Workspace for 'On the Dubinin-Radushkevich equation for adsorption in microporo

Page 1 (row 1, column 1)

modified Dubinin-Radushkevich (MDR) equation that has a proper Henry's law limit and retains the original form of the DR equation at moderate to high pressures

$$n = \beta_1\left(n_0 \exp\left[-\left(C \ln \frac{P_s}{P}\right)^2\right]\right) + \beta_2\left(n_1 \frac{P}{P_s}\right)$$

no and C (= RT/BE) are the two fitting parameters.

weighting factors, BI and B2, must be chosen such that the second term becomes significant only at very low pressures and the first term remains applicable over the rest of the pressure range up to P,.

Intu- itively, PI must be equal to zero at low pressures and unity at moderate to high pressures whereas p2 must behave

exactly in the opposite manner.

$$\beta_1 = 1 - \exp\left(-\alpha \frac{P}{P_s}\right)$$

$$\beta_2 = \exp\left(-\alpha \frac{P}{P_s}\right)$$

Alpha is an additional fitting parameter

$$n = \left[1 - \exp\left(-\alpha \frac{P}{P_s}\right)\right] n_0 \exp\left[-\left(C \ln \frac{P_s}{P}\right)^2\right] + \exp\left(-\alpha \frac{P}{P_s}\right) n_1 \frac{P}{P_s}$$

saturated vapor pressure (P,) was calculated by using the reduced Kirchoff equation,

$$P_s = P_c \exp\left[\frac{T_{nbp}}{T_c}\left(\frac{\ln P_c}{1 - T_{nbp}/T_c}\right)\left(1 - \frac{T_c}{T}\right)\right]$$