**B-AD-007**

The mesopore evaluation of porous Silica (Type IV isotherm) by the BJH method

The pore profile of mesopores using BJH-theory (Barrett-Joyner-Halenda) is analyzed based on the following three assumptions from adsorption isotherms: the pore is cylindrical in shape, it has a hemispherical meniscus with a contact angle of 0º. The condensation of adsorbates (capillary condensation) occurs because the saturated vapor pressure of adsorbates at a certain temperature becomes low due to capillarity in the meso (macro) pores. For this reason, the BJH method is calculated using the kelvin equation assuming that the adsorbed state is a liquid state (Equation 1). Usually, kelvin radius (r_c) is smaller than the actual pore radius (r_p) because adsorption occurs from the interaction between the pore surfaces and the adsorbate, followed by an increase in the adsorbed bed. Therefore, the actual pore radius is expressed using the thickness of the adsorbed layer (t) and kelvin radius (r_c) (Equation 2). Also, in isotherms with N_2@77.4 K, capillary condensation does not occur for pores smaller than the relative pressure $p/p_0 < 0.42$ (corresponding to a pore radius of 1.7 nm), so capillary

BJH Theory: Three Assumptions

① Cylinder pore shape
② Hemispherical meniscus with a contact angle of 0º
③ Correction of the adsorption layer (thickness t)
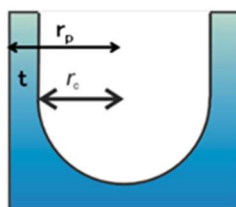
Kelvin equation for N_2 at 77K

$$r_c = \frac{-0.416}{\log(P/P^0)}$$ (Equation 1)
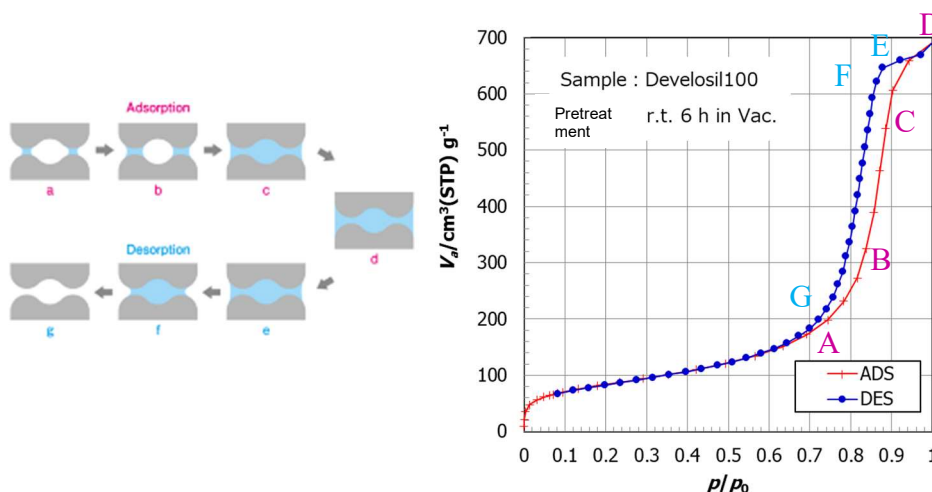
$$r_p = r_c + t$$ (Equation 2)

Fig.1 Adsorption isotherm of Develosil 100
(N_2, 77K)

condensation theory cannot be applied to materials with pores with a pore radius of 1.7 nm or less.

The N_2 adsorption-desorption isotherm @77.4 K (Fig. 1) of a Develosil100 of silica-material with mesopores shows that the isotherm rises abruptly due to capillary condensation at around $p/p_0 = 0.8$-0.9, and that the desorption isotherm exists above the adsorption isotherm (Type IV), indicating the existence of mesopores. There are various theories about why this effect, known as hysteresis occurs. In this material, the pore shape is expected to be the shape of an ink bottle. In adsorption branches (A to D), adsorption is performed from a narrow portion of pores, and in desorption branches (D to G), adsorbates are generally desorbed from large pores, but since there is a bottleneck, desorption is performed from F to G.

As a result, the BJH-plot from this isotherm (Fig. 2) shows that the total volume of mesopores in Develosil 100 was 1 $cm^3 g^{-1}$, the pore size peak of the mesopores by the adsorption branch was 16 nm, and the pore size peak of the bottleneck by the desorption branch was 12 nm. In addition, the vertical axis of Figure 2 pore size distribution has a physical meaning, and the results look quite different (Figure 3). The volume distribution (Equation 3) is heavily weighted on the large pore size, making it suitable

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for evaluation pore volumes in adsorbent development and adsorption processes. On the other hand, the area distribution (Equation 4) weights small pore diameters and is effective for comparing the area of
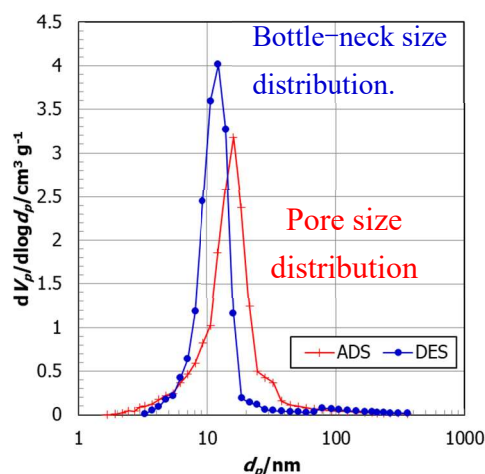

Fig.2 BJH-plot by adsorption branch or desorption branch for Develosil 100
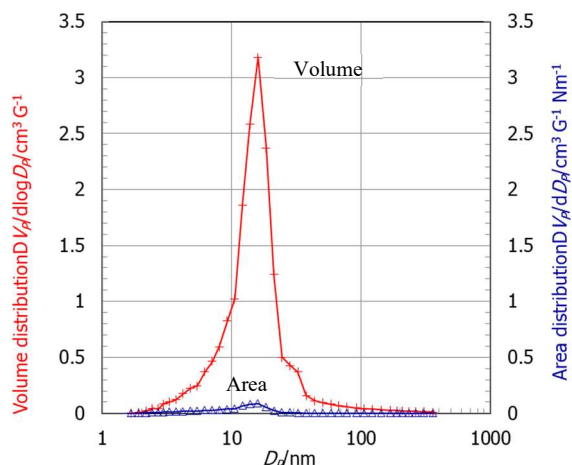

Fig.3 BJH-plot (Volume Distribution, Area Distribution)

Volume distribution $\qquad \dfrac{dV}{dlog\,(r)} = \dfrac{dV/dr}{dlog\,(r)/dr} = 2\pi r^2 L$ (Equation 3)

Area distribution $\qquad \dfrac{dV}{dr} = 2\pi r L$ (Equation 4)

reactive sites in reaction processes such as catalysts

The BET specific surface area and structural evaluation of this sample Devesil100 are introduced in Material B-AD-004(No.4) BET specific surface area evaluation) and B-AD-009 (No.9) evaluation by t-plot method).

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