# A new approach to characterization of carbon pore structure

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For years, the characterization of carbon pore size distribution (PSD) has been dominated by the analysis of nitrogen ($N_2$) isotherms measured at its boiling point (77 K). From the scientific viewpoint, however, $N_2$ is not the most appropriate molecular probe for the PSD analysis because of its significant quadrupole moment that may influence the adsorption of $N_2$ molecules due to interactions with polar surface sites. For this reason, IUPAC Technical Report 2015 [1] recommended Ar as more reliable for the PSD analysis. In practice, however, using liquid argon as a cryogen for argon adsorption measurements may be challenging due to its high cost and limited availability in various parts of the world. To reconcile this problem, we have recently proposed using $O_2$ instead of $N_2$ or Ar [2]. We have chosen $O_2$ because its quadrupole moment is less than one-third of the value reported for $N_2$. Moreover, we demonstrated a quantitative agreement between the PSD results derived from the adsorption isotherms of $O_2$ and $N_2$ measured at 77 K, and Ar at 87 K on representative carbon samples.

On the other hand the IUPAC Technical Report [1] recommended using $CO_2$ at 273 K for the analysis of ultramicroporous carbons, because at this temperature $CO_2$ diffuses faster into micropores than $N_2$ at 77 K. This recommendation, however, is inconsistent with the premise of using molecules with low susceptibility to specific interactions with polar sites, because the quadrupole moment of $CO_2$ is even larger than $N_2$.

To improve the diffusion into ultramicropores, we propose in this work to use $H_2$ in combination with $O_2$ isotherms measured at 77 K. $H_2$ molecule has a very small quadrupole moment and smaller diameter than $CO_2$. It has been shown [3] that $H_2$ isotherms may provide meaningful PSD results in an extended range of pore sizes when analyzed simultaneously with argon isotherms. In this work, we use 2D-NLDFT models to simultaneously analyze $H_2$ and $O_2$ isotherms measured at 77 K. We show comparisons of PSD results derived from single isotherms and the dual analysis of both isotherms. The approach introduced in this work is advantages compared to the earlier presented "dual analysis method"[4] based on $N_2$ and $CO_2$ isotherms, because of the lower quadrupole moments of $O_2$ and $H_2$. It is also more practically convenient because of the same cryogen, liquid $N_2$, used for both analyses.

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