Supportive Information

Mathematical Modeling and Experimental Breakthrough Curves of Carbon Dioxide Adsorption on Metal Organic Framework CPM-5

Rana Sabouni, Hossein Kazemian, Sohrab Rohani*

Department of Chemical and Biochemical Engineering, Western University, London, Ontario, Canada N6A5B9

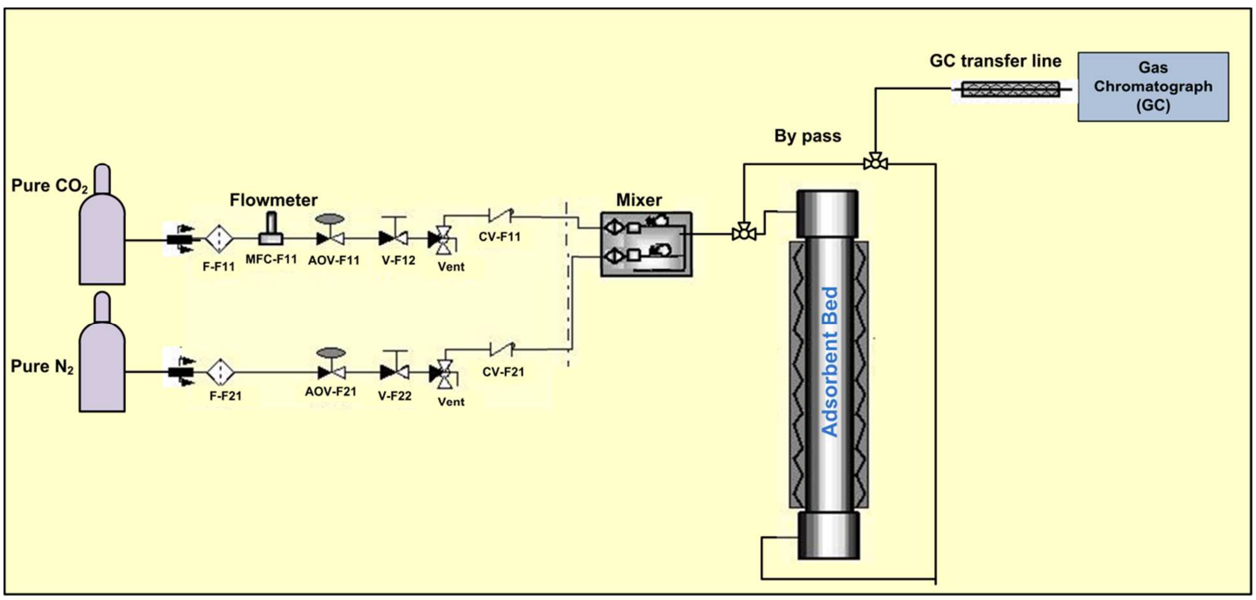

Figure S1

Figure S1: Simplified schematic diagram of the system used for adsorption experiments

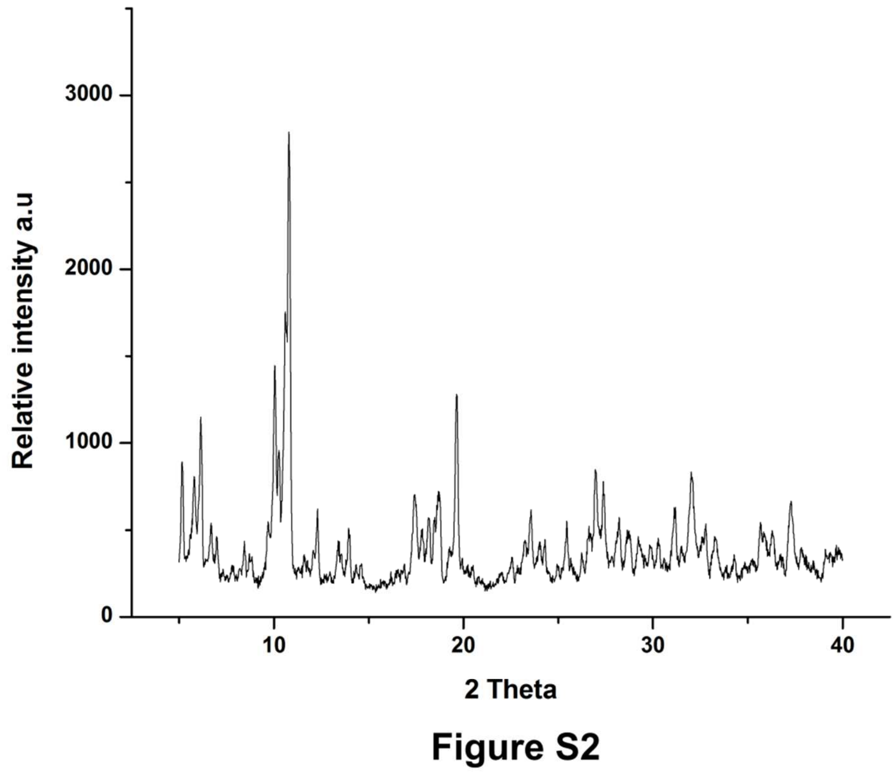

Figure S2: XRD pattern of the microwave-synthesized CPM-5

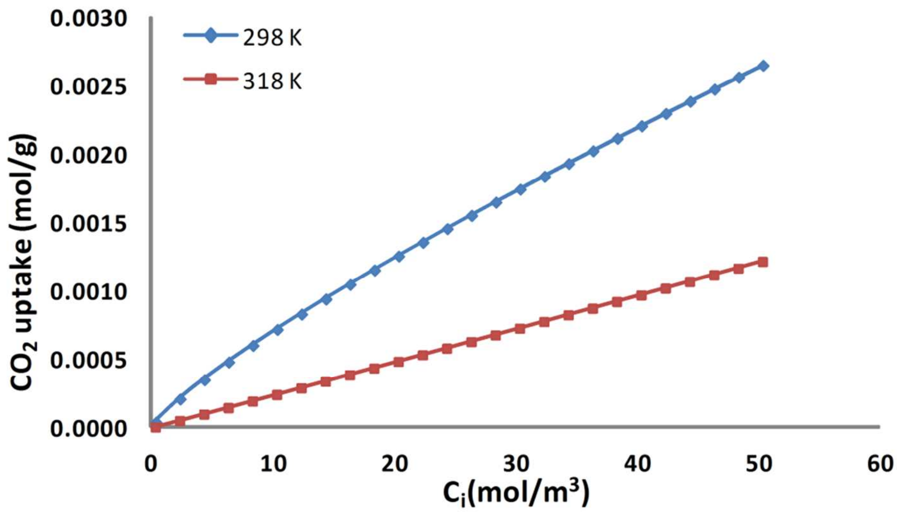

Figure S3

Figure S3: CO_2 adsorption equilibrium at different temperatures, 298 k and 318 K.

Table S1: Input parameter for the model at 298 k

Parameters	Values	Unit
□	0.406	
C_o	5.9	mol/m^3
D_L	1.85 x10^{-5}	m^2/s
R_c	1.25 x10^{-6}	m
k_t	2.44 x10^{-5}	m/s
□$_o$	1.34 x10^{-3}	m/s
L_o	0.15	m
D_c	7.92 x10^{-2}	m
K	1.1e^{-4}	(mol/g).(mol/m^3)$^{-1/n}$
n	1.2	-

Coefficient form of Partial differential equation (PDE) model

The general PDE equation, as well and the initial and boundary conditions with the vector variable *u* are as follows:

$$e_a \frac{\partial^2 y}{\partial t^2} + d_a \frac{\partial u}{\partial t} - \nabla.(c.\nabla u + \alpha.u - \gamma) + \beta.\nabla u + au = f \ in \ \Omega$$

Boundary conditions

Dirichlet type:

$$hu = r \ on \ \delta\Omega$$

Neumann type:

$$n \cdot (c.\nabla u + \alpha.u - \gamma) + au = g - h^T \mu \ on \ \delta\Omega$$

Ω is the computational domain—the union of all domains, ∂Ω is the domain boundary, and ∂Ω is the domain boundary.

The coefficient in COMSOL simulation package are as follows:

The diffusion coefficient: $c = \begin{pmatrix} 1/_{Pe} & 0 \\ 0 & 0 \end{pmatrix}$

The adsorption coefficient: $a = \begin{pmatrix} 0 & 0 \\ 0 & Sh_m \end{pmatrix}$

The mass coefficient: $e_a = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

The damping coefficient: $d_a = \begin{pmatrix} 1 & D_g \\ 0 & 1 \end{pmatrix}$

The conservative flux convection coefficient: $\alpha = \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}$

The convection coefficient: $\beta = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

The conservative flux source: $\gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

The Drichlet coefficient as follows:

$$q = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad g = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad h = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad r = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

The Neumann coefficient as follows:

$$q = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad g = \begin{pmatrix} 10 \\ 0 \end{pmatrix}$$