Lu YJ, Roskilly AP, Tang K, Wang YD, Long J, Yuan Y, Wang LW.
[Investigation and performance study of a dual-source chemisorption power generation cycle using scroll expander.](#)

Applied Energy 2017

DOI: <https://doi.org/10.1016/j.apenergy.2017.02.068>

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DOI link to article:

<https://doi.org/10.1016/j.apenergy.2017.02.068>

Date deposited:

17/03/2017

Embargo release date:

02 March 2018

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Investigation and performance study of a dual-source chemisorption power generation cycle using scroll expander

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HIGHLIGHTS

- A novel dual-source chemisorption power generation was proposed and studied
- Evaluation of the system performance using different working pairs
- Pressure controlling method was introduced to control power output
- Investigation of the dynamic system performance was conducted

Abstract

Development of novel heat recovery system attracts ever increasing attentions to convert wasted heat into useful energies. This paper reports the study of a novel dual-source chemisorption power generation cycle using scroll expander to recover dual heat sources. The proposed chemisorption power generation system contains four adsorption beds and two expansion machines for simultaneously and continuously producing electricity by recovering dual-source low grade heat energy such as solar energy and industrial waste heat into electricity. The system performance using nine Metal Chlorides-Ammonia working pairs are studied to identify the suitable operational conditions of the system using scroll expander for power generation. Results indicate that SrCl_2 as the LTS can achieve the highest thermal efficiency of the bottom part (LTS-exp₂-HTS) ranging from 11% to 7%. MnCl_2 - SrCl_2 is

This paper is a substantial extension of the short version of the conference paper presented at 8th International Conference on Applied Energy (ICAE2016) on Oct 8-11, Beijing, China. Original paper title ‘Study of a novel dual-source chemisorption power generation system using scroll expander’

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suitable to be used under the first heat source temperature ranging from 200 to 250 °C and second heat source temperature about 100 °C with the overall thermal efficiency around 10 %. The average specific energy of the system under the suggested working conditions can be as high as 102 kJ/kg(salts) in the upper cycle and 82 kJ/kg(salts) in the bottom cycle. The dynamic system performance evaluation is conducted by using the integrated adsorption mathematical model and scroll expander simulation model. Results shows that for a system using 25.2 kg MnCl₂ and 18.12 kg SrCl₂, the average electricity under the first heat source temperature at 220 °C is about 300 W within 30 minutes of upper cycle time. And the bottom cycle can produce average 500 W electricity within 22.5 minutes of bottom cycle time under the second heat source temperature at 160 °C.

Keywords

Chemisorption power generation, Scroll expander, Dual source, Electricity, Thermal efficiency

Nomenclature

C_p	Specific heat capacity [J/(mol · K)]
h	Specific enthalpy (kJ/kg)
$\dot{m}$	Mass flowrate (kg/s)
Δx	Chemical conversion ratio
P_s	Pitch of the scroll (mm)
t_s	Blade thickness of the scroll (mm)
H_s	Scroll height (mm)
r_s	Radius of basic circle (mm)
R_{gy}	Radius of gyration of the orbiting scroll (mm)
i	Number of the expansion chambers (-)
N_s	Scroll turns (-)
<i>Greek letters</i>	
η	efficiency
α	Start angle of the involute
θ	Crank angle between the fixed scroll and orbiting scroll
γ_{v_in}	Internal volumetric expansion ratio of this scroll machine
λ	Thermal conductivity [W/(m.K)]
<i>Subscripts</i>	
am	ammonia
int	Internal working condition of the fluid during expansion process
ise	Isentropic expansion process
iso	Isochoric expansion process
he_1	First heat source
he_2	Second heat source
gc	Ammonia gas channel
<i>Acronyms</i>	
$DSCP$	Dual-Source Chemisorption Power generation cycle
HTS	High Temperature Salt
LTS	Low Temperature Salt
SE	Specific energy (kJ/kg)

1. Introduction

Sorption technology, which usually be used as refrigerator or heat pump to recover low grade heat into useful energy, has attracted every increasing attentions due to the high demand of effective, alternative and environmental friendly technologies since 1970s [1, 2].

Ziegler first proposes the concept of integrating sorption technology with expansion machine for combined power and refrigeration, which emphasizes the importance on conducting basic research in this field [3]. The followed research work is conducted by Wang et al. [4], who originally propose a resorption cogeneration for refrigeration and power generation using Metal Chlorides-ammonia with expansion machine. Results indicate that the resorption cogeneration can potentially improve the overall exergy efficiency by 40-60 % compared with Goswami cycle under the same operational conditions [4]. The optimal overall exergy efficiency of the resorption cogeneration can be as high as 0.9 [4]. Lu et al. [5, 6] introduces mass and heat recovery methods to further improve the system performance of the original resorption cogeneration cycle proposed by Wang et al. [4]. The proposed solution can potentially improve the COP by 35 % using MnCl_2 as High Temperature Salt (HTS) and improve the overall electrical efficiency from 8% to 12% [5]. Continued study on the resorption cogeneration is conducted by Jiang et al. including further system performance analysis [7, 8] and experimental exploration [9]. The previous conducted researches found out the power production of the chemisorption power generation part is extremely unstable with impulse type of electricity and the electricity production can only last for several minutes [8, 9]. The further deep investigation of chemisorption power generation technology to overcome the intermittent and unstable chemical reaction processes is therefore necessary to potentially solve the technical barrier of using chemisorption power generation technology.

Other approach of using integrated physical adsorbent with expansion machine for combined power and refrigeration generation is conducted by Al-mousawi et al. [10, 11]. The prediction of the power output from the system using 8.55 kg/bed of SAPO-34 under the heat source

temperature at 160 °C is about 785 W with the turbine efficiency at 82% [10]. However, the sorption ability of chemical adsorbents is hugely larger than that of physical adsorbents such as AQSOA-Z02 (SAPO-34) zeolite and MIL101Cr Metal Organic Framework (MOF) [1, 10-12]. The adsorption-expander system proposed by Al-mousawi et al. [10, 11] requires huge physical volume of the system due to the relatively low adsorption ability of physical adsorbents, which is not desirable as a compact system. A detailed summary of integrated system using adsorption and expansion technology can be found in the following table.

Table 1

Summary of integrated system using adsorption technology and expansion machine

Author	System function	Adsorption technology	Expander	Source temp (° C)	System performance
Wang et al. [4]	Power and refrigeration generation (simulation)	Metal Chlorides-ammonia, resorption	No specific expander selected	100 - 500 °C	System performance using 12 resorption working pairs are evaluated and compared. The optimal overall exergy efficiency can be as high as 0.9 and compared with Goswami cycle, the resorption cogeneration can potentially improve the overall exergy efficiency by 40-60 %
Lu et al. [5]	Power and refrigeration generation using mass and heat recovery processes (simulation)	Metal Chlorides-ammonia, resorption	No specific expander selected	100-300 °C	First introduced mass and heat recovery processes in chemisorption combined power and refrigeration system. The proposed system can potentially improve the COP by 35 % using MnCl ₂ as High Temperature Salt (HTS) and improve the overall electrical efficiency from 8% to 12%
Long et al. [8]	Power and refrigeration with energy storage system (simulation)	MnCl ₂ - CaCl ₂ -NH ₃ with Phase change materials	Scroll expander (modified from compress or)	240 °C to heat up phase change materials	The energy storage idea using phase change material is first reported. The total energy efficiency of the cogeneration increases from 0.316 to 0.376 and exergy efficiency decrease from 0.402 to 0.391 under heat source temperature at 130 °C and evaporating temperature varies from -10 to 20 °C.
Long et al. [9]	Power and refrigeration (experiment)	MnCl ₂ -CaCl ₂ -NH ₃ (4.8 kg MnCl ₂ and 3.9 kg CaCl ₂)	Scroll expander	140 to 180 °C	The maximum cooling power 2.98 kW is able to be obtained while maximum shaft power is about 253W, when the heat source temperature at 160 oC. The total energy efficiency increases from 0.293 to 0.417 then decreases to 0.407.
Al-Mousawi et al. [11]	Power and refrigeration (simulation)	SAPO-34-water; MIL101Cr-water; Silica-gel-water	No specific expander selected	120 °C	The integrated expander system cam potentially increase the overall cycle efficiency by up to 11% and Silica-gel can achieve the maximum efficiency at 67%. The maximum values of average specific power generation (SP), specific cooling power (SCP) and cycle efficiency are 73 W/kgads, 681 W/kgads (using SAPO-34) and 67% (using Silica-gel) respectively.
Al-Mousawi et al.[10]	Power and refrigeration (simulation)	SAPO-34-water; MOF-water;	Small scale radial inflow	160 °C	The adsorption cycle for cooling and power generation is feasible and can produce up to 67 W/kgads of SP, 622 W/kgads of SCP using SAPO-34. The maximum steam mass

On the other hand, sorption technology can also potentially be integrated with Organic Rankine Cycle (ORC) to simultaneously produce cooling and power, Al-mousawi et al. studies four different adsorption-ORC systems and results show that the maximum integrated system efficiency can be as high as 70% using silica-gel/water in adsorption system and R141b in ORC [13]. The potential application of integrated ORC-resorption technology has been reported by Lu et al. [14] for the recovery of waste heat from a diesel engine into power and cooling energy. Results indicate that the overall energy efficiency of the Internal Combustion Engine can be improved by 7% and the average Brake Specific Fuel Consumption can be reduced from 205 g/kWh to 180 g/kWh at engine full load conditions [14]. However, adsorption-ORC integrated system requires relatively more complicated system design and more components compared with adsorption-expander integrated system.

In order to form an adsorption-expander integrated system, the expansion machine plays a key role in power generation system and has direct impact on the overall power generation performance of the system [15]. Scroll type of expansion machines have been widely used in small scale power generation system due to its advantages of compact size, low operational noise, high efficiency and low cost [16, 17]. Furthermore, due to relatively lower rotational speed compared with turbine machines the scroll expander can be directly connected to conventional generator for electricity generation [16, 17]. The detailed study of the scroll expander is necessary to predict the dynamic performance of the power generation system [18].

In this paper, a novel dual-source chemisorption power generation cycle using scroll expander is proposed to recover dual heat sources into electricity. System performance of nine different chemisorption working pairs are compared in the thermodynamic studies considering the overall thermal efficiency, specific energy and rotational speed of the selected scroll expander,

in order to identify the proper working pair for different operational conditions. Additionally, due to the intermittent and unstable chemical reaction processes of chemisorption technology, the dynamic system performance is critical and necessary to be studied, which has been hardly reported in previous studies. Therefore, a case study has been conducted in the second part of this manuscript in order to predict the dynamic performance of the optimal working pair using 25.2 kg MnCl_2 and 18.21 kg SrCl_2 .

2. System design

The proposed Dual-Source Chemisorption Power generation cycle (DSCP) is designed to convert two different heat sources into electricity. The system includes High Temperature Salt (HTS) to recover relatively higher heat source, Low Temperature Salt (LTS) for the recovery of relatively lower heat source, two expanders integrated with two separately electrical generators, control valves and other accessories. Two groups of HTS-LTS are designed to continuously produce power during the switching time to regenerate the adsorbents. The schematic diagram of the DSCP is shown in Fig. 1. The working principle and controlling strategies of the DSCP can be summarised as follows,

Mode 1 shown in Fig. 1 (a), Valves conditions: Open V_1, V_3, V_5, V_7 ; Close V_2, V_4, V_6, V_8

The HTS_1 is heated by the relatively higher heat source, while the ammonia desorbs and flows from the HTS_1 through V_1 , pressure control valve 1, expander 1 and V_3 to LTS_1 . The LTS_1 adsorbs the ammonia and release the adsorption heat to the environment by the cooling water. The difference of the working conditions between the inlet and outlet of the expander 1 drives the expansion machine and produce the electricity form the generator 1. Meanwhile, the LTS_2 recovers the relatively lower heat source and releases the desorbed ammonia to drive the expander 2 for power production, when the exiting ammonia from the expander 2 is adsorbed by HTS_2 . The water cooling system removes the adsorption heat from the HTS_2 to the environment.

Mode 2 shown in Fig. 1 (b), Valves conditions: Open V_2, V_4, V_6, V_8 ; Close V_1, V_3, V_5, V_7

When the chemisorption processes inside the beds completely end in Mode 1, the HTS_2 and LTS_1 are full of ammonia desorbed from LTS_2 and HTS_1 , respectively. Mode 2 works as a mirror version of Mode 1 in order to regenerate the adsorbent beds (HTS_2 and LTS_1) and restart the power generation processes. The heat source and water cooling process switches between two groups of HTS - LTS .

Fig. 1. Schematic diagram of the chemisorption power generation cycle
(a) Mode 1, Power generation pair: HTS_1 -Expander 1- LTS_1 , HTS_2 -Expander 2- LTS_2
(b) Mode 2, Power generation pair: HTS_1 -Expander 2- LTS_1 , HTS_2 -Expander 1- LTS_2

The temperature and pressure conditions of the ammonia inside the DSCP are illustrated in Clausius-Clapeyron diagram as shown in Fig. 2. Line 1-2 is on the equilibrium line of the HTS and describes the sensible heat changes of the HTS from the environmental temperature (T_{sink}) to the relatively higher heat source temperature T_{he_1} . Line 2-3 shows the expansion process of the expander 1. The exhaust pressure condition of the expander 1 is determined by the LTS under the heat sink temperature of the equilibrium line. Line 3-4 is the ammonia working condition changes from the exhaust of the expander 1 to the LTS. The second heat source is used to heat up the LTS from point 4 to point 5 and drive the expander 2 for power generation as represented in Line 5-6.

Fig. 2. Clausius-Clapeyron diagram of the dual source chemisorption power generation system

3. Thermodynamic performance analysis of the dual-source chemisorption power generation cycle using different working pairs

3.1 Evaluation methods

The performance comparison using different chemisorption salts was conducted by thermodynamic analysis to investigate the difference and identify the proper salts for different heat source conditions. The heat consumed by the salts includes the sensible heat and chemical reaction heat, which can be described and written as following two equations [5].

Δh is the specific reaction enthalpy of the salt, Δx is the chemical conversion ratio, m_{am} is the overall convertible ammonia in the chemical reaction process, and C_p is the specific heat capacity. The properties used in the equations can be found in Table 2.

$$Q_{he_1} = \underbrace{\Delta h \cdot m \cdot \Delta x}_{\text{reaction heat of HTS}} + \underbrace{C_p \cdot (T_{HTS} - T_{HTS}) \cdot m + C_p \cdot (T_{HTS} - T_{HTS}) \cdot m}_{\text{sensible heat of HTS}} \quad (1)$$

$$Q_{he_2} = \underbrace{\Delta h \cdot m \cdot \Delta x}_{\text{reaction heat of LTS}} + \underbrace{C_p \cdot (T_{LTS} - T_{LTS}) \cdot m + C_p \cdot (T_{LTS} - T_{LTS}) \cdot m}_{\text{sensible heat of LTS}} \quad (2)$$

Table 2

Thermodynamic properties of the reaction salts and ammonia [1, 19]

Molecular formula $Me_aCl_b (m-n)$	ΔH (J/mol)	ΔS [J/(mol·K)]	C_p [J/(mol·K)]	M (g/mol)	Reaction weight with per mol ammonia (g)
NH_3	22839	191.39	80.27 (liquid)	17.03	
$BaCl_2 (8-0)$	37665	227.25	75.1	208.23	26.03
$CaCl_2 (8-4)$	41013	230.3	72.52	110.98	27.74
$SrCl_2 (8-1)$	41431	228.8	75.53	158.53	22.65
$MnCl_2 (6-2)$	47416	228.07	72.86	125.84	31.46
$CoCl_2 (6-2)$	53986	228.10	78.41	129.84	32.46
$NiCl_2 (6-2)$	59217	227.75	71.6	129.6	32.40

The complex reaction between the metal chlorides and ammonia can be displayed as following equation.

P.S. $M = Ba, a=1, b=2, c=0, d=8; M = Ca, a=1, b=2, c=4, d=8;$
 $M = Sr, a=1, b=2, c=1, d=8; M = Mn, a=1, b=2, c=2, d=6;$
 $M = Co, a=1, b=2, c=2, d=6; M = Ni, a=1, b=2, c=2, d=6$

The calculation of the electricity from the scroll expansion device can be written as the following equations[20], which requires the identification of the designed working conditions of the selected scroll expansion machine. $h_{d_exp_s}$ and $P_{d_exp_s}$ respectively represents the identified internal specific enthalpy and internal pressure after isentropic expansion process of the expander. v_{d_exp} is the designed specific volume of the scroll expander. The electrical efficiency of the generator $\eta_{generator}$ is assumed at 80%.

$$W_{exp_1} = \left[(h_{he_1} - h_{d_exp_s_1}) + (P_{d_exp_s_1} - P_3) \cdot v_{d_exp_1} \right] \cdot m_{am} \cdot \Delta x \cdot \eta_{generator_1} \quad (4)$$

$$W_{exp_2} = \left[(h_{he_2} - h_{d_exp_s_2}) + (P_{d_exp_s_2} - P_6) \cdot v_{d_exp_2} \right] \cdot m_{am} \cdot \Delta x \cdot \eta_{generator_2} \quad (5)$$

In order to calculate the designed specific enthalpy, pressure and specific volume, several physical parameters of the selected scroll expander are required to be identified. A geometric study has been conducted and the geometric model of the scroll unit has been for the calculation of the physical parameters of the scroll expander including suction volume, exhaust volume, scroll turns, etc. Moreover, the geometric study of the scroll expander can reveal the relationships between the stationary and orbiting scrolls during the expansion process.

The selected scroll device SANDEN TRSA-09 has first been disassembled for the measurement of the physical parameters including scroll pitch P_s , thickness of the scroll blade t_s and height of the scroll H_s . The relationships of scroll pitch, scroll blade, radius of the basic circle r_s , start angle of the involute α and radius of gyration of the orbiting scroll R_{gy} are calculated from the following equations.

$$P_s = 2 \times \pi \times r_s \quad (6)$$

$$t_s = 2 \times r_s \times \alpha \quad (7)$$

$$R_{gy} = \frac{1}{2} \times (P_s - 2 \times t_s) \quad (8)$$

The geometric shape of the scroll blade can be described and drawn by the circle involute equation as indicated in equation (8), where r_s is the radius of the basic circle, ϕ is the involute angle and α is the start angle of the involute.

$$\begin{aligned} x &= r_s [\cos(\phi + \alpha) + \phi \sin(\phi + \alpha)] \\ y &= r_s [\sin(\phi + \alpha) - \phi \cos(\phi + \alpha)] \end{aligned} \quad (9)$$

The internal and external involute lines of the scroll unit with different start angle at $+\alpha$ and $-\alpha$ are drawn and shown as Fig. 3 (a). The comparison of the constructed geometric scroll model and the real scroll unit of SANDEN TRSA-09 is illustrated in Fig. 3 (b).

Fig. 3. Geometric study of the scroll device[21]
(a) Geometric model of a scroll, (b) Comparison of the geometric scroll model and the real scroll

The suction process in the centre of scroll expander ends and another chamber will appear when the orbiting scroll moves. The locations of the expansion chambers of the scroll expander under different crank angle between the stationary scroll and orbiting scroll are illustrated in Fig. 4.

Fig.4. Expansion process of the scroll device under different crank angles

The volume of the expansion chambers of the scroll expansion machine can be calculated by the following equation, where θ is the crank angle between the stationary scroll and orbiting scroll [22]. The number of the expansion chambers is illustrated as i in this equation. The suction volume of this scroll machine can therefore be calculated.

$$V_i = \pi \times P_s \times (P_s - 2t_s) \times H_s \times (2 \times i - 1 - \frac{\theta}{\pi}) \quad (10)$$

The geometric exhaust volume of the scroll expander $V_{exhaust}$ can be calculated by the following equation, where θ_{end} is the end angle of the expansion process[22].

$$V_{exhaust} = \pi \times P_s \times (P_s - 2t_s) \times H_s \times (2N_s - 1 - \frac{\theta_{end}}{\pi}) \quad (11)$$

The internal volumetric expansion ratio of this scroll machine can be calculated by equation (12).

$$\gamma_{v_in} = \frac{V_{exhaust}}{V_{suction}} \quad (12)$$

Both the measured and calculated physical parameters of the selected scroll expander are summarised and listed in Table 3.

Table 3

Parameters of the selected scroll device SANDEN TRSA-09 [21, 23]

Name	Symbol	Value
Scroll height	H_s	33.3 mm
Scroll turns	N_s	2.5
Radius of the basic circle	r_s	3.2 mm
Pitch of the scroll blade	P_s	20.1 mm
Start angle of the involute	α	40.29 °
Suction volume per turn	$V_{suction}$	35.04 cm ³
Exhaust volume per turn	$V_{exhaust}$	105.12 cm ³
Internal volumetric expansion ratio	r_{v_in}	3.0

The evaluation of the overall thermal efficiency, specific energy of the chemisorption power generation system, rotation speed of the scroll expander can be respectively defined by equation (13), (14) and (15).

$$\eta_{he} = \frac{W_{exp}}{Q_{he}} \quad (13)$$

$$SE = \frac{W_{exp}}{(m_{HTS} + m_{LTS})} \quad (14)$$

$$i = \frac{N}{60} \frac{V_{SV}}{v_{su}} \quad (15)$$

3.2 Results and discussion

3.2.1 Evaluation of thermal efficiency

The thermal efficiency of the upper part (HTS-exp₁-LTS) and using nine different sorption working pairs are respectively evaluated as shown in Fig.4 (a) and Fig. 4 (b). The highest thermal efficiency of the upper part (HTS-exp₁-LTS) of the system is about 10% under the heat source temperature from 160 to 180 °C with MnCl₂-SrCl₂ as the working pair. When the first heat source temperature is higher than 220 °C, the HTS using NiCl₂ and CoCl₂ can achieve higher thermal efficiency in compared with that of HTS using MnCl₂. The NiCl₂ is suitable to be used when the first heat source temperature is higher than 320 °C while the overall thermal efficiency of the upper part (HTS-exp₁-LTS) is about 8%, which is mainly determined by the LTS. When the second heat source temperature is lower than 80 °C, the highest thermal efficiency obtained from the system is around 12% using BaCl₂ to recover the heat. When the second heat source temperature is higher than 90 °C, the system using SrCl₂ as the LTS can achieve the highest thermal efficiency ranging from 11% to 7% under the second heat source temperature from 100 to 180 °C.

Fig. 5. Evaluation of thermal efficiency under various heat source temperature
(a) HTS-exp₁-LTS, recover the first heat source; (b) LTS-exp₂-HTS, recover the second heat source

3.2.2 Evaluation of specific energy

The energy density of the upper and bottom part of the system with nine chemisorption working pairs are studied and compared under different heat source conditions as shown in Fig. 6. Results indicate that the system using SrCl₂ as LTS has the highest specific energy compared with other working pairs. The highest specific energy of MnCl₂-SrCl₂ is about 102 kJ/kg(salts) when the first heat source temperature is around 210 °C. When the first heat

source temperature is higher than 320 °C, $\text{NiCl}_2\text{-SrCl}_2$ has the average energy density at 140 kJ/kg(salts). The energy density of the bottom part (LTS-exp₂-HTS) using nine chemisorption working pairs is analysed and results are plotted in Fig. 6 (b). When the second heat source temperature is higher than 60 °C, $\text{MnCl}_2\text{-SrCl}_2$ can achieve the highest specific energy compared with other working pairs. The highest specific energy obtained from the bottom part (LTS-exp₂-HTS) is about 82 kJ/kg(salts) under the second heat source temperature at 120-130 °C with $\text{MnCl}_2\text{-SrCl}_2$ as working pair.

Fig. 6. Evaluation of specific energy under various heat source temperature
(a) HTS-exp₁-LTS recover the first heat source; (b) LTS-exp₂-HTS, recover the second heat source

3.2.3 Evaluation of rotational speed

The rotational speed of the scroll expander under per kW supplied heat of the upper part (HTS-exp₁-LTS) and bottom part (LTS-exp₂-HTS) are studied to identify the optimal operational conditions of the scroll device under various heat ratios and heat source temperature conditions. For the electrical power generation system using scroll expander, the lower rotational speed can effectively reduce the cost of the electrical generator and the complexity of the system without using the transmission unit [16, 17]. Therefore, results indicate that suitable heat source temperature for MnCl_2 , CoCl_2 , and NiCl_2 as HTS is about 180 °C, 260 °C and 320 °C, respectively. Within the three candidate LTS, SrCl_2 possesses the highest rotational speed and BaCl_2 has the lowest rotational speed under the same working conditions, which indicated that BaCl_2 is preferred to be used as LTS for ultra-low temperature heat recovery in the bottom part (LTS-exp₂-HTS).

Fig. 7. Rotational speed of the scroll expander under different heat source temperature

In summary, thermodynamic analysis of the system performance indicates that the optimal thermal efficiency of the upper cycle (HTS-exp₁-LTS) is about 10 %. When the second heat source temperature is higher than 90 °C, SrCl₂ is preferred to be used in the bottom part (LTS-exp₂-HTS) with the highest thermal efficiency within the three LTS candidates. The analysis of specific energy shown SrCl₂ can potentially reduce the system weight with the same power output compared with other CaCl₂ and BaCl₂ as LTS. The thermodynamic properties of the reaction salts and ammonia of different Metal Chlorides are different as listed in Table 2, which will not only affect the overall heat demand as illustrated in equation (1) and (2), but also determine the power generation performance. The inlet and outlet working conditions of the expander, which is calculated from the Clausius-Claperyron equation as illustrated in equation (18) and in Fig. 2, are critical to determine the power generation performance. The evaluation of the rotational speed of the scroll expander pointed out the desirable operational temperature conditions of the selected chemisorption salts. In this study, MnCl₂-SrCl₂ is therefore selected for further study within the nine chemisorption working pairs because of its high overall thermal efficiency and specific energy, and suitable to be used for low grade heat recovery.

4. Study of the dynamic performance using MnCl₂-SrCl₂

4.1 Methodologies

4.1.1 Description of the adsorption mathematical model

The physical model can be simplified as a single adsorption tube unit which mainly consists of the composite adsorbents, thermal fluid, wall between adsorbent and fluid, internal gas channel and insulation material as illustrated in Fig. 8. The structure of the HTS and LTS beds can be recognized as several parallel adsorption tube units. The system can therefore be scale up of scale down by simply adding or reducing the numbers of adsorption tube units. The physical parameters of a single tube unit are listed in Table 4.

Fig. 8. Schematic diagram of a single adsorption tube unit
(a) Section A-A (b) Section B-B

Table 4

Physical parameters of the single adsorption tube unit

Description	Symbol	Value
Thickness of adsorbent	δ_{ad}	18.74mm
Thickness of wall	δ_w	3.91mm
Diameter of gas channel	d_{gc}	15.00mm
Inner diameter of wall	d_{w_in}	52.48mm
Outer diameter of wall	d_{w_out}	60.30mm
Outer diameter of thermal fluid	d_{f_out}	77.92mm

Thermal conductivity of wall material - 304 Stainless Steel	λ_w	16.2 W/(m.K)
Thermal conductivity of the selected composite salts	λ_{ad} [24]	1.5 W/(m.K) EG-MnCl ₂ 1.4 W/(m.K) EG-SrCl ₂
Length of the tube unit	L	300mm

Adsorption kinetic

The chemisorption kinetic models can be classified as three types: global, local and analytical models[1]. The analytical only consider the average value of the variable parameters and can be used to dynamic relationships between the variable parameters, which is an efficient and effective method to predict the adsorption performance[1]. The chemisorption kinetic model used in this study applies one of the analytical model, which has been widely adopted and used by previous researcher and have been proven as an effective model to predict the overall performance [8, 25-27].

$$\frac{dx}{dt} = Ar \cdot (1-x)^{Mr} \cdot \frac{P_c - P_{eq, syn}}{P_c} \quad (16)$$

$$\frac{dx}{dt} = Ar \cdot x^{Mr} \cdot \frac{P_c - P_{eq, syn}}{P_c} \quad (17)$$

The chemical kinetic adsorption model used in this study is expressed as equation (15), where Ar is the Arrhenius factor showing the correlation between the chemical reaction speed and working temperature and Mr reflects the influence of chemical reaction vacant sites[26, 27]. Likewise the principle of kinetic adsorption model, the kinetic model for desorption process can be written as equation (16).

The equilibrium pressure of the chemical adsorbent corresponding with the working temperature is calculated by the Clausius - Clapeyron equation as described in the following equation.

$$P_{eq, syn} = \exp\left(\frac{-\Delta H_r}{RT_{ad}} + \frac{\Delta S}{R}\right) \quad (18)$$

Heat transfer models

The heat transfer processes between the thermal fluid and adsorbent of the cylindrical tube can be divided into two parts: thermal fluid to wall and wall to adsorbent. In order to simplify the calculation of the heat transfer process of the tube unit, lumped parameter analysis is used, which assumes the temperatures of the materials are all uniform and can effectively predict the global changes of the heat transfer processes. The heat flow through the cylindrical adsorption tube unit can be further divided into four parts: convection between thermal fluid and outer side of the wall, conduction between outer and centre of the wall, conduction between centre and inner side of the wall, conduction between centre of the wall and centre of the adsorbent. The thermal resistances from thermal fluid to the adsorbent are illustrated and the equations of the thermal resistances are described in Fig. 9.

Fig.9. One-dimensional heat flow through the single adsorption cylindrical tube unit

The thermal resistance between thermal fluid and wall is defined as equation (18). And R_{w_ad} is the thermal resistance between wall and adsorbent as presented in equation (19).

$$R_{f_w} = \frac{1}{\pi d_{w_out} h_{f_w} L} + \frac{\ln[d_{w_out} / (d_{w_in} + \delta_w)]}{2\pi\lambda_w L} \quad (19)$$

$$R_{w_ad} = \frac{\ln[(d_{w_in} + \delta_w) / d_{w_in}]}{2\pi\lambda_w L} + \frac{\ln[d_{w_in} / (d_{w_in} - \delta_{ad})]}{2\pi\lambda_{ad} L} \quad (20)$$

The Log Mean Temperature Difference (LMTD) between the heat transfer fluid and the wall during the convection heat transfer process can be written as

$$LMTD_{f-w} = \frac{T_{f-in} - T_{f-out}}{\ln \frac{T_{f-in} - T_w}{T_{f-out} - T_w}} \quad (21)$$

Energy balance equations

The heat transfer between the thermal fluid and wall can be described by equation (21). The left of the equation is the internal energy change of the thermal fluid. And the right of the equation includes the overall energy provided/removed by thermal fluid through convection and the energy changes through conduction between fluid and wall. The specific heat capacity, volume, density, and mass flow rate of the thermal fluid is shown as C_{p-f} , V_f , ρ_f and $\dot{m}_f$, respectively.

$$\rho_f C_{p-f} V_f \frac{\partial T_f}{\partial t} = \dot{m}_f (T_{f-in} - T_{f-out}) - \frac{LMTD_{f-w}}{R_{f-w}} \quad (22)$$

The heat transfer between the wall and adsorbent includes two convection processes. The left side of the equation is the internal energy change of the wall and the right side describes two convection heat transfer processes: fluid-wall and wall-adsorbent as written below

$$\rho_w C_{p-w} V_w \frac{\partial T_w}{\partial t} = \frac{LMTD_{f-w}}{R_{f-w}} - \frac{T_w - T_{ad}}{R_{w-ad}} \quad (23)$$

In order to simplify the calculation and improve the applicability of the simulation model, the thermal mass of the fluid and wall is lumped together[28], which means the slope of the changes of T_f and T_w is the same. Therefore the equation (22) and equation (23) can be combined and written as the following equation

$$(\rho_f C_{p-f} V_f + \rho_w C_{p-w} V_w) \frac{\partial T_w}{\partial t} = \dot{m}_f (T_{f-in} - T_{f-out}) - \frac{T_w - T_{ad}}{R_{w-ad}} \quad (24)$$

The energy balance equation of the adsorbent can be written as equation (24). The first element of this equation is the internal energy change of the adsorbent and the second element

is the energy of the adsorbed/desorbed ammonia through the adsorbent. n_{ad} is the number of moles of chemical adsorbent and $(d - c)$ can be found in the chemical reaction formula in equation (3).

$$\left(\sum_{i=1}^N \rho_i C_{p_i}\right) V_{ad} \frac{\partial T_{ad}}{\partial t} - (d - c) n_{ad} M_{r_NH_3} \Delta H_{ad} \frac{dx}{dt} = \frac{T_w - T_{ad}}{R_{w_ad}} \quad (25)$$

The specific volumetric heat capacity can be written as ρC_p . The sum of specific volumetric heat capacity of the composite same can therefore be written as $\sum_{i=1}^N \rho_i C_{p_i}$, which includes the specific volumetric heat capacity of graphite, adsorbent and ammonia as shown in the following equation.

$$\sum_{i=1}^N \rho_i C_{p_i} = \underbrace{\rho_{EG} C_{p_EG}}_{\text{Graphite}} + \underbrace{\rho_{ad} C_{p_ad}}_{\text{Adsorbent}} + \underbrace{\rho_{NH_3} (d - c) n_{ad} M_{r_NH_3} C_{p_NH_3}}_{\text{Ammonia}} / V \quad (26)$$

Table 5

Parameters of the adsorption tube unit model [29]

Parameter	Symbol	Value
Mass of adsorbent in one tube unit	m_{ad}	210 g
Mass of expendable graphite in one tube unit	m_{EG}	105 g
Specific heat capacity of heat transfer fluid	C_{p_f}	1.6 kJ/(kg.K)
Specific heat capacity of metallic wall (304 ss)	C_{p_w}	0.5 kJ/(kg.K)
Specific heat capacity of ammonia	$C_{p_NH_3}$	2.06 kJ/(kg.K)
Specific heat capacity of graphite	C_{p_EG}	0.71 kJ/(kg.K)
Average density of the thermal fluid	ρ_f	0.88 g/cm ³
Density of the metallic wall (304 ss)	ρ_w	7.99 g/cm ³
Volume of the composite adsorbent	V_{ad}	595.9 cm ³
Volume flow rate of the thermal fluid	$\dot{V}_f$	26 L/min

Volume of the thermal fluid	V_f	573.8 cm ³
Volume of the wall	V_w	207.8 cm ³

Verification of the sorption model

Fig.10. Comparison of experimental data and simulation results
(a) $MnCl_2$ under $P_c=1.91$ bar (b) $SrCl_2$ under $P_c=1.91$ bar

The power generation of the dual source chemisorption power generation system mainly determines by the desorption performance of the HTS in generator 1 and LTS in generator 2. The experimental data and the simulation results of the adsorption model are verified to validate the accuracy of the simulation methods. The experimental data are obtained from an adsorption performance test rig using volumetric testing method[21], which can effectively test the dynamic chemisorption performance of the selected testing samples. The verification conducted including 160 °C and 180 °C heat source temperatures under the restricted pressure at 1.91 bar for $MnCl_2$ -NEG and 90 °C and 110 °C heat source temperature under the restricted pressure at 1.91 bar for $SrCl_2$ -NEG. The comparison of the experimental and simulation results show good agreement as illustrated in Fig. 10, which can therefore be used to predict the dynamic performance of the proposed system.

4.1.2 Simulation model of scroll expander

The scroll expander model applied here is first proposed by Lemort et al [30]. This semi-empirical model has been proven as a very effective model and used by many researchers to predict the performance of scroll expander within specific operational ranges [18, 20, 31-34]. The schematic diagram of the semi-empirical model has been shown in Fig. 11.

Fig.11. The scroll expander model[21]
(a) parameters diagram, (b) schematic diagram of the scroll expander model

The expansion process of the scroll expander are divided and described into five steps

- 1) Supply mass leakage from su to in , during this process the supply mass flow rate equals to the internal supply mass flow rate plus leaking mass flow rate
- 2) Isentropic expansion process from in to int , the first part of internal expansion process inside the expander has been recognised as isentropic process
- 3) Isochoric expansion process inside the expander from int to ex_2 , during the process, the working fluid is expanded in constant volume.
- 4) Mixing process at the exhaust of expander when the internal leakage mixes with the working fluid involving the expansion process. The condition changes has been illustrate as from ex_2 to ex_1
- 5) Exhaust losses from condition ex_1 to ex

The working condition at *int* point is defined by the specific volume v_{int} and pressure P_{int} , which can be calculated by the following equations

$$\gamma_{v_in} = \frac{V_{s_cp}}{V_{s_exp}} = \frac{v_{int}}{v_{su}} \quad (27)$$

$$P_{int} = f(v_{int}, s_{su}) \quad (28)$$

The theoretically obtained energy, which has been converted as mechanical power, of the expander can be calculated by the combination of the mechanical power during isentropic and isochoric processes as illustrated in equation (28)

$$\dot{V}_{in} = \underbrace{\dot{V}_{ise}}_{\text{isentropic}} + \underbrace{\dot{V}_{iso}}_{\text{isochoric}} \quad (29)$$

The relationship between the supply mass flow rate and rotation speed of the expander has been calculated by equation (29). v_{su} is the specific volume of the compressed air at the supply point.

$$\dot{V}_{in} = \frac{\dot{V}_{ise}}{v_{su}} + \frac{\dot{V}_{iso}}{60 \times v_{su}} \quad (30)$$

The mass balance of the simulation model can be defined as the displaced mass flow rate of the expander $\dot{V}_{out}$ equals to the overall mass flow rate $\dot{V}_{in}$ minus the internal leakage mass flow rate $\dot{V}_{leak}$. The leakage mass flow rate leaking between the clearances in the scroll can be modelled by assuming an isentropic flow through a convergent nozzle [35, 36]. A_{leak} is the leakage area and C_{throat} is the velocity at the throat of the nozzle model.

$$\dot{V}_{out} = \underbrace{\frac{N \times V_{swept}}{60 \times v}}_{\dot{V}_{in}} - \underbrace{A_{leak} \times \frac{C_{throat}}{v}}_{\dot{V}_{leak}} \quad (31)$$

The velocity of the working fluid at the throat of nozzle can be calculated by and the specific enthalpy at the throat is defined by two parameters the pressure P_{throat} and the specific entropy at the throat s_{throat} . Because the specific entropy at the throat equals to the specific entropy at the supply point s_{su} , the specific enthalpy at the throat can be calculated by

$$C_{throat} = \sqrt{2(h_{su} - h_{throat})} \quad (32)$$

$$h_{throat} = f(P_{throat}, s_{su}) \quad (33)$$

The pressure at the throat of nozzle is defined as the critical pressure when the fluid is in choked flow regime where the critical pressure is larger than the exhaust pressure. When the fluid is not in choked flow regime, the throat pressure equals to the exhaust pressure. The definition of throat pressure, critical pressure of the choked flow, heat capacity ratio γ can therefore been illustrated as

$$P_{throat} = MAX(P_{critical}, P_{ex}) \quad (34)$$

$$P_{critical} = P_{su} \times \left(\frac{2}{r+1} \right)^{\frac{r}{r-1}} \quad (35)$$

$$\gamma = \frac{C_{p_su}}{C_{v_su}} \quad (36)$$

The energy balances when the fluid mixes with the leakage flow at the exhaust point of the expander is calculated by the equation (37), where h_{ex1} is the specific enthalpy at the exhaust point before mixing with the leakage flow, h_{ex2} is the specific enthalpy of the fluid after the mixing process and h_{su} is the specific enthalpy of the leakage flow. The specific enthalpy at the exhaust point of the expander can therefore be calculated by the equation (38), where the

specific enthalpy at the exhaust point has been represented as h_{ex} and $\dot{\zeta}_{ex}$ is the overall heat losses of the expander to the environment.

$$\dot{V}_{net} = \dot{V}_{in} - \dot{V}_{loss} - \dot{V}_{fric} - \dot{V}_{leak} \quad (37)$$

$$h_{ex} = h_{ex1} + \frac{\dot{\zeta}_{ex}}{\dot{V}_{net}} \quad (38)$$

The net power output as the form of electricity equals to the theoretical power obtained by the expander minus the friction losses. The friction losses are defined as a sum of internal friction of the expander and the friction of electrical generator. The friction losses are assumed to be converted as heat losses of the expansion machine. Therefore the overall net power output from the expander can be calculated by the following equation.

$$\dot{V}_{net} = \dot{V}_{in} - \dot{V}_{loss} - \dot{V}_{fric} - \dot{V}_{leak} = \dot{V}_{in} - \dot{V}_{loss} - \dot{V}_{fric} - \dot{V}_{leak} - h_{int}) + v_{int} \times (P_{int} - P_{ex})] - \dot{\zeta}_{ex} \quad (39)$$

Determination of friction losses & leakage area

The overall friction losses include the internal friction of expander, mechanical losses between the shafts and electrical losses in the generator. The relationship between the rotational speed of the expander and friction losses based on eight experimental tests has been illustrated in Fig.12 (a). Leakage area is a predefined parameter in the nozzle model of the scroll expander simulation mode. The leakage area is used to calculate the leakage mass flow rate inside the expansion machine, which is also related to the rotation speed. The relationship between the rotation speed of the expander and leakage area under the experimental conditions has been drawn in Fig. 12 (b). The friction losses and leakage area can therefore be written as equation (39) and (40).

Fig. 12. Determination of friction losses & leakage area[21]
(a) Friction losses and rotation speed, (b) Leakage area and rotation speed

$$P_{loss} = 0.061 + 7.98908 \times 10^{-5} \times N \quad (40)$$

$$A_{leak} = -4.80027 \times 10^{-8} + 1.34374 \times 10^{-7} \times N \quad (41)$$

Verification of the scroll expander model

Fig. 13. Verification of the scroll expander model
(a) Comparison of experimental data and simulation results of the scroll expander,
(b) Relationship between electricity and inlet temperature

The simulation results are first verified with twenty six steady state experimental data with 5% error bar as shown in Fig. 13 (a). A central line has been added in the figure to illustrate the targeted position of the experimental and simulation results, which indicates that the scroll expander model can be used to effectively predict the electricity performance of this scroll expansion machine. The simulation results are further compared with the experimental results under different inlet temperature as illustrated in Fig 13 (b). The results indicate that the

simulation model has well prediction of the performance of this expander. The errors between the simulation and experimental results are within 5%.

4.2 Results and discussion

A case study was conducted with 25.2 kg MnCl_2 and 18.12 kg SrCl_2 . The system contains 120 tubes MnCl_2 and 86 tubes SrCl_2 . Each adsorption tube fills with salts and expandable graphite with the weight ratio of 2:1, which is the same as described previously.

4.2.1 Power generation performance – upper cycle $\text{MnCl}_2\text{-exp}_1\text{-SrCl}_2$

The dynamic power generation performance of the upper cycle HTS-exp1-LTS are studied. The evaluations of the electricity, rotational speed of the scroll expander and conversion ratio of the ammonia are investigated. Six restricted pressures are used to control the inlet pressure of the expansion machine. The results under the first heat source temperature at 180 and 220 °C are respectively plotted in Fig. 14. Results indicate that the lower of the restricted pressure is, the higher of the maximum rotational speed of the scroll expander will achieve. Under the first heat source temperature at 180 °C, the highest rotational speed of the scroll expander is about 7800 rpm at 7 minutes of cycle time with 2 bar restricted pressure. However, the electricity performance of the upper cycle $\text{MnCl}_2\text{-exp}_1\text{-SrCl}_2$ under 2 bar restricted pressure is relatively poor compared with that of other restricted pressures, which is mainly because the selected scroll expander does not work in the optimal working conditions under 2 bar restricted pressure. Higher heat source temperature can effectively reduce the cycle time and improve the overall electricity production, but will lead to higher rotational speed of the scroll expander as shown. Under the first heat source temperature at 180 °C, the restrict inlet pressure to the scroll expander can be set at 5 bar, and it will lead to the upper cycle time for about 1hour and can averagely produce 120 W electricity. When the upper cycle time is about 25 minutes, the upper cycle is operated under the first heat source temperature at 220 °C and the restricted supply pressure to the scroll expander can be set at 5 bar, which can averagely produce around 300 W electricity.

Fig. 14. Upper cycle $\text{MnCl}_2\text{-exp}_1\text{-SrCl}_2$ power generation performance
(a) electricity power, (b) rotational speed, (c) global conversion ratio at 180 °C
(d) electricity power, (b) rotational speed, (c) global conversion ratio at 220 °C

4.2.2 Power generation performance – bottom cycle $\text{SrCl}_2\text{-exp}_2\text{-MnCl}_2$

The bottom cycle power generation performance are analysed under six restricted pressure conditions and two heat source temperature. Under the heat source temperature at 120 °C, the highest instantaneous electricity power is about 0.55 kW at 9 minutes of cycle time under 2 bar restricted pressure. The average electricity power production from the bottom cycle under 3 bar restricted pressure can be higher than that of 2 bar restricted pressure. Similar conclusions can be drawn from this part of simulation results including, the higher of the heat

source temperature is, the more electricity can be obtained from the bottom cycle and less cycle time is required; an optimal restricted pressure condition exists and is mainly determined by the selected scroll expansion machine; the higher of the restricted pressure is, the longer of cycle time will be, and rotational speed of the scroll expander can be reduced and electricity power production can be more stable. For example, when the second heat source temperature is at 120 °C and the restricted pressure is 5 bar, the average electricity of the bottom cycle is about 150 W with 1 hour bottom cycle time and the rotational speed of the scroll expander can be kept lower than 1000 rpm. Under the same restricted pressure, when the second heat source temperature is increased at 160 °C, the average electricity of the bottom cycle can be effectively increased to about 500 W, the bottom cycle time can be reduced to 22.5 minutes and the maximum rotational speed of the expander will be increased to around 3600 rpm.

(a)

(d)

(b)

(e)

Fig. 15. Bottom cycle LTS-exp₂-HTS power generation performance
 (a) electricity power, (b) rotational speed, (c) global conversion ratio at 120 °C
 (d) electricity power, (b) rotational speed, (c) global conversion ratio at 160 °C

5. Conclusions

A novel dual-source chemisorption power generation system using scroll device as the expansion machine was proposed and studied. The system performance using nine different chemisorption working pairs were thermodynamic investigated and compared to select the proper working pair for different heat source conditions. The prediction of dynamic system performance was conducted to investigate a small scale dual source chemisorption power generation system contains 25.2 kg MnCl_2 and 18.21 kg SrCl_2 . The conclusions drawn from this study can be summarised as follows:

- The thermal efficiency of the upper cycle (HTS-exp₁-LTS) is about 10 % under the optimal first heat source conditions. When the second heat source temperature is lower than 80 °C, BaCl_2 is recommended to be used as LTS. When the second heat source temperature is higher than 90 °C, the system using SrCl_2 as the LTS can achieve the highest thermal efficiency of the bottom part (LTS-exp₂-HTS) ranging from 11% to 7% under the second heat source temperature from 100 to 180 °C.
- The specific energy analysis indicates SrCl_2 can potentially reduce the system weight with the same power output compared with other CaCl_2 and BaCl_2 as LTS. When MnCl_2 - SrCl_2 is selected as the working pair, the highest specific energy of the

system can be as high as 102 kJ/kg(salts) when the first heat source temperature is around 210 °C. The highest specific energy obtained from the bottom part (LTS-exp₂-HTS) is about 82 kJ/kg(salts) under the second heat source temperature at 120-130 °C with MnCl₂-SrCl₂ as working pair.

- The prediction of the dynamic system power generation performance using MnCl₂-SrCl₂ as the working pair indicates that the pressure controlling strategies can be used as one of the potential solutions to solve the unstable power production of the chemisorption power generation system. The optimal restricted pressure condition is mainly determined by the selected scroll expansion machine. The increase of restricted pressure will lead to longer upper/bottom cycle time, reduced rotational speed of the scroll expander and stabilized power production.
- The dual-source chemisorption power generation system using 25.2 kg MnCl₂ and 18.12 kg SrCl₂ can averagely produce 300 W electricity under 220 °C first heat source temperature with 30 minutes upper cycle time. The bottom cycle can potentially produce 500 W electricity within 22.5 minutes of bottom cycle time under the second heat source temperature at 160 °C.

The proposed dual-source chemisorption power generation system (DSCPS) has high potential to be used in the place, where the heat source conditions are different, and can convert dual heat source energy into electricity. One of the potential application areas is to be used in industry, where there are various heat sources and the heat source conditions are not stable. Another potential application area is to integrate this proposed system with Internal Combustion Engine (ICE) for the recovery of coolant and exhaust energy. The high temperature heat source (exhaust energy of ICE) can be used to heat up the HTS and the low temperature heat source (coolant energy of ICE) can be used to provide the heat for LTS.

Acknowledgements

The authors would like to thank the supports from EPSRC IAA (EP/K503885/1)-Study of engine waste heat recovery technologies, EPSRC Prosperity Outcomes Award 2016 (EP/P511201/1)-Study of carbon based Nanomaterial to Enhance heat transfer and efficiency in Chemisorption Cogeneration system (NE-Cogen) and Royal society (IE/151256). The first author also would like to thank for the encouragement and recognition on this study from China Scholarship Council for the ‘2015 Chinese Government Award for Outstanding Self-financed Students Abroad’.

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