

Appendix A: supplementary material

Influence of activation conditions on textural properties and performance of activated biochars for pyrolysis vapors upgrading

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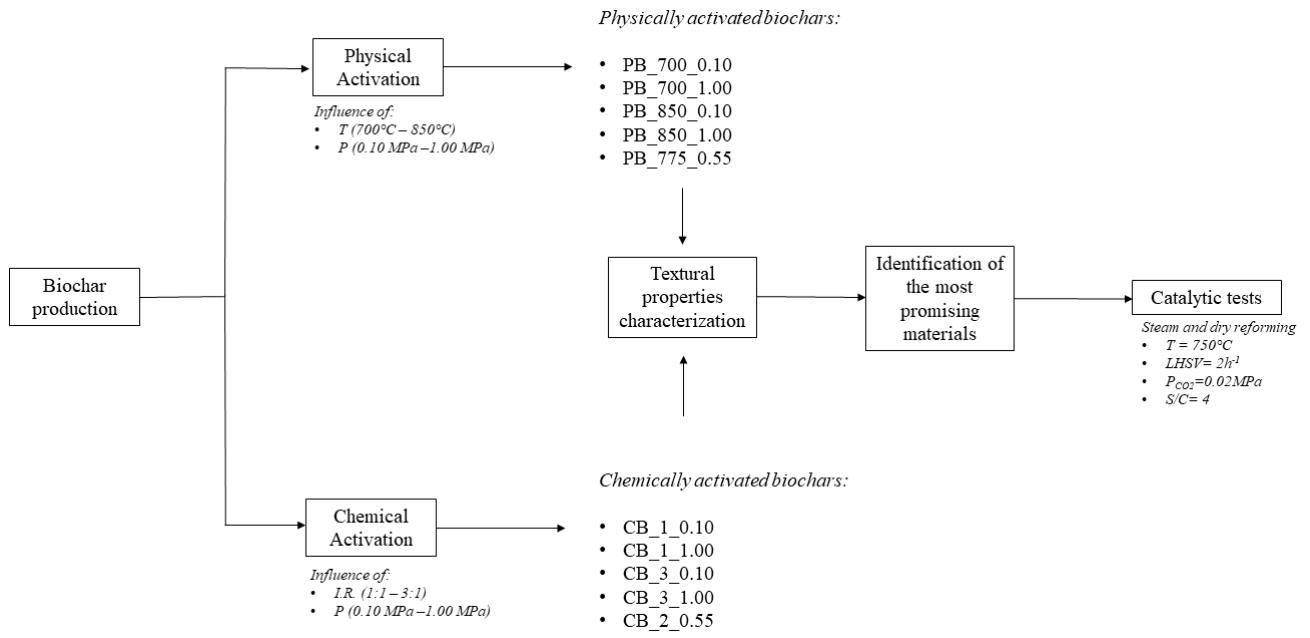


Fig. A.1. Schematic representation of the methodology followed in this study.

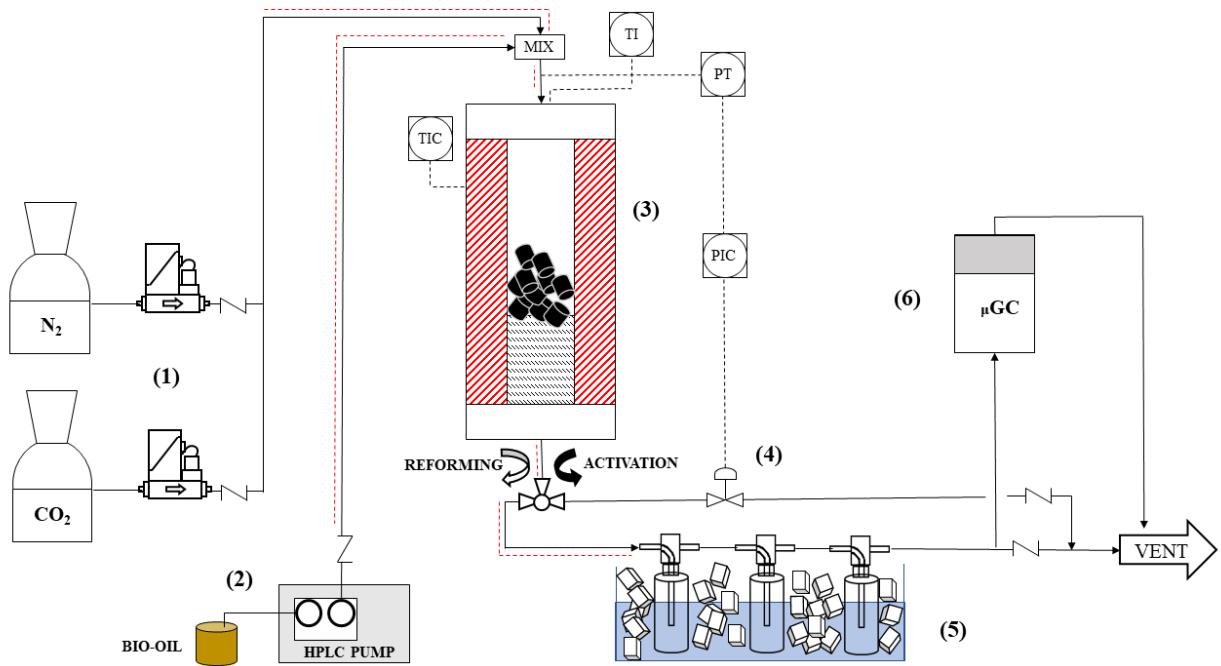


Fig. A.2. Overview of the experimental device used for activation and reforming tests: Feeding system (1); HPLC pump (2); fixed-bed reactor and furnace (3); Servo-controlled valve (4); condensation train (5); and μGC analyzer (6).

Table A.1. Results of textural characterization, proximate analysis and elemental analysis of pristine biochar derived from wheat straw

Proximate analysis (wt. %)	
<i>Moisture</i>	2.00 ± 0.08
<i>Volatile matter</i>	10.8 ± 0.63
<i>Ashes</i>	12.7 ± 0.21
<i>Fixed carbon</i>	74.5 ± 0.55
Ultimate (wt. % on a dry ash-free basis)	
<i>C</i>	92.6 ± 0.07
<i>H</i>	4.02 ± 0.05
<i>N</i>	2.01 ± 0.08
<i>O</i>	1.32
<i>Molar H:C ratio</i>	0.52
Textural characterization	
A_{BET} ($\text{m}^2 \text{ g}^{-1}$)	2.90
$S_{2D-NLDFT}$ ($\text{m}^2 \text{ g}^{-1}$)	341
$V_{0.97}$ ($\text{cm}^3 \text{ g}^{-1}$)	0.0026
V_{tot} ($\text{cm}^3 \text{ g}^{-1}$)	0.084
V_{ultra} ($\text{cm}^3 \text{ g}^{-1}$)	0.083
V_{micro} ($\text{cm}^3 \text{ g}^{-1}$)	0.083
V_{meso} ($\text{cm}^3 \text{ g}^{-1}$)	0.001 (1.28 vol. %)

Table A.2. Regression coefficients and quality-of-fit statistics for the design of experiments on chemical activation. The values in brackets correspond to the *p*-values resulting from the *t*-tests. The significant terms are marked in bold

	Response variable				
	$S_{2D-NLDFT}$	V_t	V_{meso}	V_{micro}	V_{ultra}
β_0	810.1 (0.000)	0.21605 (0.000)	0.009516 (0.003)	0.2065 (0.000)	0.16447 (0.000)
β_A (Pressure)	-12.24 (0.326)	-0.00364 (0.132)	0.000215 (0.715)	-0.00385 (0.190)	-0.00553 (0.150)
β_B (Mass ratio)	73.32 (0.016)	0.02801 (0.003)	0.002904 (0.030)	0.02511 (0.006)	0.01871 (0.016)
β_{AB}	-36.90 (0.060)	-0.1089 (0.018)	-0.000625 (0.346)	-0.01026 (0.035)	-0.00865 (0.070)
R^2_{adj} (%)	94.05	98.78	83.90	97.38	93.27
<i>Curvature</i>	(0.042)	(0.015)	(0.350)	(0.029)	(0.090)

Table A.3. Regression coefficients and quality-of-fit statistics for the design of experiments on physical activation. The values in brackets correspond to the p -values resulting from the t -tests. The significant terms are marked in bold

	Response variable				
	$S_{2D-NLDFT}$	V_t	V_{meso}	V_{micro}	V_{ultra}
β_0	884.9 (0.000)	0.29181 (0.000)	0.023189 (0.001)	0.268623 (0.000)	0.19055 (0.000)
β_A (Temperature)	−35.46 (0.017)	0.00381 (0.155)	−0.000811 (0.461)	0.004623 (0.034)	−0.01445 (0.008)
β_B (Pressure)	59.54 (0.006)	0.02250 (0.006)	0.004000 (0.047)	0.018500 (0.002)	0.01050 (0.015)
β_{AB}	−28.08 (0.027)	−0.02250 (0.006)	−0.004000 (0.047)	−0.018500 (0.002)	−0.01050 (0.015)
R^2_{adj} (%)	98.06	98.47	86.47	99.42	98.22
<i>Curvature</i>	(0.018)	(0.025)	(0.328)	(0.008)	(0.013)

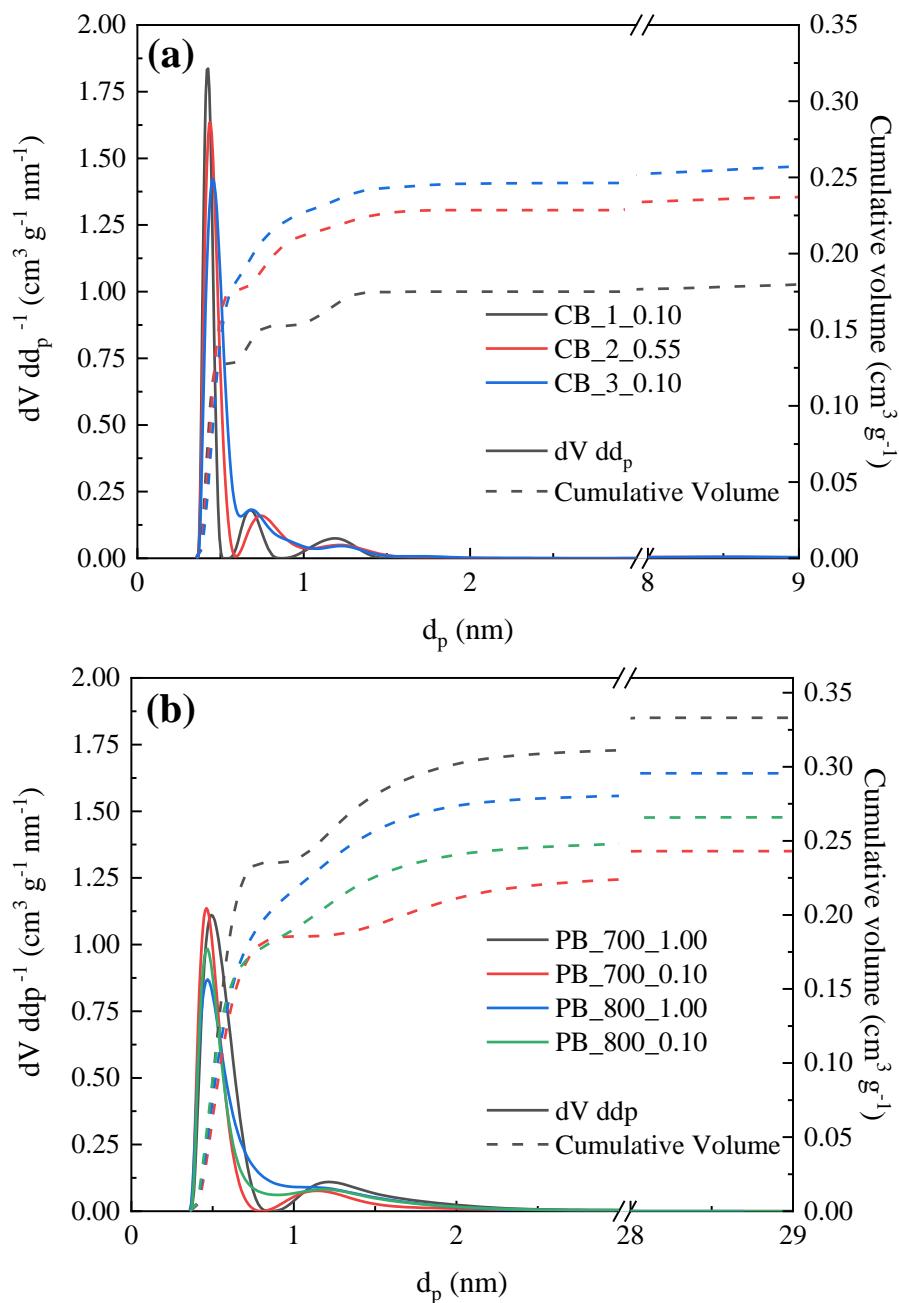


Fig. A.3. PSD and cumulative pore volume of chemical (a) and physical (b) activated biochars.

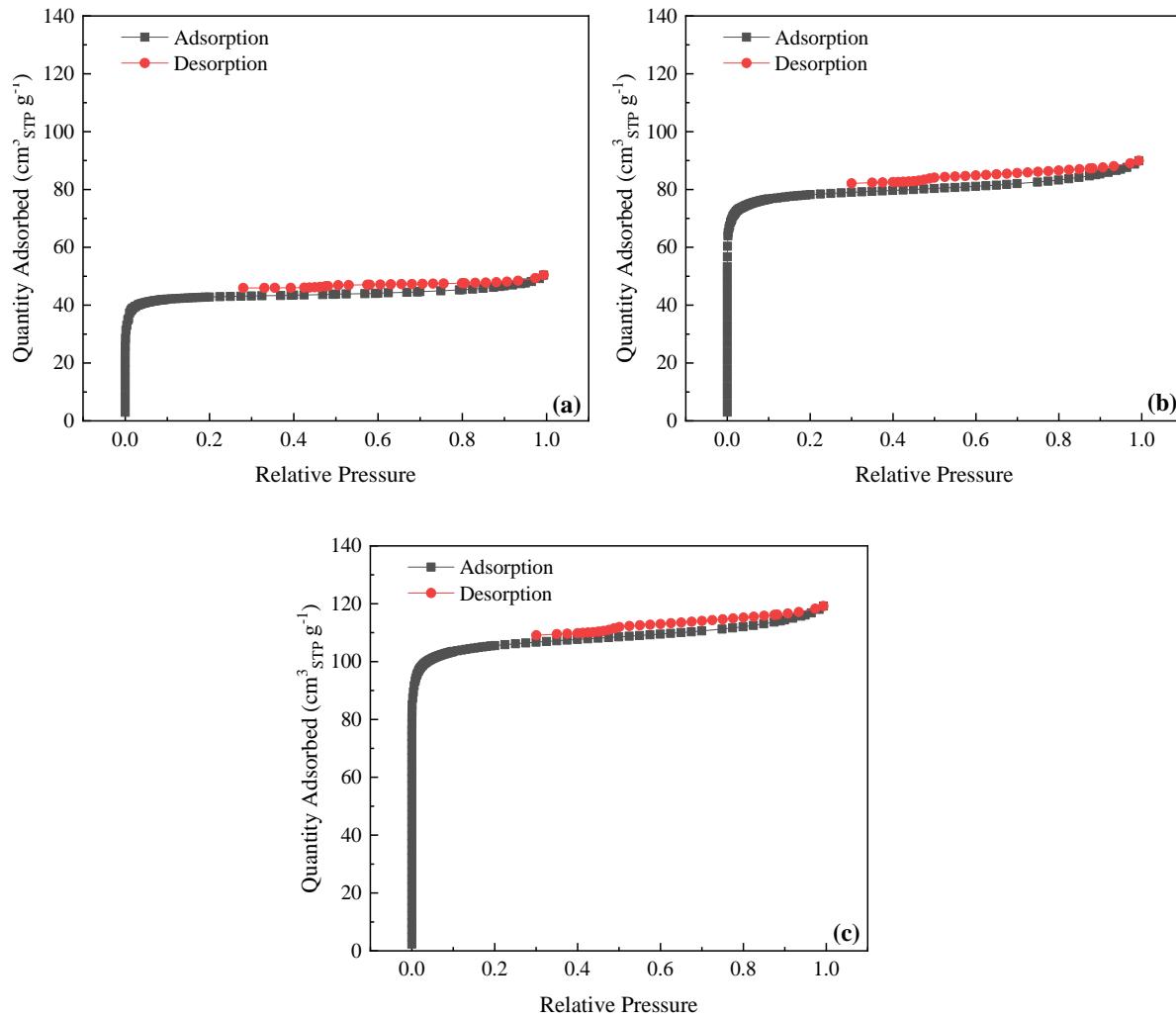


Fig. A.4. N₂ adsorption/desorption isotherms of the following chemically activated biochars: CB_3_0.10 (a); CB_2_0.55 (b); and CB_3_0.10 (c).

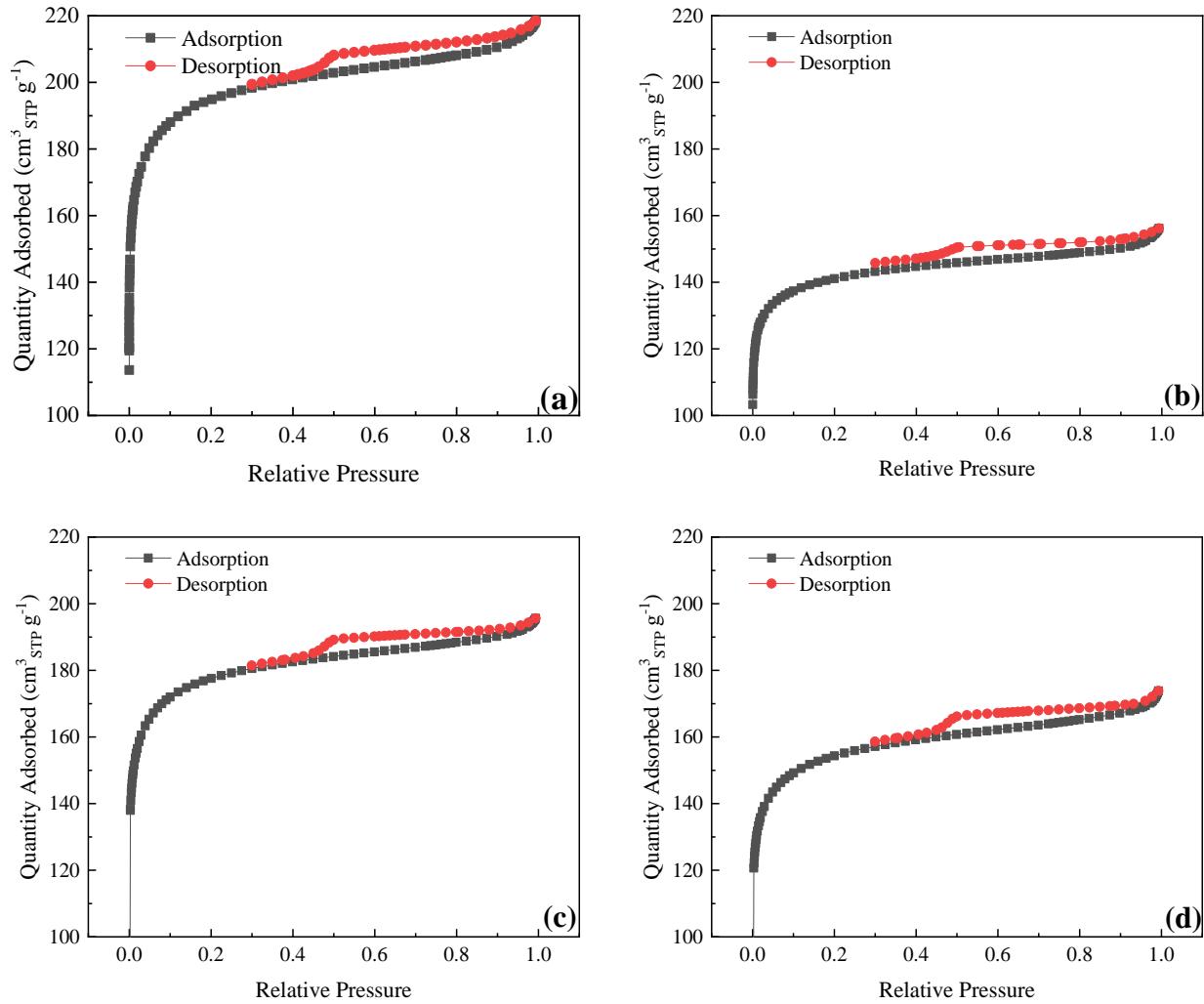


Fig. A.5. N_2 adsorption/desorption isotherms of the following physically activated biochars: PB_700_1.00 (a); PB_700_0.10 (b); PB_850_1.00 (c); and PB_850_0.10 (d).

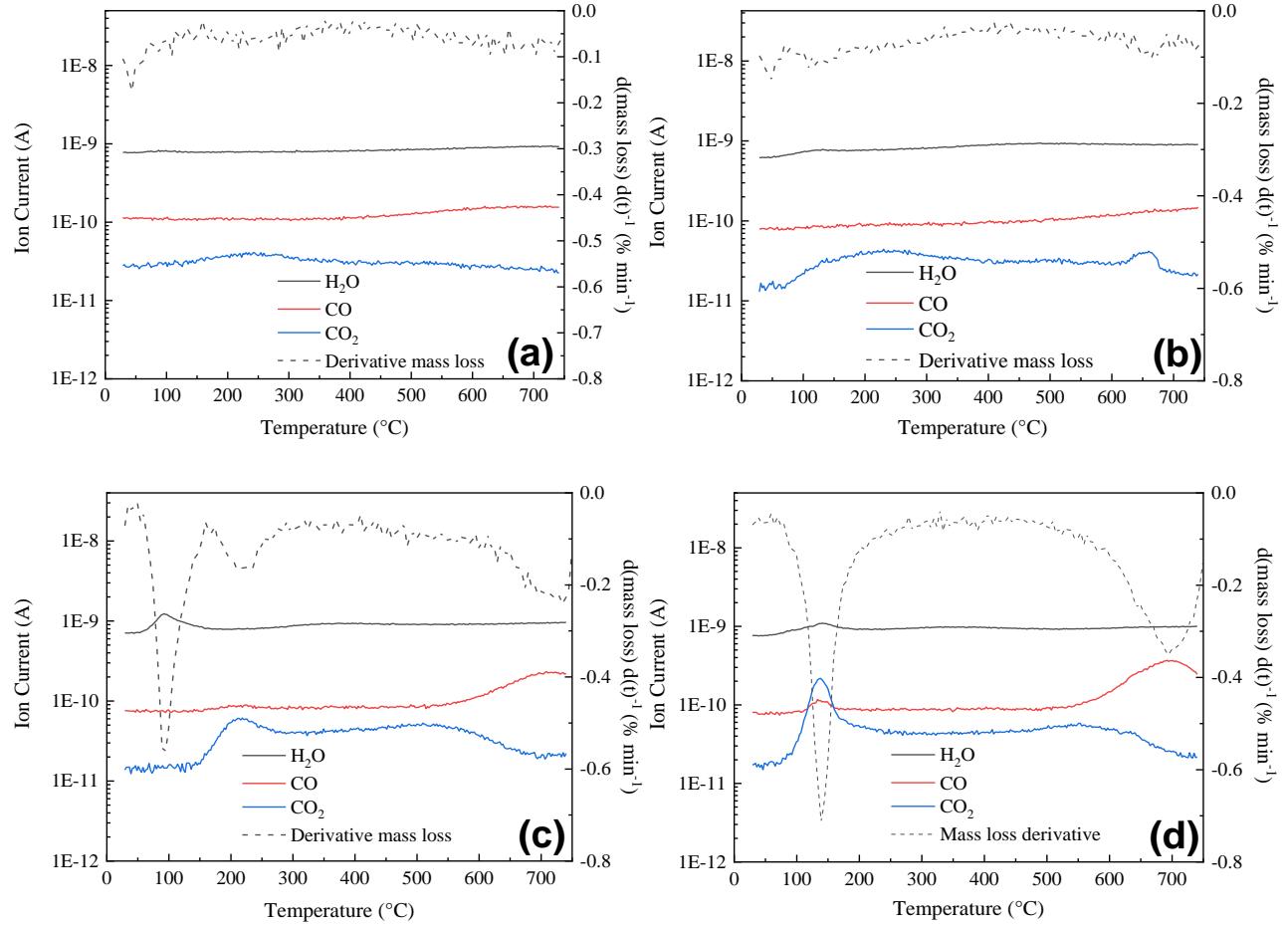


Fig. A.6. Differential thermogravimetric curves (in % of mass min^{-1}) and profiles of released species (H_2O , CO_2 , and CO) from the TPD measurements conducted for the following materials: CB_3_0.10 (a); CB_3_0.10_W (b); CB_3_0.10_R (c); and PB_700_1.00+K₂CO₃ (d).

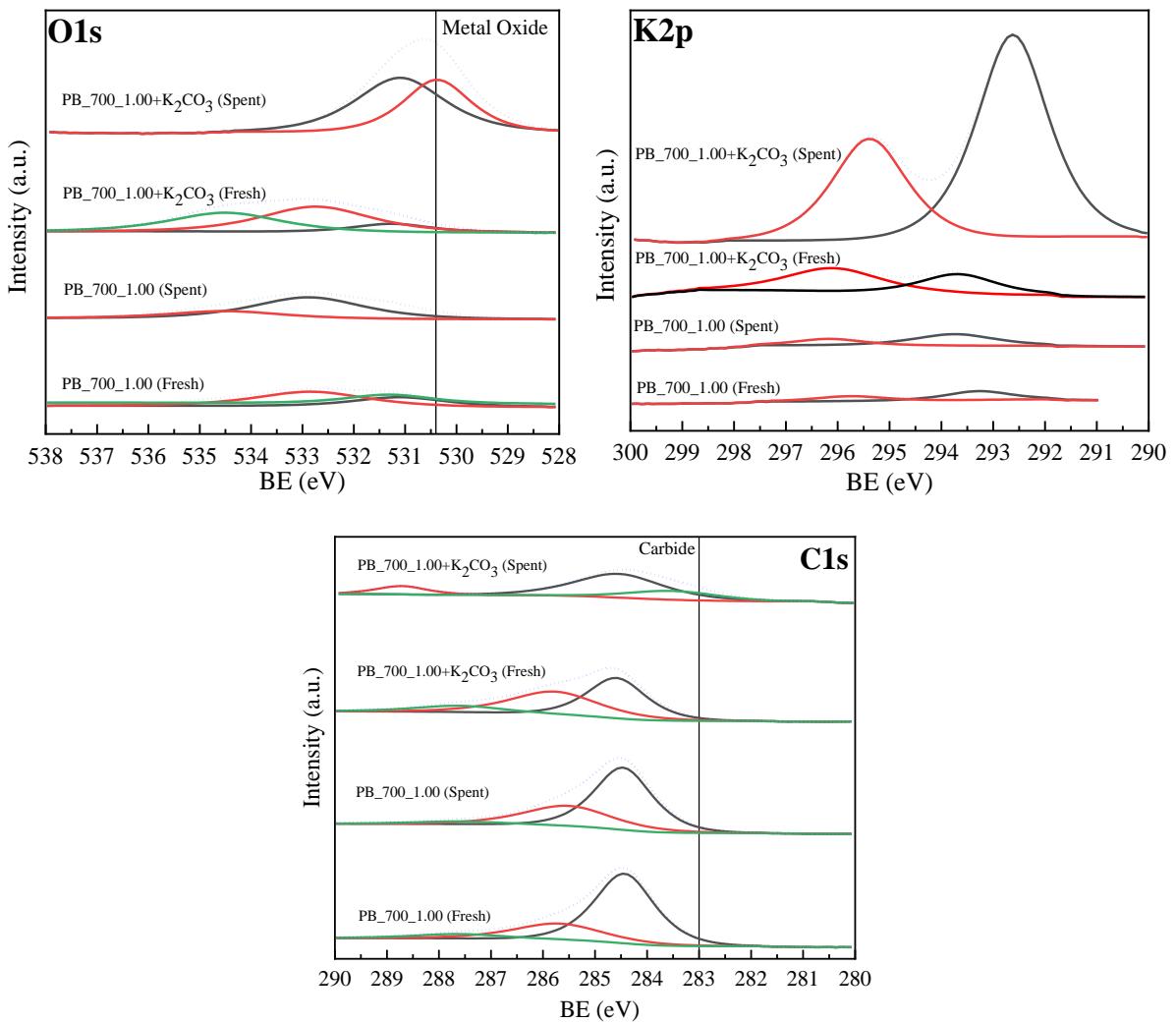


Fig. A.7. C1s, O1s and K2p spectra of fresh and spent PB_700_1.00 and PB_700_1.00+K₂CO₃.