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Improving porous properties of activated carbon from carbon gel by the OTA method

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Peak separation of TPD analysis

To estimate the amount of each type of oxygen-containing functional group, we conducted peak separation of the TPD spectra of CO and CO_2. The desorption temperature and full width at half maximum (FWHM) were determined based on the literature [1-3]. Peak separation from the obtained TPD spectra was conducted using the conditions shown in Table S1, and the peak fitting results are presented in Figure S1.

Table S1 Peak separation conditions of CO and CO_2 from TPD spectra

Functional groups	Peak temperature (°C)	FWHM (°C)	Desorption gas
Carboxylic #1	240	150	CO_2
Carboxylic #2	340	150	CO_2
Anhydride	490	130	CO_2 + CO
Lactone#1	600	130	CO_2
Lactone#2	700	130	CO_2
Phenol/Ether#1	550	125	CO
Phenol/Ether#2	640	125	CO
Phenol/Ether#3	750	150	CO
Carbonyl#1	900	150	CO
Carbonyl#2	1030	100	CO
Carbonyl#3	1125	150	CO

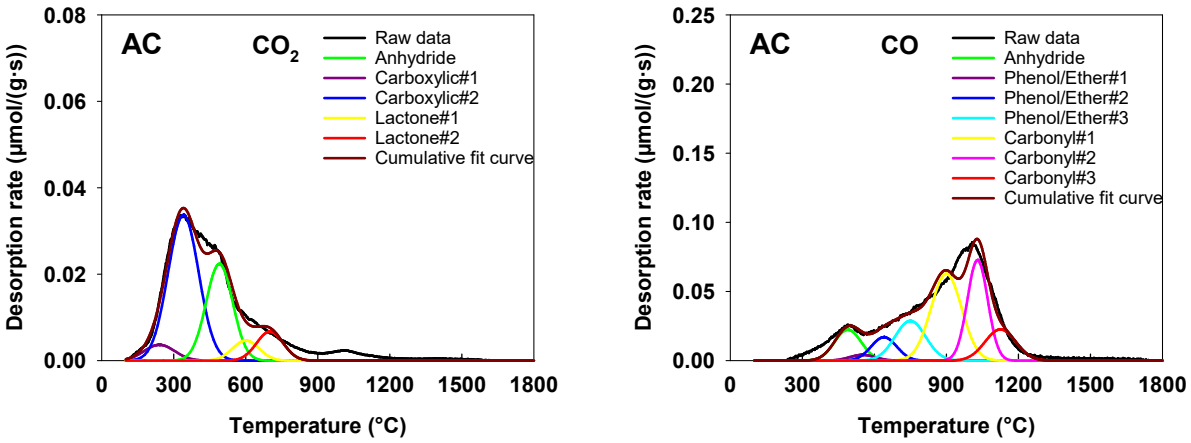

Figure S1 *Cont.*

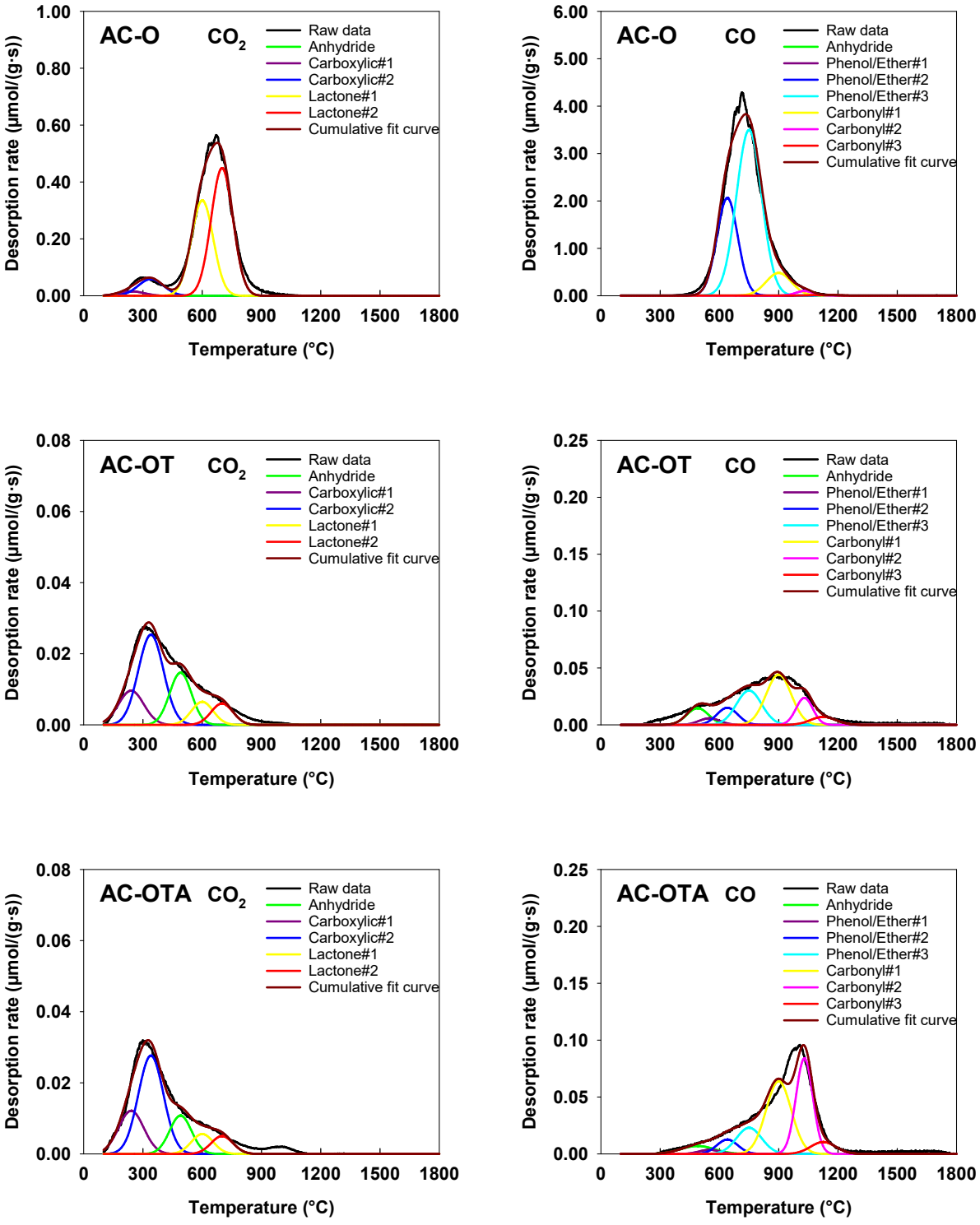

Figure S1 Peak fitting results of TPD profiles for activated carbon gels using a Gaussian function. The black lines represent the TPD experimental data, and the colored lines show the fitting profiles optimized by the Levenberg-Marquardt method.

References

1. Li, N., X. Ma, Q. Zha, K. Kim, Y. Chen, and C. Song, *Maximizing the number of oxygen-containing functional groups on activated carbon by using ammonium persulfate and improving the temperature-programmed desorption characterization of carbon surface chemistry.* Carbon, 2011. **49**(15): p. 5002-5013.

2. Ishii, T., S. Kashihara, Y. Hoshikawa, J.-i. Ozaki, N. Kannari, K. Takai, T. Enoki, and T. Kyotani, *A quantitative analysis of carbon edge sites and an estimation of graphene sheet size in high-temperature treated, non-porous carbons.* Carbon, 2014. **80**: p. 135-145.

3. Ishii, T. and J.-i. Ozaki, *Understanding the chemical structure of carbon edge sites by using deuterium-labeled temperature-programmed desorption technique.* Carbon, 2020. **161**: p. 343-349.