### **SUPPORTING INFORMATION**

# Urea-formaldehyde derived porous carbons for adsorption of CO<sub>2</sub>

Deepak Tiwari, Haripada Bhunia\*, and Pramod K. Bajpai

Deepak.tiwari@thapar.edu, hbhunia@thapar.edu, pramod.iitk77@gmail.com

Department of Chemical Engineering, Thapar University, Patiala-147004, Punjab, India

\*Correspondence to: Haripada Bhunia

 $Email\ address: \underline{hbhunia@thapar.edu}$ 

Phone: +91-9316682355; fax: +91-175-2393005

### 1. Adsorption kinetic models

Kinetics of CO<sub>2</sub> uptake give useful information about the efficiency of the adsorption process. Here three kinetic models were used for to evaluate CO<sub>2</sub> uptake on UFZ-700.

The Lagergren pseudo-first-order model expressed as:1

$$q_t = q_e \left( 1 - \exp(-k_f t) \right) \tag{1}$$

where  $k_f$ : pseudo-first-order model constant (min  $^{-1}$ ).

The pseudo-second order model is given as:1

$$q_t = \frac{k_2 q_e^2 t}{1 + k_2 q_e t} \tag{2}$$

where  $k_2$ : pseudo-second-order rate constant (g mmol  $^{-1}$  min  $^{-1}$ ).

The fractional - order rate model is given as:<sup>2</sup>

$$q_{t} = q_{e} - \frac{1}{\left[\left((n-1)k_{n}/m\right)t^{m} + \left(1/q_{e}^{n-1}\right)\right]^{1/n-1}}$$
(3)

where m and n: model constants.

Coefficient of determination  $(R^2)$  and error (%) was used for to evaluate accuracy of models,

Error (%)= 
$$\sqrt{\frac{\sum [q_{t(\exp)} - q_{t(pred)}/q_{t(\exp)}]^2}{N-1}} \times 100$$
 (4)

where,  $q_{t(pred)}$  and  $q_{t(exp)}$  are the predicted and experimental CO<sub>2</sub> loading, respectively.

#### 2. Adsorption isotherm studies

To study the adsorption equilibrium three isotherms Langmuir, Freundlich and Temkin isotherm were analyzed.<sup>3</sup>

Langmuir adsorption isotherm assumes that binding sites are homogeneously distributed over the adsorbent surface. It can be expressed as:

$$q_e = \frac{q_m K_L P}{1 + K_L P} \tag{5}$$

where  $q_m$ : maximum adsorption capacity, mmol  $g^{-1}$ , and  $K_L$ : Langmuir constant, atm<sup>-1</sup> and it indicate adsorption affinity.

Freundlich adsorption isotherm is an empirical equation used to describe heterogeneous systems. It can be given as:

$$q_e = K_F P^{1/n} \tag{6}$$

where  $K_F$  and 1/n are sorption capacity and sorption intensity, respectively. If the value of n>1, it represents favorable adsorption condition.

Temkin isotherm assumes that the heat of adsorption (function of temperature) decrease linearly rather than logarithmic with coverage. The equation can be expressed as follows:

$$q_e = B \ln(K_T P) \tag{7}$$

where  $K_T$  ( $atm^{-1}$ ) and B = RT/b with b (J mol<sup>-1</sup>) are the Temkin constants. R (8.314 J mol<sup>-1</sup> K<sup>-1</sup>) and T (K) is the temperature.

#### 3. Adsorption thermodynamics

The standard Gibbs free energy  $\Delta G^0$  (J mol<sup>-1</sup>), standard molar adsorption enthalpy  $\Delta H^0$  (J mol<sup>-1</sup>), and standard entropy change can be obtained using following equations:

$$\Delta G^{\circ} = -RT \ln \left( K_{eq} \right) \tag{8}$$

$$\ln\left(K_{eq}\right) = -\frac{\Delta H^{\circ}}{R} \frac{1}{T} + \frac{\Delta S^{\circ}}{R} \tag{9}$$

where  $K_{eq}$ : equilibrium constant for adsorption.

 $\Delta H^0$  and  $\Delta S^0$  can be calculated from the slope and intercept of van't Hoff plot, respectively. <sup>4</sup> Enthalpy of adsorption can be obtained from isosteric heat of adsorption  $Q_{st}$  which represents strength of adsobate-adsorbent interaction. The  $Q_{st}$  ( $kJ \ mol^{-1}$ ) can be expressed by Clausius-clapeyron equation:

$$Q_{st} = -R \left[ \frac{\partial \ln P}{\partial \left( \frac{1}{T} \right)} \right]_{q_s} \tag{10}$$

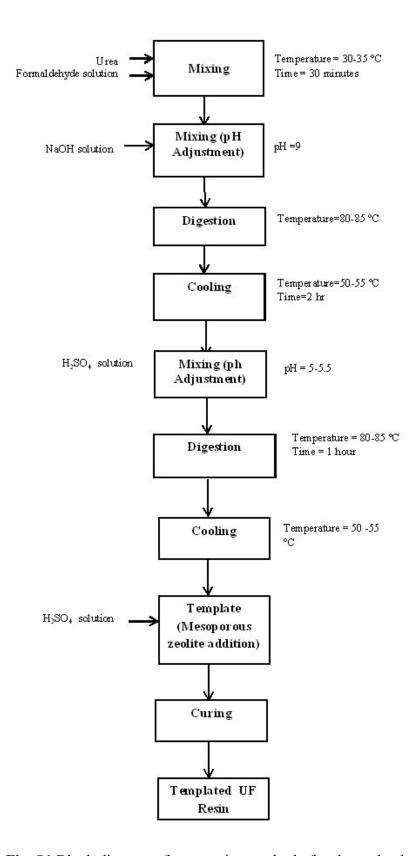


Fig. S1 Block diagram of preparation method of carbon adsorbents

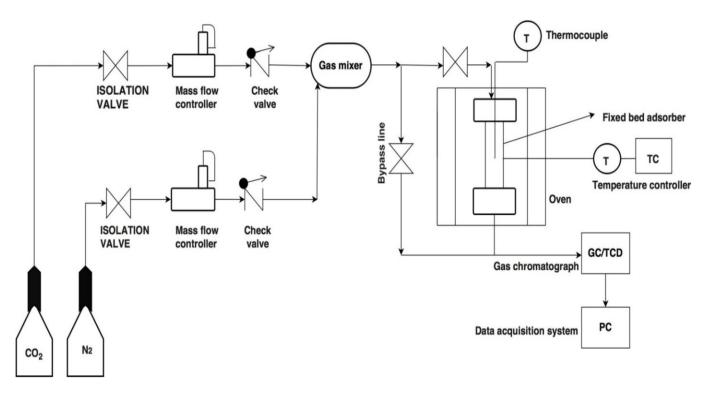


Fig. S2 Schematic experimental setup used for adsorption—desorption experimental setup<sup>5</sup>

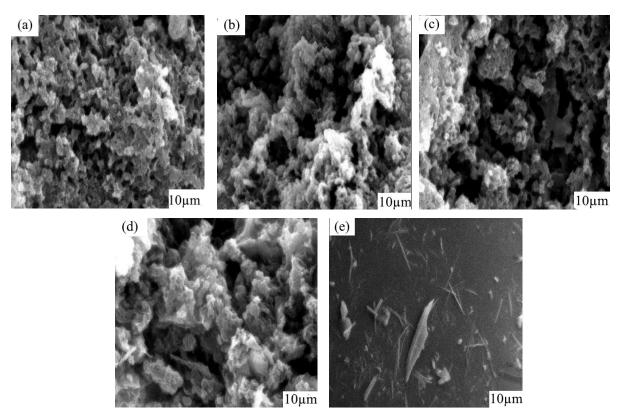


Fig. S3 SEM images of (a) UFZ-500, (b) UFZ-600, (c) UFZ-700, (d) UFZ-800 and (e) UF-700

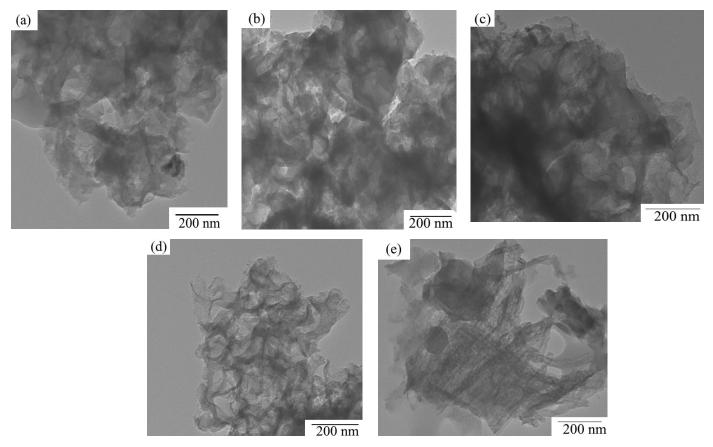


Fig. S4 TEM images of (a) UFZ-500, (b) UFZ-600, (c) UFZ-700, (d) UFZ-800 and (e) UF-700

## References

- 1. M.-S. Chiou and H.-Y. Li, *J. Hazard. Mater.*, 2002, 93, 233-248.
- 2. C. Shen, C. A. Grande, P. Li, J. Yu and A. E. Rodrigues, *Chem. Engin. J.*, 2010, 160, 398-407.
- 3. M. A. Ahmad, N. A. A. Puad and O. S. Bello, Water Resour. Indus., 2014, 6, 18-35.
- 4. C. Goel, H. Bhunia and P. K. Bajpai, *RSC Adv.*, 2015, 5, 93563-93578.
- 5. C. Goel, H. Bhunia and P. K. Bajpai, *J. Environ. Sci.*, 2015, 32, 238-248.