## Application Note - 88

## Choosing the Proper K Value for the Dubinin-Astakhov Method of Data Reduction

The value of *K* represents a constant in the Dubinin-Astakhov (D-A) equation. It is defined as an energy-to-radius conversion constant. The value of *K* is equivalent to the inverse value of beta, that is, 1/beta, where beta is the so called *affinity coefficient*, and is a shifting factor that depends on the adsorptive in use and the analysis temperature. By convention, the beta of benzene is considered as the reference value and is equal to 1.

When using the ASAP 2000 Micropore software to reduce isothermal data for the Dubinin-Astakhov micropore distribution, the *K* value must be selected properly depending on the adsorptive in use.

The default value of *K* used in the ASAP 2000 Micropore software is 3.145, which corresponds to nitrogen as the adsorptive at a temperature of 77 K. However, you must change the value of *K* when you change the adsorptive. For example, for CO2 at 195 K, the beta value is 0.461, the inverse of which produces a *K* value of 2.169. For argon, the beta value is 0.267 at 87 K; the *K* value is then 3.745.

To change the Dubinin-Astakhov *K* value in the ASAP 2000 Micropore software, refer to **6.5.3.8 Add Report Options - Dubinin Report Options** in the *ASAP 2000 Micropore Operator's Manual.* 

## **References:**

- 1. M.M. Dubinin, J. Coll. Interf. Sci. 23, 487-493 (1967).
- 2. P.J.M. Carroll and J.J. Freeman, *Carbon* 29, 499-506 (1991).
- 3. M.K. Ismail, *Carbone 90*, 30, International Carbon Conference held in Paris, July 15-20 (1990)