

REVIEW COPY

©COPYRIGHT MATERIAL, 2018

There is mathematically a point of minimum curvature that can be derived from chi theory at $P/P_{\text{vap}} = 0.3679$. However, the value of the of the monolayer does not correspond to this value. This is discussed in the next section.

The Inflection Point Method

The detailed algebra for this method is presented in the appendix II G on page 310. This method is based on quantum mechanics and has a much firmer foundation than the “B” method and requires very little judgement to perform. It works in this form only for nonporous adsorbents. The method is as follows:

1. Determine the number of moles adsorbed at the relative pressure (P/P_{vap}) of 0.3678 (the value of e^{-1} .)
2. Determine the slope of the isotherm at this point. The isotherm should be close to a straight line from a relative pressure of about 0.2 to 0.6. If it is not, then the adsorbent has some porosity and an alternative method must be used.
3. To obtain the monolayer equivalence, divide the slope by e (2.718...).
4. If the energy of adsorption for the first adsorbate molecules is required, substitute into the equation:

$$\bar{E}_a = -RT \exp\left(\frac{eP_I}{P_{\text{vap}}} - 1 - \frac{n_{\text{ads},I}}{n_m}\right) \quad (2)$$

Where $n_{\text{ads},I}$ is the number of moles adsorbed at the inflection point and P_I is the adsorptive pressure at the inflection point.

The graph in **Figure 10** illustrates this technique. The straight line fit for the tangent line is very good (within 2%) over the P/P_{vap} range of 0.2 to 0.6. It is within 0.1 % over the P/P_{vap} range of 0.30 to 0.44. How close one can get the right value is more a matter of how good the data definition is.

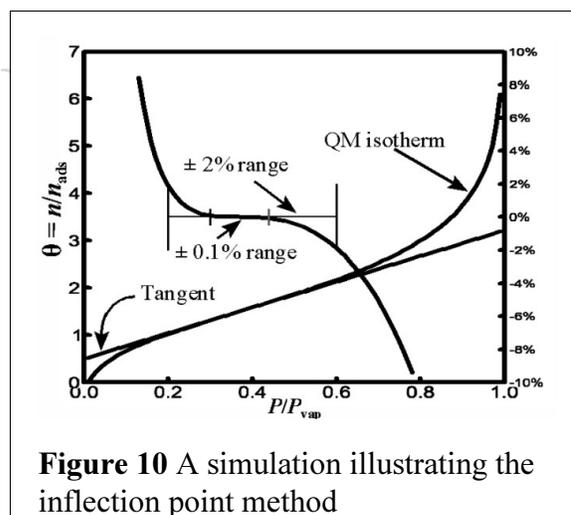


Figure 10 A simulation illustrating the inflection point method

Note: \bar{E}_a is not a function of n_{ads} . See the sections on heats of adsorption for these functions.

REVIEW COPY

©COPYRIGHT
MATERIAL, 2018

ElSevier Publishing

DO NOT COPY

DO NOT DISTRIBUTE

DO NOT DUPLICATE