Supporting Information for Publication

Effective Design of a PVSA Process to Recover Dilute Helium from a Natural Gas Source in a Methane-Rich Mixture with Nitrogen

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S1: The parameters in the DPL model of equations 4~6 are as summarized in **Table S1-a** and the parameters of Toth model are as in **Table S1-b.**

Table S1-Model parameters obtained from fitting the experimental equilibrium adsorption data for CH_4 and N_2 on zeolite 13X. S1-a- DPL Model, and S1-b-Toth Model

a- DPL Model Parameter	N_2	CH_4
$B_{1,i}$ *(K)*	3770.8	4826.2
$B_{2,i}$ *(K)*	1254.9	599.5
$b^0_{1,i}$ *(KPa^{-1})*	4.03e-09	2.60e-10
$b^0_{2,i}$ *(KPa^{-1})*	1.29e-05	1.35e-4
$q^s_{1,i}$ *(mol/kg)*	1.30	1.83
$q^s_{2,i}$ *(mol/kg)*	2.09	2.54
b- Toth Model Parameter		
ΔH_i *(Kj/mol)*	17.38	19.82
b^0_i *(KPa^{-1})*	9.29e-7	5.82e-7
q^s_i *(mol/kg)*	3.26	4.12
t_i	1.035	1.31

S2- Initial and boundary conditions for solving the PSA mathematical model at each process step are as below:

Table S2- Initial and boundary conditions used for solving the governing model equations for PSA cyclic model

Initial Conditions		
	@t=0	
$y_i= y_{feed}$ & $q_i=0$	$P=P_{Feed}$	$T_g=T_p=$

Boundary Conditions

Feed	**EqD**	**BD**	**Vac.**	**EqU**	**FP**	**PP**
@z=0: $u_g C_g = u_{feed} C_{feed}$ $T_g = T_{feed}$ $P = P_{feed}$	***@z=0 :*** *u=0* ***@z=L:*** *P= from CV Equation (14)*	***@z=0:*** *P= from CV Equation (14)* ***@z=L:*** *u=0*	***@z=0:*** *P= from CV Equation (14)* ***@z=L:*** *u=0*	***@z=0:*** *u=0* ***@z=L:*** *P= from CV Equation (14)*	***@z=0:*** $u_g C_g = u_{feed} C_{feed}$ $T_g = T_{feed}$ *P= from CV Equation (14)*	***@z=0:*** $u_g C_g = u_{product} C_{product}$ $T_g = T_{feed}$ *P= from CV Equation (14)*

S3-Derivation of Equation for Estimation of valve Coefficient (C_V):

The derivation of the expression used to estimate the linear valve constant Cv form the bed conditions and stage time starts with ideal gas equation:

$$P_B V_B = nRT_B \qquad \text{S3-1}$$

where:

P_B= Pressure of the bed

V_B= Effective volume of the bed

n= Number of moles of material in the bed

R= Gas constant

T_B= Bed temperature

The rate of change of pressure is related to the rate of change of material holdup (assuming constant temperature and volume):

$$\frac{\partial P}{\partial n} = \frac{RT_B}{V_B} \qquad \text{S3-2}$$

The flowrate through a valve can be expressed as a linear function of the pressure drop across the valve:

$$F = C_V \Delta P = C_V \left(P_B - P_{Downstream}\right) \qquad \text{S3-3}$$

Where:

F= Flowrate through the valve

C_v= Linear valve constant

$P_{Downstream}$= Pressure downstream of the valve.

This expression can be re-expressed as the molar flux:

$$\frac{\partial n}{\partial t} = C_V \left(P_B - P_{Downstream}\right) \qquad \text{S3-4}$$

Assuming a constant downstream pressure from the valve, the rate of change of pressure in the bed can be found from the following expression:

$$\frac{\partial P_B}{\partial t} = \frac{\partial P_B}{\partial n} \times \frac{\partial n}{\partial t} = \frac{RT_B}{V_B} C_V (P_B - P_{Downstream}) \qquad \text{S3-5}$$

This expression can then be integrated between the bed's start and end pressure for a given stage length and constant downstream pressure:

$$\frac{RT_B C_V}{V_B} d_t = \int_{P_{Bstart}}^{PB_{end}} \frac{1}{P_B - P_{Downstream}} dP_B \qquad \text{S3-6}$$

Giving:

$$\frac{RT_B C_V}{V_B} stag\_Time = \ln(P_B - P_{downstream})]\,_{P_{Bstart}}^{P_{Bend}} = \ln(\frac{P_{Bstar} - P_{downstream}}{P_{Bend} - P_{downstream}}) \qquad \text{S3-7}$$

By rearranging the above expression, the estimate of the constant valve C_v is given by:

$$C_V = \frac{V_B}{RT_B stage\_time} = \ln(\frac{P_{Bstart} - P_{downstream}}{P_{Bend} - P_{downstream}}) \qquad \text{S3-8}$$