

Multi-factor study of the effects of a trace amount of water vapor on the low concentration CO₂ capture by 5A zeolite particle

Hui Wang^a, Ying Yin^b, Jun-qiang Bai^{a*}, Shi-feng Wang^c

^aSchool of Aeronautics, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, China

^bMOE Key Laboratory of Thermo-Fluid Science and Engineering, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China

^cSchool of Engineering, Newcastle University, Newcastle, UK, NE1 7RU

*Corresponding Author: junqiang@nwpu.edu.cn

Table S1 L-J and particle charges of 5A zeolite and CO₂, N₂ and water molecule

(a) L-J parameters of 5A zeolite and CO₂, N₂ and water molecule

Atom	Atom	$\sigma(\text{Å})$	$\varepsilon/k_B(K)$
O_zeolite	C_CO ₂	3.193	29.116
O_zeolite	O_CO ₂	3.067	23.433
Na	C_CO ₂	2.827	66.778
Na	O_CO ₂	2.707	54.762
Ca	C_CO ₂	2.944	96.932
Ca	O_CO ₂	2.833	77.152
Al	C_CO ₂	3.366	32.215
Al	O_CO ₂	3.246	25.323
Si	C_CO ₂	3.620	49.754
Si	O_CO ₂	3.494	38.900
C_CO ₂	C_CO ₂	2.757	28.129
O_CO ₂	O_CO ₂	3.033	80.507
O_CO ₂	C_CO ₂	2.895	47.588
O_zeolite	O_TIP4P	3.421	51.734
Al	O_TIP4P	3.613	56.948
Si	O_TIP4P	3.887	87.850
Ca	O_TIP4P	3.157	171.814
Na	O_TIP4P	3.024	119.146
O_zeolite	H_TIP4P	0	0
Al	H_TIP4P	0	0
Si	H_TIP4P	0	0
Ca	H_TIP4P	0	0
Na	H_TIP4P	0	0
O_zeolite	L_TIP4P	0	0
Al	L_TIP4P	0	0
Si	L_TIP4P	0	0
Ca	L_TIP4P	0	0
Na	L_TIP4P	0	0
O_TIP4P	O_TIP4P	3.154	78.021
L_TIP4P	O_TIP4P	0	0

H_TIP4P	O_TIP4P	0	0
L_TIP4P	L_TIP4P	0	0
L_TIP4P	H_TIP4P	0	0
H_TIP4P	H_TIP4P	0	0
O_zeolite	N_N ₂	3.305	43.68065934
Al	N_N ₂	2.805	28.14249456
Si	N_N ₂	2.805	28.14249456
Ca	N_N ₂	3.16908	65.66259209
Na	N_N ₂	2.983775	23.31260603
N_N ₂	N_N ₂	3.31	36
O_zeolite	N_com	0	0
Al	N_com	0	0
Si	N_com	0	0
Ca	N_com	0	0
Na	N_com	0	0
N_com	N_com	0	0
N_com	N_N ₂	0	0
N_N ₂	O_CO ₂	3.1715	53.8354158
N_N ₂	C_CO ₂	3.0335	31.82206781
N_com	O_CO ₂	0	0
N_com	C_CO ₂	0	0
O_TIP4P	O_CO ₂	2.9555	46.847
O_TIP4P	C_CO ₂	3.0935	79.254
H_TIP4P	O_CO ₂	0	0
H_TIP4P	C_CO ₂	0	0
L_TIP4P	O_CO ₂	0	0
L_TIP4P	C_CO ₂	0	0
O_TIP4P	N_N ₂	3.232	52.99769806
H_TIP4P	N_N ₂	0	0
L_TIP4P	N_N ₂	0	0
O_TIP4P	N_com	0	0
H_TIP4P	N_com	0	0
L_TIP4P	N_com	0	0

(b) Particle charges of 5A zeolite structure and CO₂ molecule

Atom	Si	Na	Al	O_zeolite	Ca	C_CO ₂	O_CO ₂
Charge(e)	2.2124	0.9887	2.0833	-1.298	1.7166	0.6512	-0.3256
Atom	O_TIP4P	H_TIP4P	L_TIP4P	N_N ₂	N_com		
Charge(e)	0	0.52	-1.04	-0.4048	0.8096		

Table S2 Simulation parameters ¹

Property	Formula	values
Z	$Z^3 - \left(1 - \frac{bp}{RT}\right)Z^2 + \left(\frac{ap}{R^2T^2} - 3\frac{b^2p^2}{R^2T^2} - 2\frac{bp}{RT}\right)Z - \left(\frac{abp^2}{R^2T^2} - \frac{b^2p^2}{R^2T^2} - \frac{b^3p^3}{R^3T^3}\right) = 0$	–
a	$a = 0.45724 \frac{R^2T_c^2}{p_c} \left[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_c^{0.5})\right]^2$	–
b	$b = 0.07779 \frac{RT_c}{p_c}$	–
Λ	$\Lambda = \sqrt{\frac{h^2}{2\pi mkT}}$	$h = 6.626 \times 10^{-34}$ J.s $m_{CO_2} = 7.307 \times 10^{-26}$ kg $m_{N_2} = 3.32 \times 10^{-27}$ kg

References

- (1) D.Y. Peng and D. B. Robinson, A new two-constant equation of state, Ind. Eng. Chem. Fundam. 1976, **15**, 59-64.