Supplementary for 'A site energy distribution function for the characterization of the continuous distribution of binding sites for gases on heterogeneous surface'

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Derivation of the binding site energy distribution function for Jensen-Seaton isotherm

The binding site energy distribution, according the *condensation approximation method* is given by the differentiation of the Jensen-Seaton isotherm, $q(E^*)$, with respect to the binding site energy, E^*, of the adsorption sites on the adsorbent surface, $-dq(E^*)/dE^*$, given by

$$\frac{d}{dE^*}\left(Kp_s \exp\left(-\frac{E^*}{R}\right)\left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{R}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{R}\right)\right)}\right)^c + 1\right)^{-1/c}\right) \quad (Eq\ \ 1)$$

Let $u \exp\left(-\frac{E^*}{R}\right)$ and $v = \left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{R}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{R}\right)\right)}\right)^c + 1\right)^{-1/c}$; applying the product rule, $\frac{d(uv)}{dx} = \frac{d(u)}{dx}v + \frac{d(v)}{dx}u$, we get

$$= \left(Kp_s \exp\left(-\frac{E^*}{RT}\right) \left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1 + kp_s \exp\left(-\frac{E^*}{RT}\right)\right)} \right)^c + 1 \right)^{-1/c} \right) \frac{d}{dE^*}\left(\exp\left(-\frac{E^*}{RT}\right)\right) +$$

$$\exp\left(-\frac{E^*}{RT}\right) \frac{d}{dE^*} \left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1 + kp_s \exp\left(-\frac{E^*}{RT}\right)\right)} \right)^c + 1 \right)^{-1/c} \qquad (Eq\ 2)$$

if, u = -E^*/RT, applying the chain rule, $\frac{de^u}{dx} = e^u \frac{du}{dx}$, and simplifying, we get

$$= Kp_s \left(\exp\left(-\frac{E^*}{RT}\right) \frac{d}{dE^*} \left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1 + kp_s \exp\left(-\frac{E^*}{RT}\right)\right)} \right)^c + 1 \right)^{-1/c} \right) -$$

$$\exp\left(-\frac{E^*}{RT}\right) \left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1 + kp_s \exp\left(-\frac{E^*}{RT}\right)\right)} \right)^c + 1 \right)^{-1/c} \qquad (Eq\ 3)$$

if, $u = \left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1 + kp_s \exp\left(-\frac{E^*}{RT}\right)\right)} \right)^c + 1$ and n = -1/c, from the chain rule, $\frac{du^n}{dx} = nu^{n-1}\frac{du}{dx}$

and simplifying the resulting expression, we get

$$= Kp_s \left(- \frac{\exp\left(-\frac{E^*}{RT}\right)\left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}\right)^c + 1\right)^{-\frac{1}{c}-1}}{c} \right) \frac{d}{dE^*}\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}\right)^c -$$

$$\frac{\exp\left(-\frac{E^*}{RT}\right)\left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}\right)^c + 1\right)^{-1/c}}{r} \qquad (Eq\ \ 4)$$

if $u = \frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}$ and $n = c$, then from the chain rule $\frac{du^n}{dx} = nu^{n-1}\frac{du}{dx}$

$$= Kp_s \left(\left(- \frac{\exp\left(-\frac{E^*}{RT}\right)\left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}\right)^{c-1}\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}\right)^c + 1\right)^{-\frac{1}{c}-1} \frac{d}{dE^*}\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}\right)^c}{c} - \right. \right.$$

$$\left. \left. - \right) \frac{\exp\left(-\frac{E^*}{RT}\right)\left(\left(\frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1+kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}\right)^c + 1\right)^{-1/c}}{RT} \right)$$

----- $(Eq\ \ 5)$

if $u = \exp\left(-\frac{E^*}{RT}\right)$ and $v = 1 + kp_s \exp\left(-\frac{E^*}{RT}\right)$; Let $X' = Kp_s \exp\left(-\frac{E^*}{RT}\right)$;

$$Y' = \frac{Kp_s \exp\left(-\frac{E^*}{RT}\right)}{a\left(1 + kp_s \exp\left(-\frac{E^*}{RT}\right)\right)}; \quad E' = \exp\left(-\frac{E^*}{RT}\right)$$

$$= Kp_s \left(\frac{\left(X'\left((Y')^{c-1}(Y')^c + 1\right)^{-\frac{1}{c}-1} \right)\left((kp_s E'+1)\frac{d}{dE^*}(E') - E'\frac{d}{dE^*}(bp_s E'+1) \right)}{a(1+kp_s E')^2} - \frac{E'\left(\left(\frac{X'}{a(1+kp_s E')}\right)^c + 1\right)^{-1/c}}{RT} \right) \quad (Eq\ 6)$$

if $u = - E^*/RT$, and introducing the parameter, and then applying the chain rule, $\frac{de^u}{dx} = e^u \frac{du}{dx}$, and rearranging the resulting expression and substituting the appropriate parameters and simplifying, we get

$$f\left(E^*\right) = \frac{X\left((Y)^c + 1\right)^{-\frac{c+1}{c}}\left(Z\left((Y)^c + 1\right) + 1\right)}{A} \qquad (Eq\ 7)$$

where,

$$X = \exp\left(-\frac{E^*}{RT}\right)Kp_s \qquad (Eq\ 8)$$

$$Y = \frac{X}{kp_s a \exp\left(-\frac{E^*}{RT}\right) + a} \qquad (Eq\ 9)$$

$$Z = kp_s \exp\left(-\frac{E^*}{RT}\right) \qquad (Eq\ 10)$$

$$A = kp_s \exp\left(-\frac{E^*}{RT}\right)RT + RT \qquad (Eq\ \ 11)$$