

# Modelling and experimental investigation of effects of moisture and operating parameters during the adsorption of CO<sub>2</sub> onto polyaspartamide

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**Abstract** Parametric effect of moisture and influence of operating variables on the adsorption behaviour of polyaspartamide during CO<sub>2</sub> capture was investigated in this study using experimental and modelling approach. Individual effects of operating conditions (e.g. pressure, temperature and gas flow rates) as well as the effect of moisture on the adsorption capacity of polyaspartamide were methodically investigated using Dubinin–Raduskevich model. Results from the investigations reveal that the presence of moisture in the flue gas had an incremental effect on the adsorption capacity of polyaspartamide; thereby showcasing the potential of polyaspartamide as a suitable hydrophilic material for CO<sub>2</sub> capture in power plants. In addition, pressure, temperature and gas flow rates at 200 kPa, 403 K, and 1.5 mL/s, respectively, significantly influenced the CO<sub>2</sub> adsorption capacity of polyaspartamide. Physisorption and chemisorption both governed the adsorption process while equilibrium studies at different temperatures showed that Langmuir isotherm could adequately describe the adsorption behaviour of the material with best fit with  $R^2 > 0.95$ .

**Keywords** Adsorption capacity · CO<sub>2</sub> capture · Moisture · Operating variables · Polyaspartamide

## 1 Introduction

Coal is one of the world's cheapest and abundant fossil fuel with a wide range of applications in power generation, transport systems and thermal energy production (Chitsiga et al. 2018). However, the use of coal in these important sectors results in the emission of greenhouse gases (especially CO<sub>2</sub>) into the atmosphere which is a major cause of climate change. Discontinuing the use of coal especially in

power generation or switching to other alternative clean energy sources will make power generation very expensive and unaffordable in most developing countries (Sekoai et al. 2018; Yoro and Sekoai 2016). Research have shown that by applying CO<sub>2</sub> capture and storage techniques, it is possible to continue the use of coal in power generation and yet maintain a near-zero CO<sub>2</sub> emission. Adsorption of CO<sub>2</sub> is a reliable technique that can be used for CO<sub>2</sub> capture and adsorbents play a critical role during this process.

So far, variety of adsorbents such as synthetic zeolites (Cheung and Hedin 2014; Siriwardane et al. 2005), amine-grafted zeolite 13 × (Bezerra et al. 2014), amine-grafted activated carbon (Alhassan et al. 2017; Hao et al. 2017; Zhang et al. 2013), amine-modified polymethyl methacrylate (Lee et al. 2008), carbon molecular sieves (Donald-Carruthers et al. 2012; Lee and Park 2015), silica and metal oxides (Chowdhury et al. 2015; Li et al. 2015; Zhang et al. 2014b), as well as metal organic frameworks and amine-modified materials (Belmabkhout et al. 2016; Fracaroli et al. 2014; Zhang et al. 2014b) have been developed and

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studied for CO<sub>2</sub> capture under both dry and wet conditions. Before now, amine-grafted zeolite 13 × and carbon molecular sieves were used for CO<sub>2</sub> capture because of their high CO<sub>2</sub> adsorption capacities at low CO<sub>2</sub> concentration (258 mg/g for amine-grafted zeolite 13 × and 950 mg/g for carbon molecular sieves), rapid mass transfer in the particle, and other factors such as cheap preparation cost and environmental friendliness (Li et al. 2013; Samanta et al. 2012; Xu et al. 2002, 2005). However, CO<sub>2</sub> adsorption capacity of these adsorbents tend to decline rapidly in the presence of moisture with a slight increase in temperature (Xu et al. 2011). In response to these challenges, polyaspartamide was recently developed for CO<sub>2</sub> capture but the effects of operating conditions on its behaviour during the adsorption of CO<sub>2</sub> has not been adequately reported in open literature. Hence, it is investigated in this study.

Polyaspartamide is an amine-grafted polysuccinimide. It is non-toxic, biodegradable and environmentally friendly with a high degree of porosity and extended inter-particle surface area widely used in chemotherapeutic studies (Kim et al. 2012; Miyata et al. 2008; Moon et al. 2011). Its rich amine-content, high thermal stability, high adsorption capacity and ability to be regenerated after use makes it a potential material for CO<sub>2</sub> capture. Details on its preparation and cost have been reported extensively in our previous works (Ngoy et al. 2017; Chitsiga et al. 2016). Hence, it is not repeated in this work. As far as could be ascertained, no information has been provided in literature in contrast with impregnation or grafting of polyaspartamide because the material is still new in the area of CO<sub>2</sub> capture. Grafting and impregnation of polyaspartamide with other materials could be considered by future research. Since the application of polyaspartamide in CO<sub>2</sub> capture is still new; a detailed report on its behaviour during the adsorption of CO<sub>2</sub> is crucial towards attaining efficient separation. It has been identified that there is a dearth report on the behaviour of the adsorbent in the presence of moisture (Scapino et al. 2017). In-depth information on the influence of operating conditions on the adsorption capacity of adsorbents as well as the optimization of these operating conditions during CO<sub>2</sub> capture is also very pivotal in the design of adsorbents and adsorption systems to ensure a good CO<sub>2</sub> adsorption capacity. Therefore, the main objective of this study is to provide useful parametric information that could be used to optimize polyaspartamide as an adsorbent for effective CO<sub>2</sub> capture in the presence of moisture. This is because, for adsorption of CO<sub>2</sub> to be economically feasible during post-combustion CO<sub>2</sub> capture, there is a need for the development of adsorbents with high adsorption capacity and very high moisture resistance (Cuéllar-Franca and Azapagic 2015; Scapino et al. 2017).

A typical industrial flue gas contains moisture and the adsorption capacity of most adsorbents is chiefly determined by the conditions at which they are put into use. The composition of flue gas from a typical power plant is usually 68%–75% N<sub>2</sub>, 10%–15% CO<sub>2</sub>, 5%–10% moisture and 2%–5% O<sub>2</sub> with traces of NO<sub>x</sub> and SO<sub>x</sub> (Ntiamoah et al. 2016). Conventionally, the wet flue gas from power plants is usually pre-treated and dried to reduce its moisture content before adsorption process commences (Ntiamoah et al. 2016; Xu et al. 2011). This conventional approach of pre-treating and drying flue gas before capturing the CO<sub>2</sub> content is widely embraced industrially. However, this option increases the overall cost of the CO<sub>2</sub> capture process and also impacts negatively on plant efficiency (Sekoai and Yoro 2016; Yoro 2017; Zhang et al. 2014a, b, c). In addition, most adsorbents adsorb moisture alongside other gases and this makes the CO<sub>2</sub> separation selectivity to become very low during the capture process (Marx et al. 2013; Yoro and Sekoai 2016; Zhang et al. 2014a, b, c).

The key elements of a good adsorbent for CO<sub>2</sub> capture are; rapid adsorption/desorption kinetics, moisture resistance, stable adsorption capacity after repeated cycles and adequate mechanical strength of the particles (Titinchi et al. 2014; Veneman et al. 2015; Yu et al. 2017). Most of these key elements for a good adsorbent have been studied and reported in literature for most adsorbents (Alhwaige et al. 2016; Ding et al. 2016; Osler et al. 2017a, b; Singo et al. 2017; Yoro et al. 2016; Ngoy et al. 2017; Sekoai et al. 2016). The effect of moisture on adsorbents during CO<sub>2</sub> capture needs to be studied in-depth because most times, moisture usually occupy the pores of adsorbents and most adsorbents have exhibited a higher affinity for moisture than CO<sub>2</sub> (Amponsah et al. 2014; Leung et al. 2014). The effect of moisture on the adsorption capacity of adsorbents during CO<sub>2</sub> capture could be advantageous or detrimental (Marx et al. 2013). Hence, if polyaspartamide must be considered as an appropriate material for CO<sub>2</sub> capture from power plants, there is need to understand the effect of moisture on its adsorption performance during the CO<sub>2</sub> capture process (Marx et al. 2013; Qi et al. 2000).

Previous studies have speculated that amine-rich polymer-based adsorbents exhibit a high tolerance level for moisture (Chou and Chiou 1997; Hefti et al. 2014). Similarly, the effect of vapour pressure on the adsorption capacity of other CO<sub>2</sub> capture materials have been described using the popular Langmuir, Freundlich, and Dubinin–Raduskevich models in the past (Chou and Chiou 1997; Guangzhi et al. 2017; Vargas et al. 2012); as such, a similar approach was adapted and modified in the investigation reported herein to confirm the aforementioned speculation.

Synthesis and characterization of polyaspartamide have been adequately reported in our previous works (Chitsiga et al. 2016; Ngoy et al. 2017; Yoro et al. 2017). A study on

the kinetic behaviour of polyaspartamide has also been reported recently (Yoro et al. 2017), but the influence of moisture and other operating parameters on the adsorption capacity of polyaspartamide during the adsorption of CO<sub>2</sub> from a flue gas stream is rare and has not attracted adequate attention in the past. Therefore, the current study is focused on the investigating the influence of key operating variables during adsorption of CO<sub>2</sub> by polyaspartamide and the effect of moisture on its adsorption capacity during CO<sub>2</sub> capture. The modelling and experimentation approach adapted in this study is simpler, straightforward and better suited than the original graphical technique commonly used for dynamic simulation of activated carbon adsorbents and it have been confirmed to be suitable for parametric studies of this kind from related studies (Alhassan et al. 2017; Chou and Chiou 1997; Yoro et al. 2017). The outcome of this study is expected to provide useful information that could be used to optimize polyaspartamide as an adsorbent for effective CO<sub>2</sub> capture.

## 2 Materials and methods

### 2.1 Materials

The materials used in this study include; polyaspartamide, gas mixture (Composition: 15% CO<sub>2</sub>, 85% N<sub>2</sub>), and pure Nitrogen gas (100% N<sub>2</sub>). Polyaspartamide used in this study was not procured but synthesized in our laboratory according to a modified protocol described by Ngoy et al. (2014, 2017) while all gases used in this study were purchased from Afrox (Pty) South Africa and used without any further purification. The gas analyzer considered in this study is a single component CO<sub>2</sub> gas analyzer (Model: ABB-AO2020, Dimension: 485 mm × 460 mm × 135 mm, Weight: 15 kg, Precision: SO<sub>2</sub>, NO, CO, CO<sub>2</sub> ≤ ± 2%, O<sub>2</sub> ≤ ± 3%, Place of manufacture: Frankfurt, Germany). The analyzer was used to obtain the concentration of CO<sub>2</sub> adsorbed by the adsorbent.

### 2.2 Methods

The sample (polyaspartamide) was pre-treated by heating at 353–373 K under vacuum (0.01–0.05 kPa) for 1 h to desorb CO<sub>2</sub>, water and other gaseous impurities that could be present on the sample. The adsorption column temperature was then cooled down to room temperature (298 K) and re-pressurized with N<sub>2</sub> gas. Afterwards, the temperature was adjusted to the desired adsorption temperatures. Experimental data obtained from the adsorption experiments were fitted into mathematical models adapted from a similar study (Chou and Chiou 1997), and then analysed in order to describe the effect of moisture on the adsorption

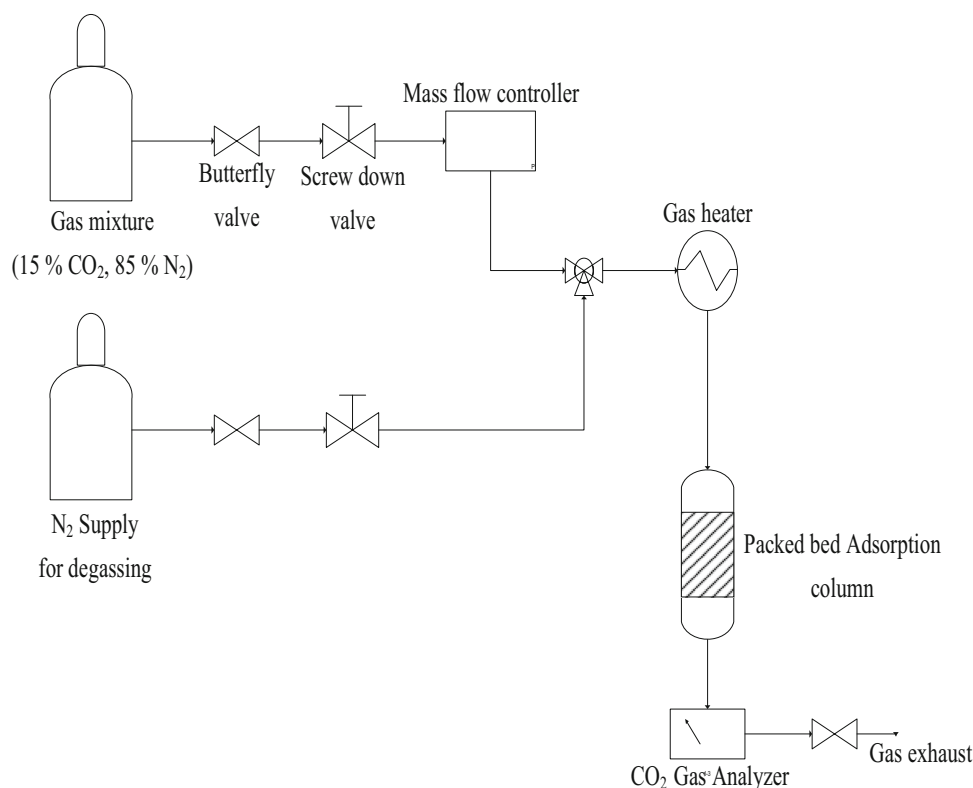
capacity of polyaspartamide while the influence of operating conditions on the adsorption capacity of polyaspartamide was studied experimentally at different operating conditions in a packed-bed adsorption system. Within the experimental conditions in this study, the adsorption capacities of polyaspartamide in both moist and dry air streams were related to the operating pressure, gas flow rate and adsorption temperature.

## 3 Experimental procedure

Experimental runs were first carried out to determine the adsorption capacity of polyaspartamide in a laboratory-scale packed-bed adsorption column at operating temperatures of 403, 418 and 433 K, as well as a pressure range of 100–200 kPa. Polyaspartamide (0.1 g) was loaded into a column and pure N<sub>2</sub> was used to purge the adsorption system at 373 K at an inlet gas flow rate of 1.5 mL/s for 10 min (600 s) to get rid of impurities within the column. To proceed with the main experimental runs, the initial temperature was lowered to 433 K and the concentrations of CO<sub>2</sub> were obtained from the digital CO<sub>2</sub> gas analyzer at different times. The feed gas (15% CO<sub>2</sub>, 85% N<sub>2</sub>) was then fed into the adsorption column while by-passing the reactor in order to obtain the initial concentrations of CO<sub>2</sub> at different temperatures. More experimental runs were repeated at 418 and 403 K, respectively. Each experimental run lasted for 1200 s at different operating conditions. At any given temperature considered, the quantity of gas adsorbed was a function of the pressure. Adsorption capacity of the material was then mathematically calculated from the mass balance in the system using experimental data obtained based on the gas flow rates, gas concentrations, and adsorption time when equilibrium was attained. The flow diagram for the experimental set-up is presented in Fig. 1.

## 4 Model description

An existing model which incorporates vapor pressure parameter was adapted from a previous study by Chou and Chiou (1997) and was used to predict the numerical effect of moisture on the adsorption capacity of polyaspartamide. The model was modified to suit the conditions in this study and experimental data were imputed into the model with respective vapor pressure parameters. A new adsorption capacity of polyaspartamide, noting the moisture presence, was then obtained from the model. Details on the assumptions, boundary conditions and full description of the Dubinin–Raduskevich model as used in this study has been reported by the original developers of the model (Chou and Chiou 1997). The adsorption of gases as a single



**Fig. 1** Flow adsorption setup for the CO<sub>2</sub> separation from simulated flue gas. (Adapted from Yoro et al. (2017))

component onto polyaspartamide was then quantified using the Dubinin–Raduskevich equation as shown in Eq. 1:

$$q_a = \rho_a W_a \exp \left[ -K_a \left( \frac{RT \ln P a_s}{P_a} \right)^2 \right] \quad (1)$$

where  $q_a$  represents the adsorption capacity;  $\rho_a$  is the density of CO<sub>2</sub>;  $W_a$  is the limiting adsorption volume for CO<sub>2</sub>;  $P a_s$  is the saturated vapor pressure of CO<sub>2</sub>;  $P_a$  is the vapor pressure in the presence of moisture;  $T$  is the temperature in Kelvin;  $R$  is the universal gas constant and  $K_a$  is the molar volume of the gas (CO<sub>2</sub>).

The experimental data obtained were further fitted to standard adsorption isotherms (Langmuir and Freundlich adsorption). The adsorption isotherm models for Langmuir and Freundlich are presented in Eqs. (2) and (3), respectively:

$$q = \frac{q_m K P_{CO_2}}{1 + K P_{CO_2}} \quad (2)$$

$$q_e = K_f C_e^{1/n} \quad (3)$$

where  $q$  is the amount of CO<sub>2</sub> adsorbed at the pressure  $P$ ;  $q_m$  is the amount of CO<sub>2</sub> adsorbed with monolayer coverage; and  $K$  is the Langmuir constant. While  $q_e$  is the equilibrium amount of CO<sub>2</sub> adsorbed;  $K_f$  is the adsorption

constant;  $C_e$  is the equilibrium concentration of CO<sub>2</sub> and  $n$  is the adsorption intensity of the Freundlich model.

## 5 Results and discussion

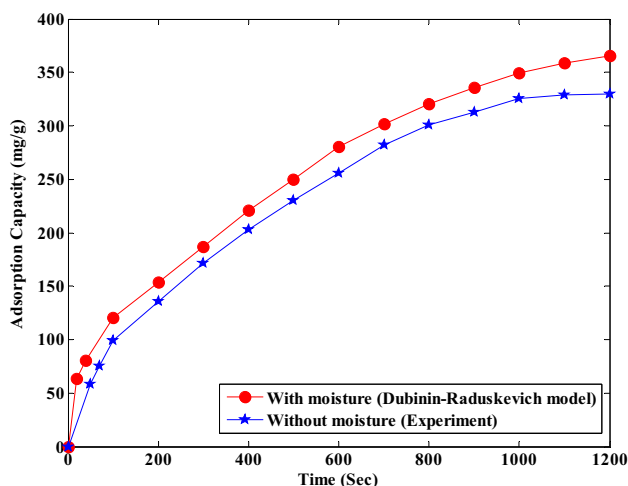
### 5.1 Effect of moisture

Most physical adsorbents for CO<sub>2</sub> capture have less tolerance for water vapour in the gas feed (Ünveren et al. 2017; Saiwan et al. 2014); but we envisage that polyaspartamide will exhibit a high tolerance level for moisture unlike other physical adsorbents because of its amine-impregnation and the fact that it can function both as a physical or chemical adsorbent. CO<sub>2</sub> uptake by polyaspartamide is expected to increase in the presence of moisture due to the interactions between amine and CO<sub>2</sub>. A bicarbonate compound is formed when CO<sub>2</sub> reacts with a primary amine group in polyaspartamide under wet conditions while carbamate is formed under dry conditions according to the schemes in the chemical Eqs. (4) and (5) presented below (Stowe et al. 2015).



Bicarbonate is a major specie formed during CO<sub>2</sub> capture via an aqueous amine process, such as monoethanolamine (MEA), diethanolamine (DEA), and other hindered amines. The result presented in Fig. 2 shows that the model predicted an adsorption capacity of 365.6 mg/g instead of 330.1 mg/g obtained using experimental approach (dry conditions). The result in Fig. 2 shows an increase in the adsorption capacity of polyaspartamide in the presence of moisture. Adsorption capacity is expected to increase to almost double in the presence of moisture. However, only a slight increase was observed in this study because most of the micro pores on the surface of the material have been occupied by CO<sub>2</sub> molecules and also saturated. Therefore, there will be no room for a further increase in the adsorption capacity of polyaspartamide. The slight increase in the adsorption capacity of polyaspartamide in this study could also be attributed to the hydration interaction of CO<sub>2</sub> and adsorbed water on the surface of the adsorbent as reported by Li et al. (2009a, b) as well as Baltrusaitis and Grassian (2005). This is in line with previous reports in literature

Findings from this study reveal that although polyaspartamide shows high tolerance for moisture (hydrophilic), its adsorption capacity improves slightly in the presence of moisture due to chemical adsorption of CO<sub>2</sub> resulting in bicarbonate formation as well as the pore structure, the surface area, the degree and type of functionalization as well as the amine impregnation of polyaspartamide. This makes polyaspartamide a very suitable material for CO<sub>2</sub> capture from flue gas streams. The findings reported in this study agrees with that of a similar study reported for a polyamine-based solid adsorbent which is a similar material to the adsorbent considered in this study (Goepfert et al. 2011). Moisture have also been reported in the past to enhance the adsorption capacity as well as the amine



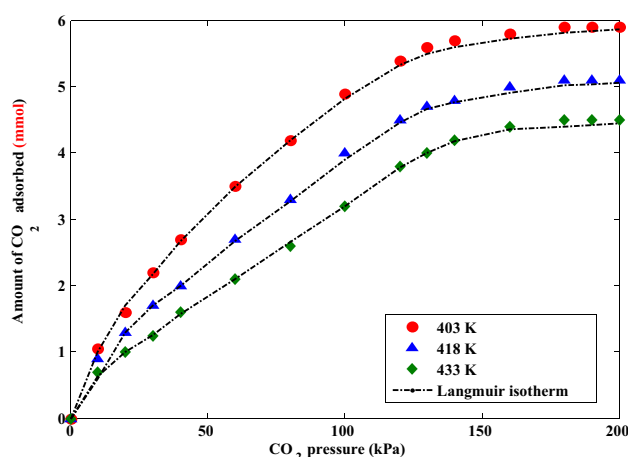
**Fig. 2** Theoretical and experimental effect of moisture on the CO<sub>2</sub> adsorption capacity of polyaspartamide

efficiency of tetraethylenepentamine (TEPA), polyethylenimine (PEI impregnated) (Yu and Chuang 2017), and 3-aminopropyltrimethoxysilane (APS) grafted silica sorbents during CO<sub>2</sub> capture (Hahn et al. 2015; Stuckert and Yang 2011). In all the aforementioned reports, enhancement effect of moisture on adsorption capacity was also attributed to the formation of bicarbonate which is very similar to the claim in this study.

## 5.2 Effect of temperature

To investigate the effect of temperature on the adsorption capacity of polyaspartamide, data obtained from the experiments conducted at 403, 418 and 433 K were analysed. These temperatures were chosen because Chitsiga et al. (2016) reported that polyaspartamide is usually thermally stable at about 210 °C (483 K). Since adsorption is a temperature dependent surface phenomenon favoured by lower temperatures, any further decrease in temperature below 403 K is expected to result to a higher adsorption capacity before equilibrium is attained and the material gets saturated. In this work, the highest adsorption capacity was observed at 403 K (the lowest temperature); hence we speculate here that the optimum temperature for this study is the lowest temperature (403 K).

The adsorption isotherms in this study exhibited a monolayer adsorption mechanism for both models. The isotherms also displayed a common behaviour notwithstanding the operating temperature as depicted in Figs. 3 and 4. The results further revealed that Langmuir isotherm shows a superior fit to the adsorption data in this study (see Fig. 3). The increase in the adsorption capacity with decrease in temperature illustrates that CO<sub>2</sub> adsorption onto polyaspartamide is an exothermic process. The adsorption isotherms presented in this study generally



**Fig. 3** CO<sub>2</sub> adsorption isotherms of polyaspartamide at various temperatures (experimental vs Langmuir isotherm)

described the influence of temperature on the amount of CO<sub>2</sub> adsorbed by polyaspartamide. The amount of CO<sub>2</sub> capturable by polyaspartamide was 5.9 mmol of CO<sub>2</sub> at 403 K while 4.5 mmol of CO<sub>2</sub> was captured by polyaspartamide at 433 K, constant pressure of 200 kPa and gas inlet flow rate of 1.5 mL/s as shown in Fig. 3. This implies that the ideal temperature for the adsorption of CO<sub>2</sub> by polyaspartamide at a laboratory level as presented in this study is 403 K. Values for the Langmuir isotherm parameters obtained in this study were compared with values recently reported in a similar study by (Khalili et al. 2016) and presented in Table 1; while values for the Freundlich isotherm parameters are presented in Table 2 and Fig. 4. The results obtained confirm that at lower temperatures, the adsorption capacity of polyaspartamide improves steadily just like other adsorbents reported in literature (Alhwaige et al. 2016; Siriwardane et al. 2005; Titinchi et al. 2014; Zhang et al. 2013, 2014c). The observations in this study are in agreement with a recent report by Auta et al. (2013); but an opposite pattern was observed with amines commonly used for CO<sub>2</sub> absorption in liquid phase polyethylenimines such as monoethanolamine and diethanolamine reported by Goepfert et al. (2010). The increasing absorption capacity of polyethylenimine-based sorbents with increasing temperature is attributed to the nature of polyethylenimines. With increasing temperature, the viscosity of polyethylenimines diminishes. Diminishing viscosity at higher temperatures improves the reaction kinetics of CO<sub>2</sub> with the amino groups of the absorbent, thereby improving the CO<sub>2</sub> adsorption. Polyaspartamide can easily be regenerated and desorption of CO<sub>2</sub> from polyaspartamide is possible when the temperature is raised slightly above 450 K. However, desorption and regeneration is not discussed in detail in this work because it does not fall within the scope of this report. It will be reported in our future research.

### 5.3 Effect of operating pressure

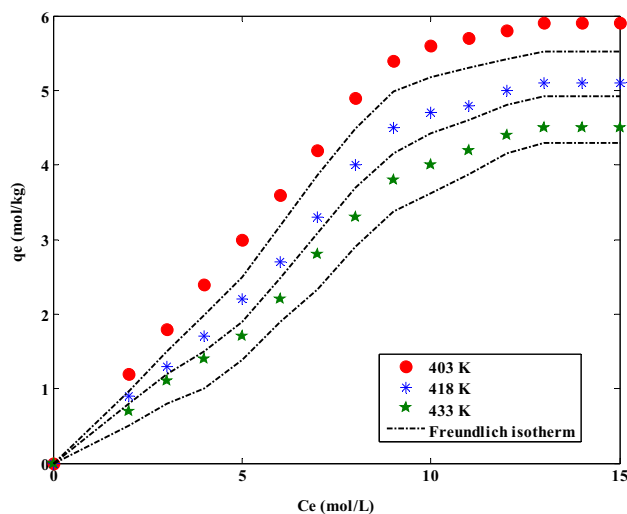
Pressure is an important parameter in studying the behaviour and adsorption capacity of solid sorbents (Yoro et al. 2017). Mathematically, the amount of CO<sub>2</sub> adsorbed by an

**Table 1** Constant model parameters for the Langmuir isotherm at different temperatures compared with literature

$T$ (K)	$q_m$ (mg/g)	$K$ (kPa <sup>-1</sup> )	$R^2$	References
288	4.131	0.026	0.984	Khalili et al. (2016)
298	3.812	0.020	0.987	Khalili et al. (2016)
308	2.879	0.018	0.992	Khalili et al. (2016)
288	7.420	0.017	0.991	This study
298	6.150	0.012	0.994	This study
308	4.985	0.005	0.998	This study

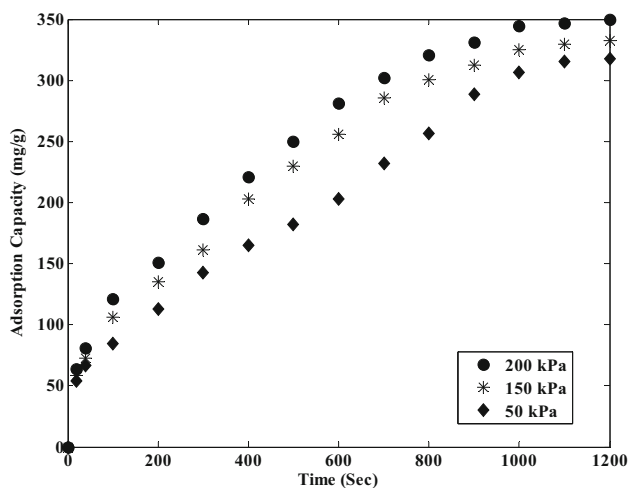
**Table 2** Constant model parameters for Freundlich isotherm at different temperatures compared with literature

$T$ (K)	$K_f$ (mg/g)	$n$	$R^2$	References
288	1.140	1.587	0.995	Khalili et al. (2016)
298	1.110	1.451	0.996	Khalili et al. (2016)
308	0.992	1.434	0.996	Khalili et al. (2016)
288	1.320	1.840	0.720	This study
298	1.224	1.690	0.800	This study
308	1.150	1.520	0.892	This study



**Fig. 4** CO<sub>2</sub> adsorption isotherms of polyaspartamide at various temperatures (experimental vs Freundlich isotherm)

adsorbent is directly proportional to the operating pressure. According to the results presented in Fig. 5, at higher operating pressure, the CO<sub>2</sub> adsorption capacity of polyaspartamide increased and lower operating pressures resulted in a decreased adsorption capacity of polyaspartamide at the same operating temperature. The adsorption capacities of polyaspartamide obtained in this study were 350, 330 and 320 mgCO<sub>2</sub>/g adsorbent at varying operating pressure of 200, 150 and 100 kPa, respectively. The adsorption capacities reported in this study were obtained from experiments conducted in a packed bed adsorption column at an operating temperature of 403 K. The maximum adsorption capacity of polyaspartamide reported in this study (350 mgCO<sub>2</sub>/g adsorbent) was obtained at the highest pressure of 200 kPa in this study using a gas composition of 15% CO<sub>2</sub> and 85% N<sub>2</sub>. This value is higher than that reported by Chitsiga et al. (2016), where the authors reported an adsorption capacity of 44 mgCO<sub>2</sub>/g using a 100% CO<sub>2</sub> source in a thermogravimetric analyzer (TGA) under the same operating conditions. The higher adsorption capacity reported herein could be attributed to



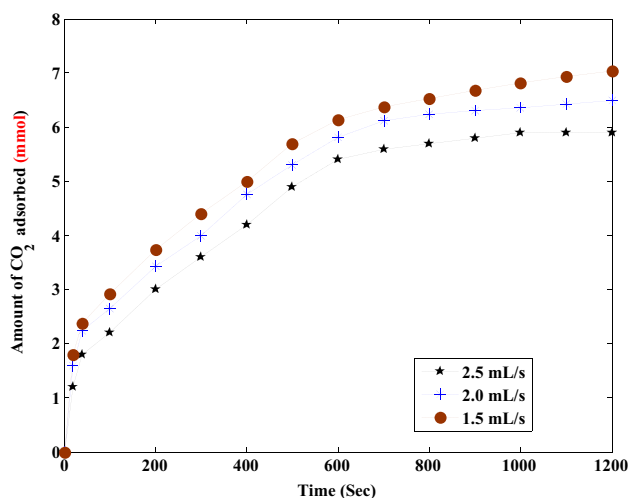
**Fig. 5** Effect of operating pressure on the adsorption capacity of polyaspartamide

the closer contact between the adsorbent (Polyaspartamide) and the adsorbate ( $\text{CO}_2$ ) within the packed bed and increased residence time due to packings in the column than in the thermogravimetric analyzer used by Chitsiga et al. (2016). The different composition of gases used in both studies also contributed to the high adsorption capacity obtained in this study. In summary, findings from this study show that higher operating pressure resulted in an improved adsorption capacity of polyaspartamide.

#### 5.4 Effect of gas flow rate

The results for adsorption of  $\text{CO}_2$  onto polyaspartamide at different gas flowrates is presented in Fig. 6. It was observed that decreasing the inlet gas flow rate increases the contact time and therefore improves the adsorption capacity of polyaspartamide. This implies that, faster flow rates decrease the retention time of  $\text{CO}_2$  molecules on polyaspartamide within the packed bed system thereby resulting in a reduced adsorption capacity. Longer residence times are required for higher adsorption capacities. Based on the results presented in Fig. 6, the maximum amount of  $\text{CO}_2$  adsorbed by polyaspartamide at different flow rates of 1.5, 2.0 and 2.5 mL/s  $\text{CO}_2$  were 7.0, 6.0 and 5.8 mg  $\text{CO}_2/\text{g}$  of adsorbent while the adsorption capacities were 350, 330 and 320 mg $\text{CO}_2/\text{g}$  adsorbent as presented in Fig. 5.

In addition, Fig. 6 shows that as the gas flow rate increases from 1.5 to 2.5 mL/s, the adsorption curve becomes steeper and the breakpoint time also decreases from 600 to 500 s. This observation is in agreement with the studies reported by Auta et al. (2013) and Tan et al. (2014). Gas flow rates of 90, 120 and 150 mL/min were compared against the adsorption capacity of a NaOH-



**Fig. 6** Effect of gas flow rates on the amount of  $\text{CO}_2$  adsorbed onto polyaspartamide

modified coconut shell activated carbon (32ACSH3) by Tan et al. (2014). The researchers also reported that the slowest flow rate of 90 mL/min produced a longer breakthrough time compared with the highest flow rate of 150 mL/min. Hence, they concluded that longer dwelling times at lower flow rates allow for slower  $\text{CO}_2$  diffusion, which leads to a higher adsorption capacity. Auta et al. (2013) also conducted a similar study with the same gas flowrates reported by Tan et al. (2014) using a sodium hydroxide modified activated alumina and the authors also arrived at the same conclusion reported in this study. Information on the effect of gas flow rate provided in this study can be used for mass transfer study as well as designing and operating an industrial-sized adsorption column.

## 6 Conclusions and recommendations

Behaviour of polyaspartamide during  $\text{CO}_2$  capture was studied under different experimental conditions; including gas flow rate, adsorption temperature, operating pressure in a packed bed adsorption column while the effect of moisture on the adsorption capacity of polyaspartamide was theoretically investigated using a mathematical modelling approach. Results obtained from the packed-bed adsorption experiments reveal that feed flow rate of 1.5 mL/s at a constant adsorbent loading of 1.0 g, operating pressure of 200 kPa and adsorption temperature of 403 K are good for the adsorption of  $\text{CO}_2$  at a laboratory scale while the Dubinin–Raduskevich model accurately predicted that the presence of moisture has a promoting effect on the adsorption capacity of polyaspartamide. Validation of the model prediction in this study using experimental approach

would be a very good topic for future research. Other major findings from this study are:

- (1) Adsorption of CO<sub>2</sub> onto polyaspartamide is controlled by both physisorption and Chemisorption.
- (2) Simply targeting high CO<sub>2</sub> adsorption capacities alone is quite inadequate to conclude on the potential of an emerging adsorbent like polyaspartamide for effective CO<sub>2</sub> capture. But when other criteria such as the influence of operating parameters are included in the specifications for new materials as described in this study, polyaspartamide looks promising as an effective material for CO<sub>2</sub> capture.
- (3) Further research should be carried out on the desorption, regeneration and application of the adsorbent reported herein towards the removal of CO<sub>2</sub> from coal-fired power plants at a pilot or industrial scale.
- (4) Economic analysis may also be performed in future research to determine how cost-effective it would be to use polyaspartamide for CO<sub>2</sub> capture on a large scale.

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#### Compliance with ethical standards

**Conflict of interest** There is no conflict of interest regarding the publication of this research article.

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#### References

- Alhassan M, Andrew I, Auta M, Umaru M, Garba MU, Isah AG, Alhassan B (2017) Comparative studies of CO<sub>2</sub> capture using acid and base modified activated carbon from sugarcane bagasse. *Biofuels*. <https://doi.org/10.1080/17597269.2017.1306680>
- Alhwaige AA, Ishida H, Qutubuddin S (2016) Carbon aerogels with excellent CO<sub>2</sub> adsorption capacity synthesized from clay-reinforced biobased chitosan-polybenzoxazine nanocomposites. *ACS Sustain Chem Eng* 4:1286–1295
- Amponsah NY, Troldborg M, Kington B, Aalders I, Hough RL (2014) Greenhouse gas emissions from renewable energy sources: a review of lifecycle considerations. *Renew Sustain Energy Rev* 39:461–475
- Auta M, Amat-Darbis ND, Moh'd-Din AT, Hameed BH (2013) Fixed-bed column adsorption of carbon dioxide by sodium hydroxide modified activated alumina. *Chem Eng J* 233:80–87

- Baltrusaitis J, Grassian VH (2005) Surface reaction of carbon dioxide at the adsorbed water—iron oxide interface. *J Phys Chem B* 109:12227–12230
- Belmabkhout Y, Guillerm V, Eddaoudi M (2016) Low concentration CO<sub>2</sub> capture using physical adsorbents: are metal–organic frameworks becoming the new benchmark materials? *Chem Eng J* 296:386–397
- Bezerra DP, Francisco WM, Pedro AS et al (2014) CO<sub>2</sub> adsorption in amine-grafted zeolite 13X. *Appl Surf Sci* 314:314–321
- Cheung O, Hedin N (2014) Zeolites and related sorbents with narrow pores for CO<sub>2</sub> separation from flue gas. *RSC Adv* 4:14480–14494
- Chitsiga T, Daramola MO, Wagner N, Ngoy J (2016) Effect of the presence of water-soluble amines on the carbon dioxide (CO<sub>2</sub>) adsorption capacity of amine-grafted poly-succinimide (PSI) adsorbent during CO<sub>2</sub> capture. *Energy Procedia* 86:90–105
- Chitsiga TL, Daramola MO, Wagner N, Ngoy J (2018) Parametric effect of adsorption variables on CO<sub>2</sub> adsorption of amine-grafted polyaspartamide composite adsorbent during post-combustion CO<sub>2</sub> capture: a response surface methodology approach. *Int J Oil Gas Coal Technol* 17:321–336
- Chou MS, Chiou JH (1997) Modeling effects of moisture on adsorption capacity of activated carbon for VOCs. *J Environ Eng* 123:437–443
- Chowdhury S, Parshetti GK, Balasubramanian R (2015) Post-combustion CO<sub>2</sub> capture using mesoporous TiO<sub>2</sub>/graphene oxide nanocomposites. *Chem Eng J* 263:374–384
- Cuéllar-Franca RM, Azapagic A (2015) Carbon capture, storage and utilisation technologies: a critical analysis and comparison of their life cycle environmental impacts. *J CO<sub>2</sub> Util* 9:82–102
- Ding N, Li H, Feng X, Wang Q, Wang S, Ma L, Zhou J, Wang B (2016) Partitioning MOF-5 into confined and hydrophobic compartments for carbon capture under humid conditions. *J Am Chem Soc* 138:10100–10103
- Donald-Carruthers J, Petruska MA, Sturm EA, Wilson SM (2012) Molecular sieve carbons for CO<sub>2</sub> capture. *Microporous Mesoporous Mater* 154:62–67
- Fracaroli AM, Furukawa H, Suzuki M, Dodd M, Okajima S, Gándara F, Reimer JA, Yaghi OM (2014) Metal-organic frameworks with precisely designed interior for carbon dioxide capture in the presence of water. *J Am Chem Soc* 136:8863–8866
- Goeppert A, Meth S, Prakash GKS, Olah GA (2010) Nanostructured silica as a support for regenerable high-capacity organoamine-based CO<sub>2</sub> sorbents. *Energy Environ Sci* 3:1949–1960
- Goeppert A, Czaun M, May RB, Prakash GKS, Olah GA, Narayanan SR (2011) Carbon dioxide capture from the air using a polyamine based regenerable solid adsorbent. *J Am Chem Soc* 133:20164–20167
- Guangzhi Y, Jinyu Y, Yuhua Y, Zhihong T, DengGuang Y, Junhe Y (2017) Preparation and CO<sub>2</sub> adsorption properties of porous carbon from camphor leaves by hydrothermal carbonization and sequential potassium hydroxide activation. *RSC Adv* 7:4152–4160
- Hahn MW, Steib M, Jentys A, Lercher JA (2015) Mechanism and kinetics of CO<sub>2</sub> adsorption on surface bonded amines. *J Phys Chem C* 119:4126–4135
- Hao W, Björnerbäck F, Trushkina Y, Oregui-Bengoechea M, Salazar-Alvarez G, Barth T, Hedin N (2017) High-performance magnetic activated carbon from solid waste from Lignin conversion processes. 1. Their use as adsorbents for CO<sub>2</sub>. *ACS Sustain Chem Eng* 5:3087–3095
- Hefti M, Marx D, Joss L, Mazzotti M (2014) Model-based process design of adsorption processes for CO<sub>2</sub> capture in the presence of moisture. *Energy Procedia* 63:2152–2159
- Khalili S, Ghoreyshi AA, Jahanshahi M, Khoshandam B (2016) Predictions of the adsorption equilibrium of CO<sub>2</sub>/O<sub>2</sub> mixture on



- multi-walled carbon nanotube using ideal adsorbed solution theory. *J Water Environ Nanotechnol* 1:9–17
- Kim HJ, Oba M, Pittella F, Nomoto T, Cabral H, Matsumoto Y, Miyata K, Nishiyama N, Kataoka K (2012) PEG-detachable cationic polyaspartamide derivatives bearing stearyl moieties for systemic siRNA delivery toward subcutaneous BxPC3 pancreatic tumor. *J Drug Target* 20:33–42
- Lee SY, Park SJ (2015) A review on solid adsorbents for carbon dioxide capture. *J Ind Eng Chem* 23:1–11
- Lee S, Filburn TP, Gray M, Park J, Song H (2008) Screening test of solid amine sorbents for CO<sub>2</sub> capture. *Ind Eng Chem Res* 47:7419–7423
- Leung DY, Caramanna G, Maroto-Valer MM (2014) An overview of current status of carbon dioxide capture and storage technologies. *Renew Sustain Energy Rev* 39:426–443
- Li G, Xiao P, Webley P (2009a) Binary adsorption equilibrium of carbon dioxide and water vapor on activated alumina. *Langmuir* 25:10666–10675
- Li G, Xiao P, Webley PA, Zhang J, Singh R (2009b) Competition of CO<sub>2</sub>/H<sub>2</sub>O in adsorption based CO<sub>2</sub> capture. *Energy Procedia* 1:1123–1130
- Li B, Duan Y, Luebke D, Morreale B (2013) Advances in CO<sub>2</sub> capture technology: a patent review. *Appl Energy* 102:1439–1447
- Li K, Jiang J, Tian S, Yan F, Chen X (2015) Polyethyleneimine–nano silica composites: a low-cost and promising adsorbent for CO<sub>2</sub> capture. *J Mater Chem A* 3:2166–2175
- Marx D, Joss L, Hefti M, Pini R, Mazzotti M (2013) The role of water in adsorption-based CO<sub>2</sub> capture systems. *Energy Procedia* 37:107–114
- Miyata K, Oba M, Nakanishi M, Fukushima S, Yamasaki Y, Koyama H, Nishiyama N, Kataoka K (2008) Polyplexes from poly (aspartamide) bearing 1, 2-diaminoethane side chains induce pH-selective, endosomal membrane destabilization with amplified transfection and negligible cytotoxicity. *J Am Chem Soc* 130:16287–16294
- Moon JR, Kim MW, Kim D, Jeong JH, Kim JH (2011) Synthesis and self-assembly behavior of novel polyaspartamide derivatives for anti-tumor drug delivery. *Colloid Polym Sci* 289:63–71
- Ngoy JM, Wagner N, Riboldi L, Bolland O (2014) A CO<sub>2</sub> capture technology using multiwalled carbon nanotubes with polyaspartamide surfactant. *Energy Procedia* 63:2230–2248
- Ngoy JM, Daramola MO, Chitsiga TL, Falcon R, Wagner N (2017) CO<sub>2</sub> adsorption using water-soluble polyaspartamide. *S Afr J Chem Eng* 23:139–144
- Ntiamoah A, Ling J, Xiao P, Webley PA, Zhai Y (2016) CO<sub>2</sub> capture by temperature swing adsorption: use of hot CO<sub>2</sub>-rich gas for regeneration. *Ind Eng Chem Res* 55:703–713
- Osler K, Dheda D, Ngoy J, Wagner N, Daramola MO (2017a) Synthesis and evaluation of carbon nanotubes composite adsorbent for CO<sub>2</sub> capture: a comparative study of CO<sub>2</sub> adsorption capacity of single-walled and multi-walled carbon nanotubes. *Int J Coal Sci Tech* 4:41–49
- Osler K, Twala N, Oluwasina OO, Daramola MO (2017b) Synthesis and performance evaluation of chitosan/carbon nanotube (chitosan/MWCNT) composite adsorbent for post-combustion carbon dioxide capture. *Energy Procedia* 114:2330–2335
- Qi S, Hay KJ, Cal MP (2000) Predicting humidity effect on adsorption capacity of activated carbon for water-immiscible organic vapors. *Adv Environ Res* 4:357–362
- Saiwan C, Muchan P, Montigny D, Tontiwachwutikul P (2014) Carbon dioxide adsorption. II. Effect of amine functionalization. *Energy Procedia* 63:2317–2322
- Samanta A, Zhao A, Shimizu GKH, Sarkar P, Gupta R (2012) Post-combustion CO<sub>2</sub> capture using solid sorbents: a review. *Ind Eng Chem Res* 51:1438–1463
- Scapino L, Zondag HA, Van-Bael J, Diriken J, Rindt CCM (2017) Sorption heat storage for long-term low-temperature applications: a review on the advancements at material and prototype scale. *Appl Energy* 190:920–948
- Sekoai PT, Yoro KO (2016) Biofuel development initiatives in sub-Saharan Africa: opportunities and challenges. *Climate* 4:33
- Sekoai PT, Yoro KO, Daramola MO (2016) Batch fermentative biohydrogen production process using immobilized anaerobic sludge from organic solid waste. *Environments* 3:38
- Sekoai PT, Yoro KO, Bodunrin MO, Ayeni AO, Daramola MO (2018) Integrated system approach to dark fermentative biohydrogen production for enhanced yield, energy efficiency and substrate recovery. *Rev Environ Sci Bio/Technol* 17:501–529
- Singo MC, Molepo XC, Oluwasina OO, Daramola MO (2017) Chitosan-impregnated Sod-Metal Organic Frameworks (SOD-ZMOF) for CO<sub>2</sub> Capture: Synthesis and Performance Evaluation. *Energy Procedia* 114:2429–2440
- Siriwardane RV, Shen MS, Fisher EP, Losch J (2005) Adsorption of CO<sub>2</sub> on zeolites at moderate temperatures. *Energy Fuels* 19:1153–1159
- Stowe HM, Vilčiauskas L, Paek E, Hwang GS (2015) On the origin of preferred bicarbonate production from carbon dioxide (CO<sub>2</sub>) capture in aqueous 2-amino-2-methyl-1-propanol (AMP). *Phys Chem Chem Phys* 17:29184–29192
- Stuckert NR, Yang RT (2011) CO<sub>2</sub> capture from the atmosphere and simultaneous concentration using zeolites and amine-grafted SBA-15. *Environ Sci Technol* 45:10257–10264
- Tan YL, Islam MA, Asif M, Hameed BH (2014) Adsorption of carbon dioxide by sodium hydroxide-modified granular coconut shell activated carbon in a fixed bed. *Energy* 77:926–931
- Titinchi SJJ, Piet M, Abbo HS, Bolland O, Schwiager W (2014) Chemically modified solid adsorbents for CO<sub>2</sub> capture. *Energy Procedia* 63:8153–8160
- Ünveren EE, Monkul BO, Sarıođlan S, Karademir N, Alper E (2017) Solid amine sorbents for CO<sub>2</sub> capture by chemical adsorption: a review. *Petroleum* 3:37–50
- Vargas DP, Giraldo L, Moreno-Piraján JC (2012) CO<sub>2</sub> adsorption on activated carbon honeycomb-monooliths: a comparison of Langmuir and Tóth models. *Int J Mol Sci* 13:8388–8397
- Veneman R, Frigka N, Zhao W, Li Z, Kersten S, Brilman W (2015) Adsorption of H<sub>2</sub>O and CO<sub>2</sub> on supported amine sorbents. *Int J Greenh Gas Control* 41:268–275
- Xu X, Song C, Andresen JM, Miller BG, Scaroni AW (2002) Novel polyethylenimine-modified mesoporous molecular sieve of MCM-41 type as high-capacity adsorbent for CO<sub>2</sub> capture. *Energy Fuels* 16:1463–1469
- Xu X, Song C, Miller BG, Scaroni AW (2005) Influence of moisture on CO<sub>2</sub> separation from gas mixture by a nanoporous adsorbent based on polyethylenimine-modified molecular sieve MCM-41. *Ind Eng Chem Res* 44:8113–8119
- Xu D, Zhang J, Li G, Xiao P, Webley P, Zhai Y (2011) Effect of water vapor from power station flue gas on CO<sub>2</sub> capture by vacuum swing adsorption with activated carbon. *J Fuel Chem Technol* 39:169–174
- Yoro KO (2017) Numerical simulation of CO<sub>2</sub> adsorption behaviour of polyaspartamide adsorbent for post-combustion CO<sub>2</sub> capture. M. Sc. thesis. University of the Witwatersrand
- Yoro KO, Sekoai PT (2016) The potential of CO<sub>2</sub> capture and storage technology in South Africa's coal-fired thermal power plants. *Environments* 3:24
- Yoro KO, Singo M, Daramola MO, Mulopo JL (2016) Mathematical modeling of adsorption behaviour of SOD-ZMOF/chitosan adsorbent during post-combustion CO<sub>2</sub> capture. In: Proceedings of the 33rd annual international pittsburgh coal conference. Omnipress, Capetown, South Africa

- Yoro KO, Singo M, Mulopo JL, Daramola MO (2017) Modelling and experimental study of the CO<sub>2</sub> adsorption behaviour of polyaspartamide as an adsorbent during post-combustion CO<sub>2</sub> capture. *Energy Procedia* 114:1643–1664
- Yu J, Chuang SSC (2017) The role of water in CO<sub>2</sub> capture by amine. *Ind Eng Chem Res* 56:6337–6347
- Yu Q, de la Delgado JP, Veneman R, Brillman DWF (2017) Stability of a benzyl amine based CO<sub>2</sub> capture adsorbent in view of regeneration strategies. *Ind Eng Chem Res* 56:3259–3269
- Zhang C, Song W, Sun G, Xie L, Wang J, Li K, Sun C, Liu H, Snape CE, Drage T (2013) CO<sub>2</sub> capture with activated carbon grafted by nitrogenous functional groups. *Energy Fuels* 27:4818–4823
- Zhang W, Liu H, Sun C, Drage TC, Snape CE (2014a) Performance of polyethyleneimine–silica adsorbent for post-combustion CO<sub>2</sub> capture in a bubbling fluidized bed. *Chem Eng J* 251:293–303
- Zhang Z, Yao ZZ, Xiang S, Chen B (2014b) Perspective of microporous metal–organic frameworks for CO<sub>2</sub> capture and separation. *Energy Environ Sci* 7:2868–2899
- Zhang Z, Wang B, Sun Q (2014c) Fly ash-derived solid amine sorbents for CO<sub>2</sub> capture from flue gas. *Energy Procedia* 63:2367–2373