thickness of the packed bed sections (s=11 mm), while screening of the contact thermal conductance γ showed that 150 $Wm^{-2}K^{-1}$ can be considered an appropriate recommended value. These parametric studies, however, resulted in a maximum increase of +0.8% in turbine power output. The implementation of a genetic algorithm allowed the introduction of a multi-objective optimization approach, quickly finding the optimal packed bed and channel geometry, which resulted in a +3.0% increase in power output, with room for further improvement.

Keywords: Carnot Battery; chemical heat storage; calcium hydroxide; supercritical carbon dioxide; Brayton cycle; multi-objective optimization

Nomenclature

bed	packed bed
comp	compressor
cond	condenser
conv	convection
hyd	hydration
turb	turbine
sCO_2	supercritical CO_2
a	horizontal size of channel [m]
b	vertical size of channel [m]
c	specific heat capacity [J $kg^{-1}K^{-1}$]
D_{eq}	equivalent diameter [m]
f	friction coefficient [-]
h	specific enthalpy [kJ kg^{-1}]
L	length of the channel [m]
m’	mass flow [kg s^{-1}]
n	number of channels [#]
Nu	Nusselt number [-]
P	pressure [kPa]
Pr	Prandtl number [-]
Q	heat power [W]
Re	Reynolds number [-]
s	half-thickness of the packed bed reactor [m]
t	time [s]
T	temperature [°C]
v_m	mean velocity of sCO_2 flow [m s^{-1}]
W	Mechanical power [W]
x	reacted fraction [-]
α_{conv}	convection heat transfer coefficient [$Wm^{-2}K^{-1}$]
γ	thermal contact conductance [$Wm^{-2}K^{-1}$]
Δt	time step [s]
ΔH	hydration reaction enthalpy, 1404 [kJ/kg]
ε	efficiency of the packed bed reactor heat exchanger [-]
η	thermal efficiency of the Brayton cycle [-]
λ	thermal conductivity [$Wm^{-1}K^{-1}$]
μ	viscosity [Pa s]
ξ	efficiency of regenerator [-]
ρ	density [kg m^{-3}]

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1. Introduction

Renewable energy sources such as solar and wind power play a crucial role in decarbonizing society. However, their generation is not easily scheduled based on energy demand, necessitating the need for energy storage to manage surplus energy and ensure grid stability. Battery storage, such as lithium-ion, sodium sulfur, or flow batteries, is one option extensively reviewed by Koohi-Fayegh et al. [1]. Another alternative is Carnot batteries, which convert electricity to heat, store it, and convert it back to electricity on demand through a thermodynamic cycle, as reviewed by Dumont et al. [2]. Sensible or latent heat accumulators are commonly used in these systems. Zamengo et al. [3] proposed a calcium hydroxide-based thermochemical heat storage for a Carnot battery, coupled with a supercritical CO_2 (sCO_2) Brayton cycle. Initial analysis estimated a theoretical round-trip efficiency of 42% by leveraging the heat pump effect of chemical heat storage. However, the model lacked a detailed analysis of heat transfer in the packed-bed reactor and its components, which is crucial for efficient design. While some packed-bed reactors with heat exchangers have been experimentally tested, like in Schmidt et al. [4], a comprehensive design methodology is still lacking. In this study, a genetic algorithm is employed for multi-objective optimization of the cycle and the packed-bed reactor heat exchanger. This approach was previously applied by Zamengo et al. [5] for optimizing composite materials in a packed-bed reactor. The current work extends this methodology to include the packed-bed reactor heat exchanger and thermodynamic cycle. The optimization algorithm aims to determine the optimal size of the heat exchanger to maximize turbine power output and cycle efficiency. The model is versatile and can be adapted to other geometries and cycles. This proposed methodology holds promise as a valuable tool for the efficient design of new energy storage systems.

2. Experimental

2.1. Description of the Carnot Battery system

Figure 1 a) shows the schematic of the Carnot battery system with thermochemical heat storage, while **Figure 1 b)** presents the corresponding thermodynamic states on a T-s diagram. This study focuses on the output mode with hydration reaction occurring in the packed bed. The exothermic reaction between CaO and water vapor releases heat, transferred to an sCO_2 stream for a closed-loop Brayton cycle. Heat storage mode (dehydration reaction) is not addressed here, it is assumed that heat storage operation is accomplished by resistive heating in an earlier stage. Funayama et al. [6] provide a lab-scale implementation of this chemical heat storage material using calcium hydroxide pellets. **Figure 1 c)** displays the structure of the packed-bed heat exchanger, where water vapor is evenly distributed for the hydration reaction.

2.2. Numerical model of the Carnot Battery system

The Carnot battery of Figure 1 a) can be modeled numerically by evaluating the enthalpy balance of each component. The relationships are listed below:

Compressor:

$$W_{comp} = m' \cdot (h_2 - h_1) \tag{1}$$

Regenerator:

$$m' \cdot (h_3 - h_2) = m' \cdot \xi \cdot \left(h_{6,max} - h_5\right) \tag{2}$$

Reactor:

$$Q_{hyd} = m' \cdot (h_4 - h_3) \tag{3}$$

Turbine:

$$W_{turb} = m' \cdot (h_5 - h_4) \tag{4}$$

Condenser:

$$Q_{cond} = m' \cdot (h_1 - h_6) \tag{5}$$

This study aims to optimize heat transfer between the packed-bed reactor and an sCO_2 stream, which acts as both the heat transfer fluid and the working fluid in a Brayton cycle. The focus is on multi-objective optimization to determine the ideal combinations of dimensions (*a*, *b*, and *s*) while maintaining a fixed reactor length of 1000 mm with 10 channels. The numerical model incorporates kinetics of the hydration reaction, convection heat transfer between the heated bed and sCO_2 flow, and associated pressure drop. The system of Eqs. (1) through (5) is iteratively solved over a 5-second time interval, updating the reactor temperature and related thermophysical properties and states of the materials. The numerical model primarily emphasizes heat transfer, combining the heat transfer equation with heat generation from the chemical reaction in the solid packed bed and fluid flow in a heat exchanger.

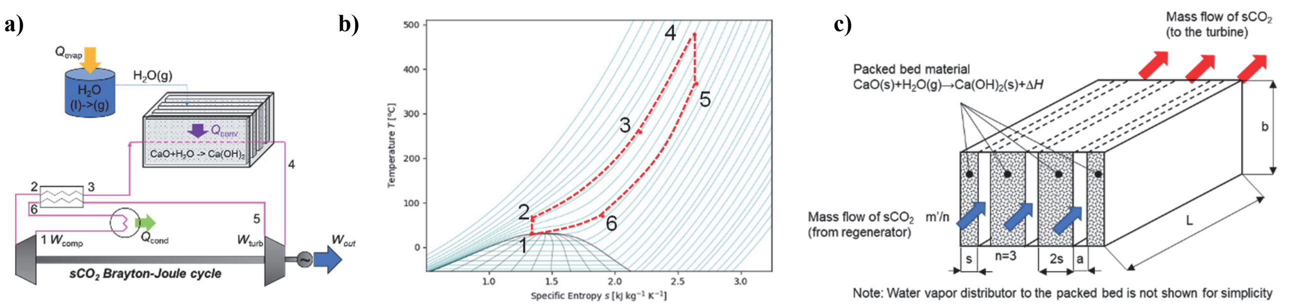

Figure 1. a) The schematic of the Carnot Battery (output mode) comprising packed bed reactor heat exchanger investigated in this work, b) the T-s diagram of the cycle, c) The schematic of the packed bed object of optimization.

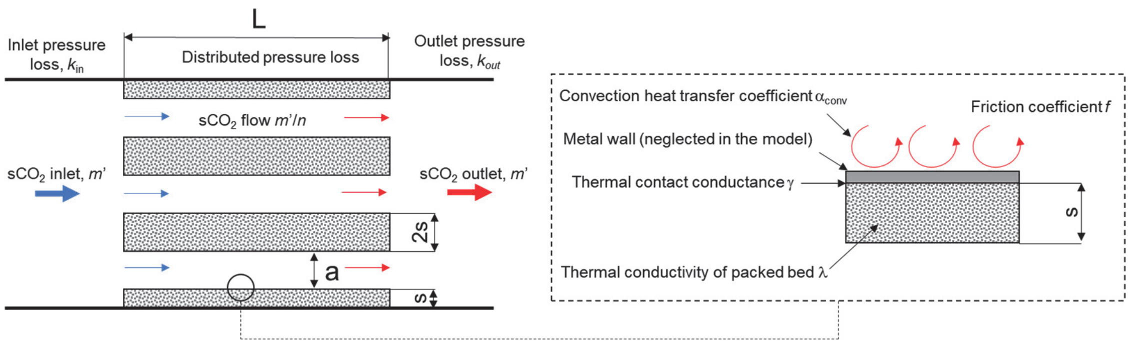

Figure 2. The schematic of the main aspects included in the numerical model of heat transfer with chemical reaction and pressure loss on sCO_2 flow.

The influence of thermal contact conductance γ on overall performance and pressure losses in the sCO_2 flow are also considered. **Figure 2** illustrates the main aspects analyzed in the model.

The global heat transfer coefficient K to be updated at each time step is provided by the following relationship:

$$K = \frac{1}{\frac{1}{\alpha_{conv}} + \sum \frac{s}{\lambda} + \frac{1}{\gamma}} \tag{6}$$

A coefficient of thermal contact conductance $\gamma = 50$ $Wm^{-2}K^{-1}$ is considered constant between the packed bed material and the reactor wall. As for the thermal diffusion in the packed bed, the analysis assumes a change in the thermal conductivity of the packed bed from 0.2 $Wm^{-1}K^{-1}$ of CaO to 0.4 $Wm^{-1}K^{-1}$ of $Ca(OH)_2$ as a function of the progress of the hydration reaction x_h. The half-thickness of the packed-bed reactor s is considered in the equation, while the metallic wall thickness and its thermal conductivity are neglected because they are considered to be smaller than the other terms. In this analysis, the temperature calculated from kinetics is assumed to be homogeneous within each reactor partition. Edge effects and heat losses to the environment are also not included in this study. The flow velocity v_m in each of the n reactor channels is expressed by the following relationship:

$$v_m = \frac{m'/n}{\rho_{sCO_2} \cdot a \cdot b} \tag{7}$$

where m' is the total mass flow rate of sCO_2. The channel's cross-section has a rectangular shape (a x b), therefore the equivalent diameter is given by:

$$D_{eq} = \frac{4(a \cdot b)}{2(a+b)} \tag{8}$$

The Reynolds number is then obtained:

$$Re = \frac{\rho_{sCO_2} \cdot v_m \cdot D_{eq}}{\mu_{sCO_2}} \tag{9}$$

Depending on the resulting value of Re, the flow can be categorized as laminar ($Re < 2100$) or turbulent. This affects both the heat transfer coefficient α_{conv} and the pressure drop of the reactor. In case of laminar flow, the friction coefficient is given by:

$$f = 64/Re \tag{10}$$

while in case of turbulent flow the Blasius relation for smooth tubes is:

$$f = 0.316 \cdot Re^{-0.25} \tag{11}$$

The distributed pressure loss ΔP [kPa] is calculated using the Colebrook-White equation (k=1):

$$\Delta P = k \cdot f \cdot \frac{L}{D_{eq}} \cdot \rho_{sCO_2} \cdot \frac{v_m^2}{2} \tag{12}$$

Moreover, the localized pressure loss at the inlet and the outlet of the packed bed reactor are estimated and summed to the distributed ones by using respectively k_{inlet}=0.5 and $k_{outlet} = (1-\beta)^2$ on Eq. (12) where:

$$\beta = \frac{flow\ cross\ section}{total\ cross\ section} = \frac{a \cdot b \cdot n}{b \cdot (a+2s) \cdot n} \tag{13}$$

Concerning the heat transfer coefficient, α_{conv}, it is necessary to determine the Nusselt number, Nu, accordingly to the following relationships (Gnielinski [7]) valid for single-phase flow between parallel plates:

$$\begin{cases} Nu = 3.78 \ \text{when } \mathrm{Re} \cdot \mathrm{Pr} \cdot \frac{a}{L} < 100 \\ Nu = 1.468 \cdot \sqrt[3]{Re \cdot Pr \cdot \frac{a}{L}} \ \text{when } \mathrm{Re} \cdot \mathrm{Pr} \cdot \frac{a}{L} > 100 \end{cases} \tag{14}$$

Then, α_{conv} is obtained from Nu as follows:

$$\alpha_{conv} = Nu \cdot \frac{\lambda_{sCO_2}}{a} \tag{15}$$

The kinetics of hydration reaction is obtained from the following relationships found on Schaube et al. [8]:

$$\frac{dx_{hyd}}{dt} = 1.0004 \cdot 10^{-34} e^{\left(\frac{53.332 \cdot 10^3}{T_{bed}}\right)} \cdot \left(\frac{P}{10^5}\right)^6 \cdot (1 - x_{hyd}) \quad (16)$$

The pressure of water vapor P is assumed 95.6 kPa (saturation temperature of 98°C), while T_{bed} is the temperature of the packed bed (assumed uniform in the whole sections). The packed bed reactor temperature is estimated at each time step: its value satisfies the heat balance between the exothermic heat of hydration generated during the time interval Δt, the heat transferred to the sCO_2 and the sensible heat accumulated on the packed bed accordingly to Eq. 17.

$$T_{bed} = T_{bed}^0 + \frac{\Delta H \Delta x_h}{c_{bed}} - \frac{Q_{conv} \Delta t}{\varrho_{bed} c_{bed} ((2s + a) \cdot n \cdot b \cdot L)} \quad (17)$$

The packed bed reactor heat exchanger is designed using the ε-NTU method. After having determined the values of global heat transfer coefficient K, the extension of the heat exchange surface and the heat capacity of the sCO_2 flow, the value of NTU can be determined as:

$$\mathrm{NTU} = \frac{K(2 \cdot b \cdot L \cdot n)}{m' \cdot c_{sCO_2}} \quad (18)$$

And then the efficiency ε:

$$\varepsilon = 1 - e^{-NTU} \quad (19)$$

Considering the heat capacity of the flowing stream of sCO_2, it is possible to calculate the values of enthalpy at the outlet of the packed bed reactor heat exchanger using the following equation in replacement of Eq. 3.

$$Q_{conv} = m' \cdot \varepsilon \cdot \left(h_{@T_{bed}} - h_3\right) \quad (20)$$

Based on the energy balance between the packed bed and the sCO_2 flow, certain temperature and pressure conditions are obtained at the turbine inlet, which affect the power output W_{turb} and the thermal efficiency of the cycle η:

$$\eta = \frac{W_{turb} - W_{comp}}{h_4 - h_3} \quad (21)$$

A constant isentropic expansion efficiency value of 0.92 was assumed for the turbine and 0.89 for the compressor. Thermophysical properties of sCO_2 were obtained from the implementation of the CoolProp library in the Python environment [9]: their values were updated in function of the time-dependent temperature evolution.

2.3. Multi-objective optimization algorithm.

The NSGA-II algorithm present in the OPTUNA Python library by Akiba et al. [10] was included as a part of the numerical model to propose at each iteration a new set of selected values of the parameters being optimized: these are the size of the channels, a and b, and the half-thickness of the packed bed, s. The algorithm selects by genetic sorting the best combinations of parameters that can simultaneously maximize the average turbine power output and Brayton cycle efficiency. For the optimization study, the minimum and maximum limit values for each parameter are established (summarized in **Table 1**). The total number of combinations is more than $1.125 \cdot 10^6$, but the algorithm converges to the optimal values within a much smaller number of trials.

Table 1. Parameters and boundaries utilized for the multi-objective optimization.

Parameters and boundaries for optimization	Minimum	Maximum	Step
Channel width, a [mm]	1	50	1 [mm]
Channel height, b [mm]	100	1000	1 [mm]
Half-thickness of packed bed, s [mm]	5	30	1 [mm]

3. Results and discussion

The numerical model of the Brayton cycle with regeneration was first validated against a literature example found in Todreas et al. [11] and showed no discrepancies from the reported values. Then, it was modified to include the packed-bed reactor and corresponding heat exchanger to heat the sCO_2 stream through the exothermic heat of the CaO hydration reaction. The starting temperature of the sCO_2 stream and heat exchanger of the packed-bed reactor is considered to be 460°C. As an example of the results obtained, the temperature evolution in the packed bed and sCO_2 stream is shown in **Figure 3(a)**. The graph includes also the total reacted fraction x_{hyd} in the packed bed sections. The corresponding values of turbine output power W_{turb} and thermal efficiency η are shown in **Figure 3(b)**. The results indicate that the power output is almost constant and decreases as soon as the reaction reaches full conversion (x_{hyd}=1). The plot in **Figure 4a** illustrates the results of a parametric study on the packed bed half-thickness, s. The optimal value was determined to be s=11 mm, resulting in a +0.1% increase in power compared to the example in Figure 3, where s=20 mm. Additionally, varying the thermal contact conductance γ while applying the model led to the results shown in **Figure 4b**. Using γ=300 $Wm^{-2}K^{-1}$ yielded a benefit of +0.8% increase in the original power output. It was observed that for γ values greater than 150 $Wm^{-2}K^{-1}$, there was no further improvement in the contact condition between the wall and packed bed materials. Attaining such elevated values can also pose a challenge as chemical heat storage materials are commonly comprised of compacted powders or pellets. Furthermore,

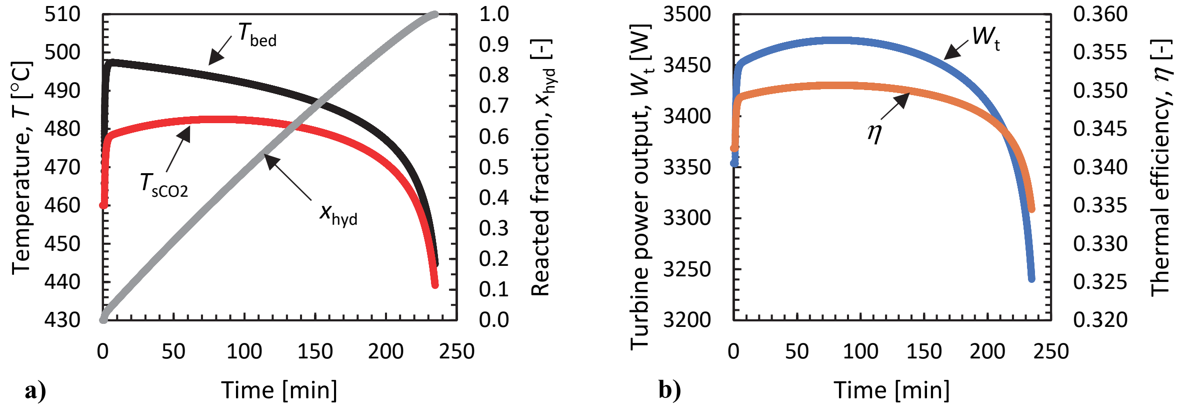

Figure 3. a) Temperature evolution in the packed bed sections and on the sCO_2 flow, b) the corresponding power output from the turbine, W_t, and thermal efficiency η of the Brayton cycle. In this example a=3 mm, b=500 mm, c=1000 mm, s=15 mm, n=10 and m'=0.03 kg/s.

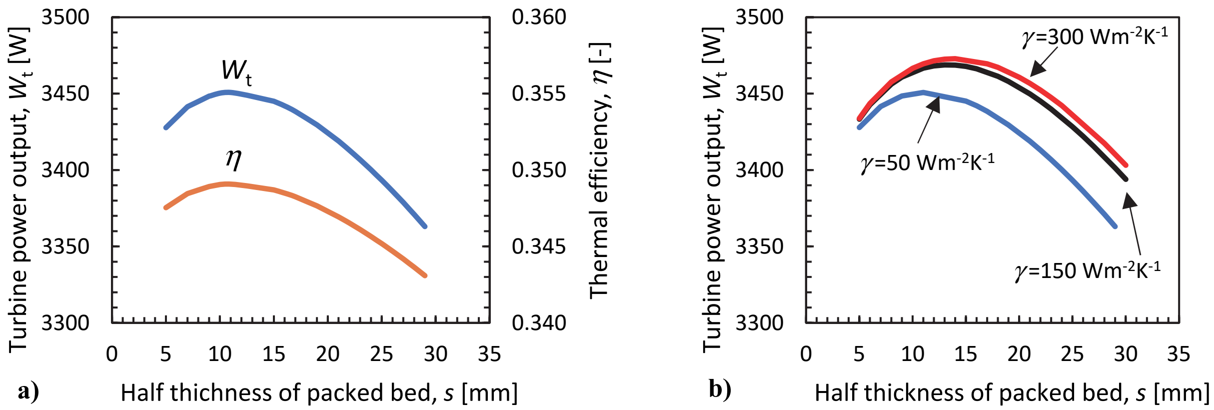

Figure 4. a) Results of the parametric study on the half-thickness of the packed bed, s, b) Results the of parametric study on the value of thermal contact conductance γ. In both the study, a= 3 mm, b =500 mm, c=1000 mm, n=10 and m'=0.03 kg/s.

Table 2. Results of parametric studies and from the multi-objective optimization.

Parameter	Original	Bed size (parametric study)	Bed size and thermal contact (parametric study)	Bed and channel sizes (optimization with NSGA-II)
Channel width, a [mm]	3	3	3	1
Channel height, b [mm]	500	500	500	958
Channel length, L [mm]	1000	1000	1000	1000
Half-thickness of packed bed, s [mm]	20	11	14	21
Number of channels, n [#]	10	10	10	10
Mass flow rate, m' [kg/s]	0.03	0.03	0.03	0.03
Thermal contact conductance γ[Wm^{-2}K^{-1}]	50	50	300	50
Average power W_{turb} [W]	3445	3451(+0.1%)	3473(+0.8%)	3547 (+3.0%)
Average thermal efficiency η [-]	0.349	0.349	0.350	0.355
Ratio of surface for heat exchange [-]	1	1	1	1.916
Ratio of pressure loss [-]	1	1.008	1.022	0.537

it was noted that higher thermal contact conductance allowed for the utilization of thicker beds, with the optimal value of s being 14 mm.

However, this parameter screening did not significantly enhance performance, as indicated by the results in **Table 2**, where pressure losses increased proportionally compared to the original configuration. To comprehensively screen all multiple parameters, including the full geometry of channels, extensive computational efforts are required, and finding the optimal configuration through cross comparisons can still be complex. By implementing the NSGA-II algorithm, the best channel dimensions (a, b) and the half-thickness of the packed bed (s) were determined in just 200 iterations. The results in Table 2 demonstrate that the NSGA-II-optimized geometry can increase power output by +3.0% compared to the original configuration by maximizing heat transfer between the packed bed and the sCO_2 stream while reducing pressure losses. This optimization aims to achieve the highest enthalpy (h_4), corresponding to higher temperature and pressure. It was found that the NSGA-II-optimized configuration had a larger surface area for heat exchange and reduced pressure losses, emphasizing the significance of heat transfer in overall performance.

4. Conclusion

A numerical model was developed for the study of a Carnot battery system using thermochemical heat storage. Under certain design constraints, a parametric study identified the optimal value of the half-thickness as 11 mm. The effect of thermal contact conductance was also analysed, showing that a conductance higher than 150 $Wm^{-2}K^{-1}$ does not affect performance, inferring that the limitations to heat transfer are given by the thermal conductivity of the packed bed. Finally, it was shown that multi-objective optimization of the heat transfer of the packed-bed reactor can play an important role in the efficient design of components and maximization of cycle performance for Carnot batteries. The genetic algorithm quickly converges to the optimal solutions, enabling rapid design of the packed-bed reactor heat exchanger: it was shown that, for a fixed number of channels n and length c, the optimized sizes of a, b, and s provided a 3.0% power increase rather than optimizing performance by acting on a single parameter. The methodology is general and can be further extended by setting other parameters to be optimized, such as the amount of filler to increase the thermal conductivity of packed bed materials.

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