# Thermodynamic Simulation of CO$_2$ – Adsorbent Based Sorption Refrigeration System

**Shajiullah Naveed Syed**

Research Scholar
School of Mechanical Engineering
Vellore Institute of Technology, Vellore,
India

**Vinod Kumar Sharma**

Associate Professor
School of Mechanical Engineering
Vellore Institute of Technology, Vellore,
India

*Different materials like activated carbon, metal organic frameworks, silica, etc. have ability to adsorb (exothermic process) and desorb (endothermic process) CO$_2$. These heat interactions during adsorption and desorption processes can be utilized for the development of gas – adsorbent based sorption refrigeration system. Therefore, in the present work, this concept is employed to analyze the thermodynamic performance of CO$_2$ – adsorbent based sorption refrigeration system (CO$_2$-A SRS). The chosen adsorbents for thermodynamic simulation are Activated Carbon (Norit RB3), Pore Expanded Mesoporous Silica Materials (PE MSM 41), Amine Tethered Mesoporous Silica Materials (AT MSM 41) and Amine Functionalized Silica (AF Silica). The working pairs are developed based on the available pressure difference between coupled adsorbent to allow sufficient amount of CO$_2$ to flow between the coupled materials in the operating temperature range of 0°C (refrigeration output), 25°C (ambient) and 100°C (heat source). The thermodynamic performance of refrigeration system is compared for two adsorbent pairs. The thermodynamic performance includes refrigeration effect, specific refrigeration power, coefficient of performance, refrigeration capacity and second law of efficiency. The refrigeration effect of Activated Carbon – PE MSM 41 pair is observed double that of AT MCM 41 – AF Silica pair. In addition, the thermodynamic performance of CO$_2$-A SRS is compared with the performance of CO$_2$ – adsorbent based vapour adsorption refrigeration system (CO$_2$-A VARS) available in literature. The COP of CO$_2$-A SRS is observed higher than CO$_2$-A VARS.*

*Keywords: Adsorbent; COP; CO$_2$ adsorbent based sorption refrigeration system; CO$_2$ storage; Reaction enthalpy; Specific refrigeration power.*

## 1. INTRODUCTION

Carbon dioxide has adverse effect on the environment, since Green House Gases contains 77% of CO$_2$ [1]. Therefore, the concept of storage and sequestration of CO$_2$ from environment or waste exhaust gases received much interest of researchers worldwide. It is observed from several studies that CO$_2$ can be captured by adsorption in different materials like activated carbon, zeolite, silica, etc. These technologies become promising solution for the benefit of future generations. Several studies on characterisation of adsorbent materials to identify its CO$_2$ storage capacity are available in literature [2-30]. Development of any sorption based thermodynamic system demands for the knowledge of adsorption/desorption characteristics, reaction kinetics and thermal stability of materials used.

Vinod and Anil [2] have experimentally and theoretically studied the CO$_2$ adsorption and desorption characteristics of three different type of activated carbons

namely Norit RB3 (steam activated rod), Norit Darco (100 mesh size), and Norit Darco (12 -20 US mesh size).They have observed that CO$_2$ adsorption capacity increased with increase in supply pressure. Later, the experimentally measured isotherm are simulated using D-A Model. Several researchers [12-14] theoretically studied the CO$_2$ adsorption phenomena on solid adsorbent. Young and Crowell [15] estimated the thermodynamic properties of solid adsorbents and revealed the importance of surface area and spreading pressure on the physical adsorption process. The development of several amine-tethered mesoporous silica materials to enhance the CO$_2$ adsorption capacity at lower partial pressures are presented by different researchers [16-20]. In other studies [28-30], novel pore expanded mesoporous silica materials are suggested as promising support for amine tethering. It allows exploitation of internal space, which is not possible with zeolite, MSM-41, SBA-15 and KIT-6 [21, 22]. On the other hand, Loganathan et al. [27] have investigated the CO$_2$ adsorption and desorption isotherms on PE-MSM-41 at different temperatures and at the pressure range of 0-25 bar and it was observed that the adsorption and desorption are reversible in nature as the isotherms coincide with each other.

The experimental investigation on CO$_2$ storage and reaction rates of pitch-based activated carbon at 303 to

423 K temperature and 0-1 bar pressure is reported by Shen et al. [23]. Balsamo et al. [24] have reported that reaction kinetics directly proportional to supply pressures whereas inversely proportional temperatures. It is observed by Zhang et al. [25] on experimental investigation of $CO_2$ storage and reaction kinetics of activated carbon and zeolite 13X at 298, 308, 318 and 328 K, and up to 30 bar pressure that the adsorption rates of zeolite 13X at low pressures are comparatively more than activated carbon whereas at higher pressures the adsorption capacities are observed lower in zeolite 13X compared to activated carbon.

$CO_2$ storage capacities of different adsorbent materials are widely investigated for several operating conditions whereas less effort has been given on the development of $CO_2$ – adsorption based thermodynamic systems. $CO_2$ – adsorption based thermodynamic systems like cooling system can be operated using waste heat as input whereas the heat of desorption during endothermic process can be utilized as cooling output. The development of any solid – gas sorption thermodynamic system demands for the several thermodynamic and thermo physical properties like gas storage, reaction kinetics, thermodynamic properties, etc. of adsorbent materials [31]. The selection of suitable working pairs depends on the adsorption isotherms, kinetics, and heat of adsorption and desorption, specific heat capacity, internal energy, etc. In addition to high adsorption capacity and fast kinetics, activated carbon exhibits high surface area, better pore size distribution and thermal stability. Therefore, it is more suitable for adsorption of $CO_2$ compared to other solid adsorbents [3–6, 26]. It can also be adopted easily for many applications due to its economical suitability for large quantity use and non-reactive to moisture. Activated carbons are also studied for the suitability of different applications like separation and purification of $CO_2$; sorption based thermodynamic devices systems, cryo-coolers and energy storage systems [7–11]. Recently, thermo-dynamic analysis of $CO_2$ and activated carbon based cooling system has been conducted by Vinod and Anil [2] and obtained maximum COP of 0.09 with $CO_2$-Norit RB3, pair at driving source temperature of 80°C with the evaporator temperature of 15°C. On the other hand, Banjac et al. [32] have discussed about the geothermal ground source heat pump for low temperature hydronic heating system. Jitendra and John Rajan [33] have presented the recent advancement in cooling technologies for solar PV systems.

Though several adsorbent materials are used to study their $CO_2$ adsorption capacity, activated carbons are reported to be most suitable for $CO_2$ storage applications due to its high $CO_2$ storage capacity. Also, activate carbons are used to study the thermodynamic performance of $CO_2$ – adsorbent based vapour adsorption refrigeration systems ($CO_2$-A VARS) by several researchers. But, the observed COP and cycle efficiency of $CO_2$-A VARS are quite low that necessitates the further investigations on system performance improvement. Therefore, in the present study, the concept of gas – solid sorption is employed to propose a new thermodynamic cycle of $CO_2$ – adsorbent based sorption refrigeration system ($CO_2$-A SRS). The sorption refrige-

ration system works with the employment of working pairs (adsorption/absorption materials) of one high pressure type and one low pressure type materials [34-39]. The useful cooling effect can be produced through adsorption/desorption of gas to/from working materials. Such systems do not require mechanical moving parts. There is no need of compressor to increase gas pressure, this (pressure increase or decrease) can be done through sensible heating and sensible cooling of charged materials. In addition, sorption systems are environmental friendly due to absence of harmful refrigerants. The refrigeration effect in $CO_2$-A SRS can be obtained by utilizing the heat interactions involved during $CO_2$ transfer between coupled adsorbent materials. This type of gas – solid sorption refrigeration system is never studied in literature using $CO_2$ as working fluid. Therefore, we proposed a concept of gas – solid sorption refrigeration system to theoretically analysis (thermodynamic simulation) the thermodynamic performance of such sorption system using $CO_2$ as working fluid. In the present study, two pairs of adsorbent materials are used to estimate the performance of $CO_2$-A SRS and compared their suitability for the development of $CO_2$-A SRS. The adsorbent pairs used for thermodynamic simulation of $CO_2$-A SRS are "Activated Carbon - PE MSM 41" and "AT MSM 41 - AF Silica". The performance of $CO_2$-A SRS is estimated in terms of refrigeration effect, refrigeration capacity, specific refrigeration power, COP and cycle efficiency.

## 2. WORKING PRINCIPLE OF $CO_2$ – ADSORBENT BASED REFRIGERATION SYSTEMS

### 2.1 $CO_2$ – Adsorbent based sorption refrigeration system ($CO_2$-A SRS)

Figures 1 and 2 show the thermodynamic cycle and scheme of $CO_2$ – A SRS respectively working in the temperature range of $T_{ref}$ = 0°C (refrigeration output temperature), $T_a$ = 25°C (ambient temperature) and $T_{reg}$ = 100°C (heat source temperature). A $CO_2$ – A SRS consists of two $CO_2$ transfer processes; refrigeration process and regeneration process, and one sensible heating process and one sensible cooling process. $CO_2$ – A SRS needs a pair of two adsorbent materials that eliminates the requirement of expansion device, heat exchangers, etc., which are required in $CO_2$-A VARS (Fig. 3). The $CO_2$ – A SRS system utilizes the reaction heats involved during adsorption/desorption of $CO_2$ on /from adsorbent materials to produce refrigeration effect.

Refer to Figs. 1 and 2; $A_1$ and $A_{1'}$ are adsorbents used at high-pressure side and $A_2$ and A2' are adsorbents at low-pressure side. In refrigeration process, adsorbent $A_1$ at point 1 desorbs $CO_2$ at $T_{ref}$, which is adsorbed by adsorbent $A_2$ at point 2 at temperature $T_a$. The desorption (endothermic) heat absorb by adsorbent $A_1$ is responsible for producing refrigeration effect ($Q_{ref}$) at $T_{ref}$ and the adsorption (exothermic) heat ($Q_a$) released by adsorbent $A_2$ is rejected to ambient at $T_a$. Simultaneously, in regeneration process, the adsorbent $A_{2'}$ desorbs $CO_2$ by taking the required heat ($Q_{reg}$) of desorption from waste heat source at $T_{reg}$ that $CO_2$ is

adsorbed by adsorbent $A_1$, by rejecting heat of adsorption ($Q_a$') to ambient at $T_a$. Thereafter, by sensibly cooling adsorbent $A_1$, from $T_a$ to $T_{ref}$ and adsorbent $A_2$, from $T_{reg}$ to $T_a$, and sensibly heating of adsorbent $A_1$ from $T_{ref}$ to $T_a$ and adsorbent $A_2$ from $T_a$ to $T_{reg}$, system can be ready for next cycle.
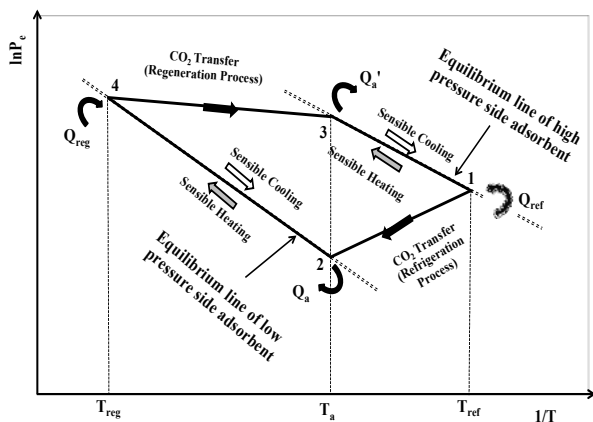


**Figure 1. Thermodynamic cycle of $CO_2$ – adsorbent based sorption refrigeration system**
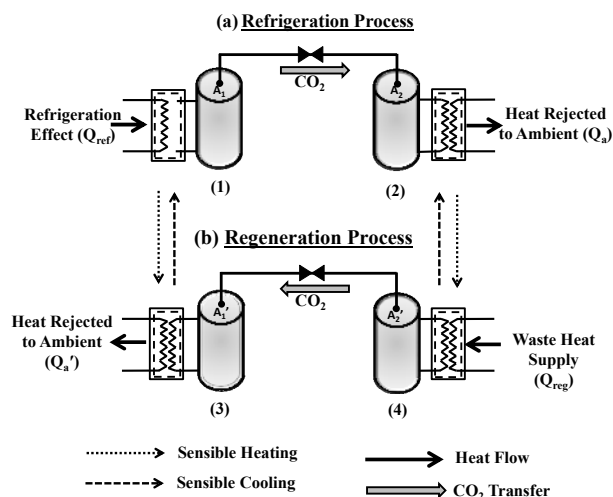


**Figure 2. Scheme of $CO_2$ – adsorbent based sorption refrigeration system**

## 2.2 $CO_2$ – Adsorbent based vapour adsorption refrigeration system (CO2-A VARS)

Figure 3 shows the scheme of $CO_2$ – adsorbent based vapour adsorption refrigeration system. This system consists of a condenser, an evaporator, an expansion valve and one sorption reactor. Firstly, $CO_2$ gets evaporated in an evaporator producing refrigeration effect ($Q_{ref}$). Then, the low-pressure $CO_2$ transferred to the adsorber and get adsorbed on adsorbent at low temperature. Since, the process of adsorption is exothermic, certain amount of heat ($Q_a$) is rejected to ambient. Adsorber is then disconnected from the evaporator heat exchanger and is sensibly heated to required condenser temperature and corresponding pressure. After reaching to equilibrium condition, $CO_2$ get desorbed from adsorbent using waste heat source ($Q_s$). The desorbed $CO_2$ condensed in the condenser by rejecting $Q_c$ amount of heat. The operation completes by expansion of $CO_2$ through expansion valve between condenser and evaporator.
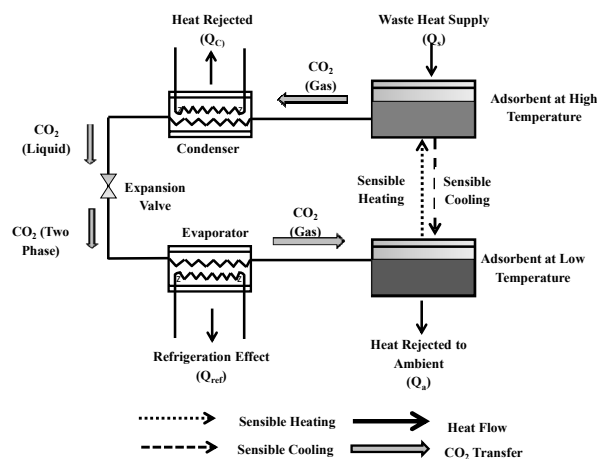


**Figure 3. Scheme of $CO_2$ – adsorbent based vapour adsorption refrigeration system**

## 3. SELECTION OF ADSORBENT PAIRS

Typically, the desirable properties of adsorbents suitable for $CO_2$ – A SR system are (a) high $CO_2$ storage capacity that increases the amount of $CO_2$ transmission, (b) fast reaction kinetics to reduce overall cycle time, (c) sufficient pressure difference between coupled sorption beds at operating temperature range, (d) and favourable thermodynamic properties, generally, high desorption heat for adsorbent at high pressure side to increase refrigeration output and low desorption heat for adsorbent at low pressure side to reduce regeneration input. In this view, different adsorbent materials characterised for $CO_2$ storage application available in literature are chosen to identify the best-suited adsorbent pairs of the development of $CO_2$ – A SRS. The chosen adsorbent materials are Activate Carbon (Norit RB3) (AC1), Activated Carbon (Norit Carco, 100 mech size) (AC2), Activated Carbon (Norit Darco, 12 × 20 US mesh size) (AC3) [2], Pore Expanded Mesoporous Silica Materials (PE MSM 41) [26], Amine Tethered Mesoporous Silica Materials (AT MSM 41) [30], Amine Functionalized Silica (AF Silica) [40], 13X Zeolite [41] and MIL 101 [42].

The isotherm data of above mentioned adsorbent materials are taken from respective references and van't Hoff plots are constructed for each adsorbent material. Van't Hoff plot is a relation between logarithmic equilibrium pressure and inverse of absolute temperature. The equilibrium pressures for all the adsorbent materials are chosen at fixed $CO_2$ concentration at different temperatures. For the selection of equilibrium pressure, $CO_2$ concentration was kept fixed to ensure the uniformity in measurements. The constructed plots are linear where its slope and intercept can be used to evaluate reaction enthalpy and reaction entropy respectively using van't Hoff equation. Fig. 4 shows the van't Hoff plots of all adsorbent materials chosen for present study. The equations of van't Hoff lines and, estimated reaction enthalpy and entropy are listed in Table 1.

As mentioned earlier, the working temperature range for $CO_2$ – A SRS is selected as $T_{ref} = 0°C$, $T_a = 25°C$ and $T_{reg} = 100°C$. We have proposed the refrigeration system which can able to discharge the waste heat at ambient temperature. Therefore, the heat sink is chosen as 25°C while the refrigeration output temperature (0°C)

and heat source temperature (100°C) are chosen in such a way that there exist sufficient pressure difference between coupled reactors to allow sufficient $CO_2$ transfer between them. Also, high pressure difference increases rate and amount of $CO_2$ transfer. Therefore, to select the suitable working pair for $CO_2$ – A SRS, all adsorbent materials are examined on the basis of available pressure difference between coupled adsorbent beds for a given temperature range (see Fig. 4) because sufficient pressure differential is required to allow $CO_2$ transfer between them and also for fast kinetics. Based on van't Hoff data, out of eight adsorbent materials are found suitable for the development of $CO_2$ – A SRS. The selected adsorbent materials and their possible pairs are Activated Carbon – PE MSM 41 (pair 1) and AT MSM 41 – AF Silica (pair 2). Activated carbon and AT MCM – 41 are considered as high pressure adsorbents due to their higher equilibrium pressures relative to PE MCM – 41 and AF Silica equilibrium pressures respectively at given operating temperatures. In the proceeding sections, thermodynamic cycles and simulation are discussed for these selected adsorbent pairs.
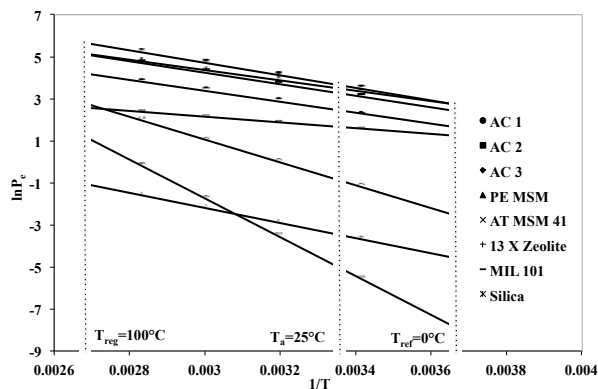


**Figure 4. Van't Hoff plots for chosen adsorbent materials**

As mentioned earlier, the working temperature range for $CO_2$ – A SRS is selected as $T_{ref}$ = 0°C, $T_a$ = 25°C and $T_{reg}$ = 100°C. We have proposed the refrigeration system which can able to discharge the waste heat at ambient temperature. Therefore, the heat sink is chosen as 25°C while the refrigeration output temperature (0°C) and heat source temperature (100°C) are chosen in such a way that there exist sufficient pressure difference between coupled reactors to allow sufficient $CO_2$ transfer between them. Also, high pressure difference increases rate and amount of $CO_2$ transfer. Therefore, to select the suitable working pair for $CO_2$ – A SRS, all adsorbent materials are examined on the basis of available pressure difference

between coupled adsorbent beds for a given temperature range (see Fig. 4) because sufficient pressure differential is required to allow $CO_2$ transfer between them and also for fast kinetics. Based on van't Hoff data, out of eight adsorbents, only four adsorbent materials are found suitable for the development of $CO_2$ – A SRS. The selected adsorbent materials and their possible pairs are Activated Carbon – PE MSM 41 (pair 1) and AT MSM 41 – AF Silica (pair 2). Activated carbon and AT MCM – 41 are considered as high pressure adsorbents due to their higher equilibrium pressures relative to PE MCM – 41 and AF Silica equilibrium pressures respectively at given operating temperatures. In the proceeding sections, thermodynamic cycles and simulation are discussed for these selected adsorbent pairs.

### 3.1 Results and discussion

For operation of $CO_2$ – A SRS, a pair of high-pressure and low-pressure type adsorbent materials is required. In the present study, Activated Carbon and AT MSM 41 are considered as high-pressure type, and PE MSM 41 and AF Silica as low-pressure type adsorbent. The thermodynamic cycles for $CO_2$ – A SRS constructed based on van't Hoff plots for working pairs Activated Carbon – PE MSM 41 and AT MSM 41 – AF Silica are shown in Figs. 5 and 6, respectively.
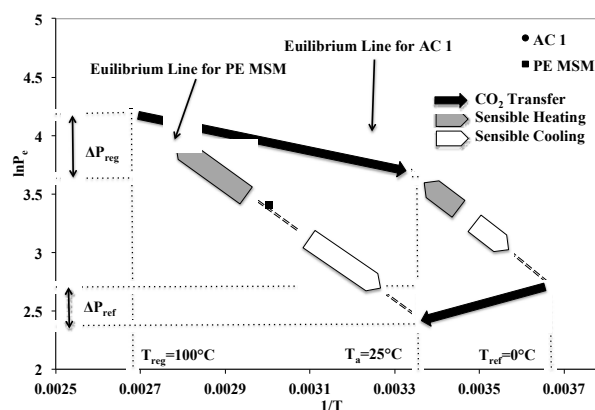


**Figure 5. $CO_2$ – A SRS thermodynamic cycle using Activated Carbon – PE MSM 41 pair**

In Fig. 5, $\Delta P_{ref}$ and $\Delta P_{reg}$ are the available pressure differences between the coupled adsorbent materials for refrigeration and regeneration processes respectively. The estimated pressure differences between coupled adsorbent materials are $\Delta P_{ref}$ = 4.14 bar, $\Delta P_{reg}$ = 30 bar, which are sufficient to allow $CO_2$ transmission during refrigeration and regeneration processes.

**Table 1. Estimated reaction enthalpy and entropy values**

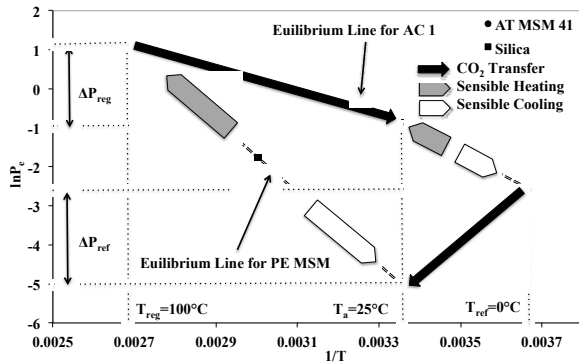| Adsorbent Materials | Van't Hoff Equations | Reaction Enthalpy; ΔH (kJ/mol) | Reaction Entropy; ΔS (kJ/mol K) |
|---|---|---|---|
| Activated Carbon-1 | $lnP_e$ = -2971.4/T + 13.621 | 24.7 | 0.113 |
| Activated Carbon-2 | $lnP_e$ = -2733.8/T + 12.438 | 22.7 | 0.103 |
| Activated Carbon-3 | $lnP_e$ = -2457.4/T + 11.737 | 20.4 | 0.098 |
| Pore Expanded PE MCM-41 | $lnP_e$ = -1983.1/T + 8.7686 | 16.5 | 0.073 |
| Amine Tethered PE MCM-41 | $lnP_e$ = -5423.9/T + 17.329 | 45.1 | 0.144 |
| 13X Zeolite | $lnP_e$ = -3589/T + 8.5758 | 29.8 | 0.071 |
| MIL 101 Powder Form | $lnP_e$ = -1367.3/T + 6.2506 | 11.4 | 0.052 |
| Amine Functionalized Mesoporous Silica | $lnP_e$ = -9226.1/T + 25.939 | 65.1 | 0.216 |

Figure 6. $CO_2$ – A SRS thermodynamic cycle using AT MCM 41 – AF Silica pair

On the other hand, in Fig. 6, for pair of AT MSM 41 – AF Silica materials, the refrigeration process occurs in sub atmospheric pressure whereas regeneration occurs at above atmospheric pressure and the pressure difference is $\Delta P_{reg}$ = 2.5 bar. It is clear from Figs. 5 and 6 that both the pairs are suitable for the development of $CO_2$ – A SRS because there exist sufficient pressure difference between paired adsorbent materials to facilitate the $CO_2$ transfer for the working of sorption refrigeration system. The decrease in $\Delta P$, in case of AT MSM 41 – AF Silica pair is responsible for decrease in $CO_2$ transfer rate, which significantly increases cycle time; it also decreases the transferrable $CO_2$ between paired adsorbents. On comparison, it is observed that the pair of Activated Carbon – PE MSM 41 materials is more suitable than AT MSM 41 – AF Silica pair due to its capacity of working on above atmospheric pressure with higher pressure differentials that improve system efficiency by reducing cycle time.

### 3.2 Thermodynamic analysis of CO2 adsorption based sorption refrigeration system

The thermodynamic analysis of $CO_2$ – A SRS is carried out using Activated Carbon – PE MSM 41 and AT MSM 41 – AF Silica pairs to check their suitability for the development of $CO_2$ – A SRS. The adsorbent to reactor mass ratio is assumed to be 1:0.75, the specific heat of adsorbent and reactor as 0.7 kJ/kg K and 0.46 kJ/kg K respectively [2, 34]. The cycle time is assumed to be 30 minutes for 1 kg of each adsorbent. The thermodynamic properties and transferrable $CO_2$ of chosen adsorbent materials are available in Table 2.

The thermodynamic performance of $CO_2$ – A SRS are estimated using following equations:
Refrigeration effect

$$Q_{ref} = n\Delta H_{ref}$$
$$- [(m_{ref}C_{ref} + m_{r,ref}C_{r,ref})(T_a - T_{ref})] \tag{1}$$

Regeneration heat supplied

$$Q_{reg} = n\Delta H_{reg}$$
$$+ [(m_{reg}C_{reg} + m_{r,reg}C_{r,reg})(T_{reg} - T_a)] \tag{2}$$

Coefficient of performance:

$$COP = \frac{Q_{ref}}{Q_{reg}} \tag{3}$$

Specific refrigeration power

$$SRP = \frac{Q_{ref}}{t_{half-cycle}(m_{ref} + m_{reg})} \tag{4}$$

Refrigeration capacity

$$RC = \frac{Re\,frigeration\,load}{Cycle\,time} = \frac{2Q_{ref}}{t_{cyl}} \tag{5}$$

Second law efficiency

$$\eta_E = COP\frac{(T_a/T_{ref})-1}{1-(T_a/T_{reg})} \tag{6}$$

Upon thermodynamic simulation of $CO_2$ – adsorbent based sorption refrigeration system, the estimated thermodynamic performance viz. refrigeration effect ($Q_{ref}$), regeneration heat supplied ($Q_{reg}$), coefficient of performance (COP), specific refrigeration power (SRP), refrigeration capacity (RC) and second law efficiency ($\eta_E$) are listed in Table 3 for both the pairs. It is observed from the literature that the thermodynamic performance of any gas – solid sorption system significantly influences by reaction heat of the material employed. Also, for better refrigeration effect, the reaction heat of the refrigeration adsorbent material should be higher whereas the reaction heat of the regeneration adsorbent material should be lower. These together result in higher COP of the thermodynamic system. In the present study, it is observed that inspite of having higher reaction heat (AT MSM 41) than Activated Carbon, the refrigeration effect of $CO_2$ – A SRS using Activated Carbon – PE MSM 41 pair is higher than that of using AT MSM 41 – AF silica pair. This is due to the availability of higher transferrable $CO_2$ between Activated Carbon – PE MSM 41 pair (due to higher $CO_2$ storage capacity of these adsorbents) than AT MSM 41 – AF silica pair. Also, in Activated Carbon – PE MSM 41 pair, the reaction heat of regeneration materials i.e. PE MSM 41 is lower than that of refrigeration material i.e. Activate Carbon, which gives rise in COP whereas on the other hand, for AT MSM 41 – AF silica pair, the reaction heat of AF Silica (regeneration material) is higher than that of AT MSM 41 (refrigeration material).

Table 2. Properties of adsorbent materials [2, 27, 40, 43]

| S. No. | Absorbent Materials | Reaction Enthalpy; ΔH ( kJ/mol) | Transferrable $CO_2$ (mol/gm) | Average Specific Heat (KJ/kgK) |
|--------|---------------------|---------------------------------|-------------------------------|--------------------------------|
| 1 | Activated Carbon | 18.63 | 0.02499 | 0.7 |
| 2 | PE MSM-41 | 16 | 0.006 | - |
| 3 | AT MSM-41 | 45 | 0.002 | - |
| 4 | Amine Functionalized Silica | 65 | 0.0012 | - |

Therefore, the SRP, cooling capacity and second law efficiency are also observed greater for the pair Activated Carbon – PE MSM 41. Based on the above observations for available pressure differential, reaction heat and transferrable $CO_2$ i.e. overall thermodynamic performance, the pair of Activated Carbon – PE MSM 41 is considered to be a best suited working pair for the development of $CO_2$ – adsorbent based sorption refrigeration system.

**Table 3. Performance of CO2 based solid sorption cooling system**

| Pairs → | Activated Carbon - PE MCM | AT MCM - AF Silica |
|---|---|---|
| $CO_2$ Exchange (moles) | 6 | 1.2 |
| $\Delta H_{ref}$ (kJ/mol) | 18.63 | 45 |
| $\Delta H_{reg}$ (kJ/mol) | 16 | 65 |
| $Q_{ref}$ (kJ) | 98.65 | 40.87 |
| $Q_{reg}$ (kJ) | 135.37 | 117.37 |
| COP | 0.72 | 0.34 |
| SRP (W/kg) | 54.8 | 22.7 |
| RC (kW) | 0.1 | 0.04 |
| $\eta_E$ (%) | 33.18 | 15.86 |

It is also observed in the literature [2] that the performance of $CO_2$ – adsorbent based vapour adsorption refrigeration system have been analysed using adsorbent materials as Activate Carbon. The schematic and working principle of the $CO_2$ – adsorbent based vapour adsorption refrigeration system is given in Fig. 3 and section 2.2. The thermodynamic performance of $CO_2$-A VARS was reported as the maximum COP of 0.04, SRP of 7.4 W/kg and second law efficiency of 2.33% for evaporator temperature of 0°C and condenser temperature of 80°C. The thermodynamic performance was estimated using the same values of transferrable $CO_2$ and reaction heat presented in Table 2 for Activated Carbon. Whereas in the present study, authors have estimated the maximum COP of 0.72, SRP of 54.8 W/kg and second law efficiency of 33.18% for the temperature range of 0°C, 25°C and 100°C with adsorbent pair of Activated Carbon – PE MSM 41.

Based on the above observations, the basic criterion for the selection of adsorbent pair to achieve best refrigeration performance can be suggested. The selection of adsorbent pair depends on the adsorbent isotherms, thermal stability and reaction kinetics at the refrigeration system operating temperature range. The general properties required are high transferrable $CO_2$ capacity, fast reaction rates, good thermal stability. The adsorbent placed at refrigeration side should possess higher reaction heat to increase refrigeration effect and the adsorbent placed at regeneration side should possess low reaction heat to reduce the regeneration heat supplied consequently together increases COP. In addition, the pressure differences between the coupled adsorbent reactors strongly influence the $CO_2$ transfer rate and amount. The higher-pressure difference between coupled adsorbents is responsible for high refrigeration capacity and reduces cycle time.

## 4. CONCLUSIONS

The study on thermodynamic simulation of $CO_2$ – adsorbent based sorption refrigeration system and vapour adsorption system led to the following conclusions:
- The materials suitable for storage of $CO_2$ are considered to check their suitability for the development of gas-solid sorption refrigeration system.
- Out of several $CO_2$ storage materials, Activated Carbon, PE MSM 41, AT MSM 41 and AF Silica are found suitable for $CO_2$ – A SRS.
- The pair of Activated Carbon – PE MSM 41 is found best suitable for the development $CO_2$ – A SRS compared to AT MSM 41 – AF Silica pair, which can produce 197 kJ of refrigeration load with 33% of second law efficiency for 1 kg of absorbents and cycle time of 30 minutes.
- The refrigeration performance of $CO_2$ – A SRS can be improved with high transferrable $CO_2$ capacity, sufficient pressure difference between coupled adsorbents, high reaction heat of refrigeration adsorbent and low reaction heat of regeneration adsorbent.
- High refrigeration performance is observed for $CO_2$ – A SRS using the pair of Activated Carbon – PE MSM 41 compared to $CO_2$-A VARS using activated carbon as working material.

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## NOMENCLATURE

| | |
|---|---|
| A SRS | adsorbent based sorption refrigeration system |
| A VARS | adsorbent based vapour adsorption refrigeration system |
| COP | coefficient of performance |
| SRP | specific refrigeration power |
| RC | refrigeration capacity |
| C | specific heat; kJ/kg K |

| | |
|---|---|
| $\Delta H$ | reaction enthalpy; kJ/mol |
| m | mass of adsorbent; kg |
| n | moles of $CO_2$; mol |
| $P_e$ | equilibrium pressure; bar |
| $\Delta P$ | pressure differential; bar |
| Q | heat load; kJ |
| T | absolute temperature; °C |
| t | time; sec |
| η | efficiency |

*Subscripts*

| | |
|---|---|
| a | ambinet |
| cyl | cycle |
| ref | refrigeration |
| reg | regeneration |
| s | waste heat source |
| c | condenser |
| r | reactor |

## ТЕРМОДИНАМИЧКА СИМУЛАЦИЈА СИСТЕМА СОРПЦИОНОГ ХЛАЂЕЊА БАЗИРАНОГ НА АДСОРБЕНТУ CO₂

### С.Н. Сајед, В.К. Шарма

Различити материјали као што су активни угљ, метално органски оквири, кварц и др. имају способност адсорпције и десорпције CO2. Топлотна интеракција током ових процеса може да се користи за развој система сорпционог хлађења на бази адсорбента гаса. У раду је ова концепција примењена за анализу термодинамичких перформанси система сорпционог хлађења базираног на адсорбенту CO2. Као адсорбенти су коришћени активни угаљ Norit RB3, PE MSM 41, AT MSM 41 и AF Silica. Од наведених адсорбената направљени су парови на основу разлике у притиску која омогућава довољан проток CO2 између два адсорбента на радној температури хлађења од 0⁰С, амбијенталној од 25⁰С и извора топлоте од 100⁰С. Термодинамичке перформансе система хлађења су упоређиване по паровима адсорбената. Анализом су обухваћене следеће перформансе: ефекат хлађења, специфична снага хлађења, коефицијент перформансе, капацитет хлађења и други закон степена искоришћености. Ефекат хлађења код пара активни угаљ – PE MSM 41 је двоструко већи него код пара AT MSM 41 – AF-Silica. Такође је извршено поређење перформанси пара CO2 – A-SRS и пара CO2 – A-VARS што је доступно и у литератури. Утврђено је да је коефицијент перформансе код пара CO2-A STS већи него код пара CO2 – A VARS.