SUPPLEMENTARY MATERIAL

Tables S1 and S2 present the number of states (n), search step (w), and brun in (aq) for the parameter estimation of the Thomas, Yoon-Nelson, Adams-Bohart, and Yan models using the Markov Chain Monte Carlo method. Estimates were conducted at different initial concentrations, with and without the estimation of the maximum adsorption capacity (q_s, N_0) for the adsorption of hydrogen sulfide gases (Table S1) and carbon dioxide (Table S2).

Table S1 – Elements used for parameter estimation of models for hydrogen sulfide (H_2S) gas

Models	Parameters	(q_s, N_0) Estimated (Present Work)		(q_s, N_0) Deterministic [29]	
	C_0 (mg/L)	1.327	2.577	1.327	2.577
Thomas	n	2,000	2,000	2,000	2,000
	w	0.003	0.003	0.003	0.003
	aq	400	400	400	400
Yoon-Nelson	n			2,000	2,000
	w			0.003	0.003
	aq			600	600
Adams-Bohart	n	2,000	2,000	2,000	2,000
	w	0.03	0.003	0.03	0.003
	aq	200	600	200	400
Yan	n	2,000	2,000	2,000	2,000
	w	0.003	0.003	0.003	0.003
	aq	300	600	200	600

Table S2 – Elements used for parameter estimation of models for hydrogen sulfide (CO_2) gas

Models	Parameters	(q_s, N_0) Estimated (Present Work)			(q_s, N_0) Deterministic [30]		
	C_0 (mg/L)	18	29	35	18	29	35
Thomas	n	3,000	6,000	2,000	2,000	1,000	2,000
	w	0.03	0.03	0.03	0.03	0.03	0.03
	aq	500	1,000	200	200	100	400
Yoon-Nelson	n	-	-	-	2,000	2,000	2,000
	w	-	-	-	0.03	0.03	0.03
	aq	-	-	-	300	400	400
Adams-Bohart	n	2,000	10,000	5,000	2,000	2,000	2,000
	w	0.03	0.03	0.03	0.03	0.03	0.03
	aq	600	1,000	1,000	300	400	100
Yan	n	2,000	10,000	3000	2,000	2,000	2,000
	w	0.003	0.003	0.003	0.003	0.003	0.003
	aq	400	400	200	400	100	200

SUPPLEMENTARY MATERIAL 2

The steps 1-6 present the mathematical modeling for H_2S and CO_2 gases developed in the works of [29] and [30], using the Linear Driving Force (LDF) model.

Step 1 – The authors considered the following assumptions: isothermal process; constant physical properties; constant bed porosity; constant interstitial velocity; gas phase behavior as an ideal gas; thermodynamic equilibrium at the fluid-solid interface (described by the isotherm model); negligible radial and angular dispersion in the fixed bed column.

Step 2 – Adsorption kinetics and equilibrium were evaluated through mass balances in the gas and solid phases according to Equation 1:

$$\frac{\partial C}{\partial t} + \frac{\rho_B}{\varepsilon_B}\frac{\partial q}{\partial t} + v_0\frac{\partial C}{\partial z} - D_{ax}\frac{\partial^2 C}{\partial z^2} = 0 \quad (1)$$

where C is the concentration of H_2S in the gas phase (mg/L), q is the concentration in the solid phase (mg/g), ρ_B is the bed density (g/L); ε_B is the bed porosity (dimensionless); v_0 is the interstitial gas velocity in the bed (cm/min) and D_{ax} is the axial dispersion (cm^2/min).

Step 3 – To describe the mass transfer term between the gas and solid phases (rate term), it was considered that the overall mass transfer rate is controlled by diffusive effects. Thus, the approach that considers the mass transfer rate proportional to the concentration difference in the solid phase relative to the equilibrium condition is called the Linear Driving Force (LDF) model, expressed by Equation 2:

$$\frac{dq}{dt} = K_G(q_e - q) \quad (2)$$

Where K_G is the overall mass transfer coefficient (min^{-1}) and q_e is the concentration of H_2S in the solid phase at equilibrium (mg/g).

Step 4 – To complete the mathematical model, the Langmuir isotherm equilibrium model was used, represented by Equation 3, where q_{max} is the maximum adsorption (mg/g), b is the affinity constant, associated with the dynamic equilibrium between adsorption and desorption (L/mg), and q_e and C_e are the concentrations of H_2S in the solid phase (mg/g) and in the gas phase (mg/L) at equilibrium, respectively.

$$q_e = \frac{q_{max} b C_e}{1 + b C_e} \tag{3}$$

Step 5 – For solving the mathematical model, composed of the mass balances in the gas phase (Equation 1), in the solid phase (Equation 2), and the equilibrium relationship (Equation 3), the initial conditions (4-5) were used:

$$C(z, 0) = C_0 \tag{4}$$

$$q(z, 0) = 0 \tag{5}$$

Step 6 – Two boundary conditions were applied, respectively, at the inlet of the bed, namely the Danckwerts boundary condition (Equation 6) and at the outlet of the bed (Equation 7).

$$D_{ax} \left.\frac{\partial C}{\partial z}\right|_{z=0} = v_0 (C(t, 0) - C_0) \tag{6}$$

$$\left.\frac{\partial C}{\partial z}\right|_{z=L} = 0 \tag{7}$$

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