

Supplementary for 'Characterization of adsorption site energies and heterogeneous surfaces of porous materials'

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Table 1: Different adsorption isotherms and their site energy distribution functions according to a condensation approximation method (This list is not extensive; rather it contains the most widely used isotherms). These functions can produce only approximate site energy distribution functions from the corresponding adsorption isotherm constants.

Adsorption isotherm	Theoretical expression	Isotherm constants	Site energy distribution function
Sips Isotherm ¹	$n = \frac{n_{max} K_s P^{m_s}}{1 + K_s P^{m_s}}$	n_{max} K_s, m_s	$f(E^*) = \frac{\exp\left(-\frac{m_s E^*}{RT}\right) k_s m_s n_{max} p_s^{m_s}}{\left(\exp\left(-\frac{m_s E^*}{RT}\right) k_s p_s^{m_s} + 1\right)^2 RT}$

Redlich-Peterson isotherm ²	$q = \frac{Ap}{1+Bp^g}$	A, B, g	$f(E^*) = \frac{A \exp(-\frac{E^*}{RT}) p_s \left[\left(B p_s^g (g-1) \exp(-\frac{gE^*}{RT}) \right) - 1 \right]}{RT \left(B p_s^g \left[\exp(-\frac{E^*}{RT}) \right]^g + 1 \right)^2}$
Jensen and Seaton isotherm ³	$n = Kp \left[1 + \left(\frac{Kp}{a(1+Kp)} \right)^c \right]^{-\frac{1}{c}}$	K, a, c	$f(E^*) = \frac{X((Y)^c + 1)^{\frac{-c+1}{c}} (Z((Y)^c + 1) + 1)}{A}$ $X = \exp\left(\frac{-E^*}{RT}\right) K p_s$ $Y = \frac{X}{K p_s a \exp\left(\frac{-E^*}{RT}\right) + a}$ $Z = K p_s \exp\left(\frac{-E^*}{RT}\right)$ $A = K p_s \exp\left(\frac{-E^*}{RT}\right) RT + RT$
Fritz-Schluender isotherm ³	$q_e = \frac{\alpha_1 p^{\beta_1}}{1 + \alpha_2 p^{\beta_2}} \beta_1 \quad \beta_2 \ll 1$	$\alpha_1, \beta_1, \beta_2$	$f(E^*) = \frac{\alpha_1 \left(p_s \exp(-\frac{E^*}{RT}) \right) \left(\beta_1 \alpha_2 p_s^{\beta_2} \exp(-\frac{\beta_2 E^*}{RT}) \right) - \beta_2 \alpha_2 p_s^{\beta_2} \exp\left(-\frac{\beta_2 E^*}{RT}\right) + \beta_1}{\left(\alpha_2 p_s^{\beta_2} \exp(-\frac{\beta_2 E^*}{RT}) \right)^2 RT}$
Fritz and Schluender isotherm ³	$q_e = \frac{\frac{\alpha_1}{c} p}{\frac{1}{c} + (\alpha_2/c) p^{\beta_2}} = \frac{A p^{\beta_2}}{B + D p^{\beta_2}}$	A, B, D, β_2	$f(E^*) = \frac{A \left(p_s \exp(-\frac{E^*}{RT}) \right) \left(\beta_1 \left(D p_s^{\beta_2} \exp\left(-\frac{\beta_2 E^*}{RT}\right) \right) + B \right) - D \beta_2 p_s^{\beta_2} \exp\left(-\frac{\beta_2 E^*}{RT}\right)}{\left(D p_s^{\beta_2} \exp\left(-\frac{\beta_2 E^*}{RT}\right) \right) + B)^2 RT}$

Freundlich isotherm ³	$q_e = (A/D) p^{\beta_1 - \beta_2}$	A, D, β_1, β_2	$f(E^*) = \frac{A/D(\beta_1 - \beta_2) \left(p_s \exp\left(-\frac{E^*}{RT}\right) \right)^{\beta_1 - \beta_2}}{RT}$
Radke-Prausnitz isotherm ³	$q_e = \frac{\alpha_1 p^{\beta_1}}{1 + \alpha_2 p^{\beta_1 - 1}}$	$\alpha_1, \alpha_2, \beta_1$	$f(E^*) = \frac{\alpha_1 \left(\exp\left(-\frac{E^*}{RT}\right) \right)^{\beta_1 + 1} \left(\alpha_2 p_s^{\beta_1} \exp\left(-\frac{\beta_1 E^*}{RT}\right) \right) + \beta_1 p_s \exp\left(-\frac{E^*}{RT}\right)}{\left(\alpha_2 p_s^{\beta_1} \exp\left(-\frac{\beta_1 E^*}{RT}\right) \right) + p_s \exp\left(\frac{E^*}{RT}\right)^2 RT}$
Toth isotherm ⁴	$q_e = \frac{q_m p}{(b + p^t)^{1/t}}$	q_m, b, t	$f(E^*) = \frac{q_m b p_s \exp\left(-\frac{E^*}{RT}\right) \left(\left(p_s \exp\left(-\frac{E^*}{RT}\right) \right)^t + b \right)^{-\frac{t+1}{t}}}{RT}$
Toth isotherm ⁴	$q_e = \frac{q_m b p}{(1 + (bp)^t)^{1/t}}$	q_m, b, t	$f(E^*) = \frac{q_m b p_s \exp\left(-\frac{E^*}{RT}\right) \left(\left(p_s b \exp\left(-\frac{E^*}{RT}\right) \right)^t + 1 \right)^{-\frac{t+1}{t}}}{RT}$
Langmuir-Freundlich (LF) ⁵	$q = \sum_{i=1}^N q_m \left[\frac{bp^n}{1 + (bp)^n} \right]$	$q_m, b, n,$ $N = 2$ for dual-site LF isotherm	$f(E^*) = \sum_{i=1}^N \frac{q_m n (bp_s)^n}{RT} \exp\left(\frac{-nE^*}{RT}\right) \left[1 + (bp_s)^n \exp\left(\frac{-nE^*}{RT}\right) \right]^{-2}$

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