



Article Effect of Physico-Chemical Properties Induced by N, P Co-Doped Biomass Porous Carbon on Nitrous Oxide Adsorption Performance

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Abstract: The adsorption and enrichment of greenhouse gases on biomass porous carbon is a promising approach. Herein, a simple type of nitrogen and phosphorus co-doped biomass porous carbon (NPPC), which was derived from fast-growing eucalyptus bark, was reported via one-step method of carbonization and activation, and the nitrous oxide (N₂O) adsorption performance and the adsorption mechanism of the NPPCs were also investigated. The results showed that NPPC-800-2 demonstrated a high specific surface area (1038.48 m²·g⁻¹), abundant micropores (0.31 cm³·g⁻¹), and enriched content of N and P (4.17 wt.% and 0.62 wt.%), which also exhibited a high N₂O adsorption capacity of 0.839 mmol·g⁻¹. Moreover, the addition of N enhanced the surface polarity of carbon, thereby altering its pore structure. And P doping induced changes in the structural orientation of carbon, resulting in an increased presence of N-P functional groups. This finding reveals that the eucalyptus bark-based N and P co-doped porous carbon shows great potential for wide applications in N₂O capture and provides effective guidance for the design and development of waste biomass adsorbent.

Keywords: porous carbon; N, P co-doped; N₂O; adsorption

1. Introduction

To our knowledge, the emission of nitrous oxide (N₂O) arises from the nitrogen (N) element transformation processes occurring in the natural environment, resulting in its release into the atmosphere as an intermediate product via nitrification and denitrification. In recent decades, the extensive utilization of N-containing chemicals in agricultural and industrial production processes has resulted in the massive release of N₂O, which has resulted in damage to the ozone layer and formation of ozone holes, exposing humans and other organisms to harmful ultraviolet radiation from the sun. Moreover, N₂O is a great potent greenhouse gas with a warming potential approximately 300 times higher than that of CO₂ on a per molecule basis, significantly accelerating global warming [1–6]. To effectively address this environmental issue, it is imperative to develop efficient technologies with low-energy consumption and cost-effectiveness for capturing and enriching N₂O.

As a conventional method, the adsorption process is characterized by its simplicity [7–10]; moreover, the adsorption serves as the initial step in catalysis and has been extensively investigated for gas separation and purification [11–13]. Among them, the chemical absorption method employs specific chemical solutions to react with the target gas, facilitating its separation from the gas. However, the requirement for a large amount of chemical reagents may cause secondary pollution [14–16]. Moreover, the principle of



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Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). physical absorption lies in utilizing the difference in solubility between different gases in a specific liquid, which was conducted to achieve selective capture of gaseous pollutants. Although this method is relatively environmentally friendly, further improvements in adsorbent recovery and reuse techniques are required [17–19]. It is concluded that achieving high-efficiency, low energy consumption and economic technology for N₂O capture and enrichment is a research hotspot which has always been full of challenges in the field of N₂O adsorption. Many previous studies have proved that the proper porous carbon has shown the great adsorption performance of greenhouse gases, such as carbon dioxide (CO₂). Du et al. [20] achieved a CO₂ adsorption capacity of 3.01 mmol·g⁻¹ by the prepared biochar, which derived from grapefruit peel with high nitrogen (N) content. Li et al. [21] conducted a study to enhance CO₂ adsorption capacity, where collected bio-oil residue and incorporated urea were used to synthesize porous carbon, demonstrating an impressive adsorption capacity of 6.22 mmol·g⁻¹. Therefore, it is important to use a suitable porous carbon with appropriate modifications that has demonstrated impressive N₂O adsorption performance.

Given the diminishing availability of traditional wood resources, numerous agricultural and forestry waste biomasses as raw materials have been reported for producing porous carbon via various processes and methods [22,23]. These low-cost biomass sources are excellent raw materials for preparing porous carbon because of their high carbon content and abundant availability. More importantly, the adsorption performance of biomass porous carbon is largely determined by the surface functional groups and pore structure characteristics of the carbon material itself [24,25], and the incorporation of heteroatoms has been proved to promote the physico-chemical properties of porous carbon, which has had a significant influence on the adsorption capacity [26,27]. Among them, the introduction of N-containing oxygen functional groups can impart strong polarity to the carbon surface and generate a greater number of active sites, thereby enhancing the adsorption heat between guest molecules and adsorbents [28]. Luo et al. [29] utilized eucalyptus bark as the primary feedstock and incorporated urea as a dopant to synthesize nitro-functionalized porous carbon possessing an exceptional CO₂ adsorption capacity, exhibiting an impressive adsorption capability of 6.98 mmol·g⁻¹ at 0 °C. Akram [30] synthesized nitrogen-doped porous carbon (NAC), which exhibited an optimal micropore size below 1 nm and a high CO_2 adsorption capacity of 6.25 mmol·g⁻¹ with an exceptional selectivity. Meanwhile, the phosphorus (P) atom can also be considered as a common doping candidate, and the P-containing functional groups of the porous carbon also play a pivotal role in the adsorption performance. Wu et al. [31] synthesized P-doped microporous carbon via using MCM-22 as the template, sucrose as the precursor, and phosphoric acid as the P source, respectively. The maximum adsorption capacity of CO₂ reached 63 mg·g⁻¹. Gong [32] used F108 (polyethylene glycol-polypropylene glycol-polyethylene glycol) as the template and phosphoric acid as the P source to prepare P-doped multi-level porous carbon and achieved efficient CO₂ capture. In addition, P doping can promote the formation of active N (pyridine, pyrrole) and a reduction in graphite-N [33-35]. N and P co-doped porous carbon was synthesized by Xiao et al. [36] through the pyrolysis and activation of a selfassembled chitosan aerogel precursor induced by phytic acid, and the phytic acid served as a P source, an acid regulator, and a structure guide agent. This was conducted to promote the formation of mesopores and micropores, resulting in the production of more marginal pyrrole and pyridine N (bases) in N-doped carbon and enhanced porosity in the carbon material. In addition, the choice of activator also has a great impact on the characteristics of porous carbon materials. KOH was generally selected as a commonly used activator which has good solubility and ionic conductivity. It could well change the void results of carbon materials at high temperature and also remove impurities and oxides in the materials. In summary, it is expected to prepare biomass porous carbon with high N₂O adsorption by co-doping of N, P reasonably.

To further clarify the promotion of N-P co-doped in N_2O adsorption and achieve the excellent adsorption capacity of N_2O , in this paper, we reported a simple and universal

method of fast-growing eucalyptus bark-based N, P co-doped porous carbon preparation, the N₂O adsorption performance of the modified porous carbon was explored, and the influence of N, P functional groups on N₂O adsorption was also investigated. The received findings not only illustrated the vital function of heteroatoms on N₂O adsorption but also provided guidance for the design of an adsorbent with high N₂O adsorption capacity.

2. Materials and Methods

2.1. Preparation of N-P Co-Doped Biomass Porous Carbon

Figure 1 presents the preparation process of N, P co-doped porous carbon. The eucalyptus bark used in this experiment was sourced from a rural area of Nanning, China. The bark was washed with deionized water, sun-dried, and subsequently ground into a fine powder using a grinder. A specific weight of the eucalyptus bark powder was measured and subjected to pre-carbonization by heating it to 500 °C (5 °C·min⁻¹) under an N_2 atmosphere (100 mL·min⁻¹) in a tubular furnace. Next, 2 g of pre-carbonized carbon, 2 g of phytic acid, and 2 g of melamine were thoroughly mixed together. Subsequently, varying amounts of KOH (0 g, 2 g, 4 g or 6 g) along with an appropriate quantity of deionized water were added into the mixture for stirring and then immersed for a duration of 10 h. The resulting mixture was then placed in an oven at 105 °C for a period of 12 h before being ground into powders, and then the powders were subsequently activated at 700 °C, 800 °C, and 900 °C (5 °C·min⁻¹) under N₂ atmosphere within the tubular furnace for a duration of two hours each. After cooling down to room temperature, the samples were neutralized by washing them with 5%HCl solution and followed by drying in an oven at 105 °C. These obtained materials were designated as NPPC-T-n, where T (=700, 800, 900 °C) represented the activation temperature, and n denoted the mass ratio between KOH and pre-carbonized carbon (simplified as n = 0, 1, 2, 3). Additionally, in order to facilitate comparison with aforementioned samples, a control sample incorporating melamine and phytic acid without either compound was also prepared individually. These additional samples were denoted as NPC-T-n, PPC-T-n, and PC-T-n.



Figure 1. Schematic diagram of preparation of N, P co-doped porous carbon (Scale bar of employed instrument: 1:50).

2.2. Characterization of Materials

The crystal structure of NPPCs was investigated by using X-ray diffraction (XRD, Bruker D8 Venture, Ettlingen, Germany), and the scanning range was set from 5° to 80° with a step length of $0.02^{\circ} \cdot s^{-1}$. The Raman (LabRAM HR Evolution, Edison, NJ, USA) spectrum of NPPCs was tested by using a 455 nm laser as the excitation source. The micromorphology of the samples was observed by using a scanning electron microscope (SEM, Gemini SEM, Jena, Germany), which operated at an acceleration voltage of 15 kV. Nitrogen adsorption and desorption isotherms were measured by using a surface area analyzer (Micromeritics ASAP 2460, Norcross, GA, USA), employing ultra-high purity N₂ for determination purposes. Before measurement, the sample underwent degassing in vacuum conditions at 200 °C for at least 8 h. Subsequently, based on adsorption data, specific surface area (S_{BET}) was calculated via multi-point Brunauer–Emmet–Teller (BET) method within the relative pressure range of 0.01 to 0.1. Qualitative analysis of functional groups was performed by Fourier transform infrared spectroscopy (FTIR, Nicolet iS50, Pittsfield, MA, USA). Surface chemical composition analysis of porous carbon was conducted through X-ray photoelectron spectroscopy (XPS, K-ALPHA, Beijing, China).

2.3. Gas Phase Adsorption Test

The adsorption experimental system is divided into three main components: a gas inlet device, an adsorption device, and a gas detection device. The N₂O adsorption capacity of all the samples at 25 °C and 1 bar was measured by using Gas Chromatograph (GC-7920, CEAULIGHT Co., Beijing, China). Before the adsorption test, N₂O and N₂ were introduced into the system and allowed to stabilize. Next, degassed samples were placed in the adsorption column until the adsorption saturation was achieved, at which the outlet concentration was equal to the inlet concentration. Then, the N₂O breakthrough curves of the samples were obtained by monitoring the concentration at each function of time. The N₂O adsorption capacity was calculated as follows:

$$Q = \frac{C_0 V (T - T_0)}{m} \tag{1}$$

where C_0 is N₂O initial concentration; *V* is the pipeline gas velocity; T_0 and *T* are the beginning and ending times of adsorption; and *m* is the mass of the adsorbent material.

3. Results and Discussion

3.1. NPPCs Characterization

The XRD spectrum of the samples is depicted in Figure 2. It can be seen that the scattering peaks were both displayed at $2\theta = 5^{\circ}$ to 10° , suggesting that a significant degree of micropore structure was present within the NPPCs. Furthermore, a broad distinct diffraction peak at 22.5° and 43° corresponded to the (002) and (100) graphite plane, respectively [37,38], indicating the presence of a characteristic amorphous carbon structure.



Figure 2. XRD spectra of the samples.

The defect degree of the NPPCs was analyzed via Raman spectroscopy. As depicted in Figure 3, the Raman spectra of all samples exhibited two broad bands at 1350 cm⁻¹ and 1595 cm⁻¹, corresponding to the disordered peak (D band) and the graphite peak (G band), respectively. To further investigate the impact of heteroatom doping on the extent of structural defects in NPPCs, the intensity ratios between the G band and the D band (I_D/I_G) were tested [39]. As shown in Figure 3, the I_D/I_G strength of NPPCs was greater than the other samples, indicating an increase in disordering, and the presence of defects was a result of the N, P co-doped modification. Meanwhile, due to the introduction of N and P, the etching and redox reaction between KOH and the carbon framework was intensified at elevated activation temperatures, which significantly amplified the magnitude of carbon framework defects.



Figure 3. Raman spectra of the samples.

The FTIR spectra of the NPPCs in the range of $500-4000 \text{ cm}^{-1}$ are presented in Figure 4, which shows a similar shape to a certain extent. The characteristic peak at about 3450 cm⁻¹ was assigned to the tensile vibration of O-H. The intense bands observed at 2923 cm⁻¹ and 1625 cm⁻¹ were attributed to the stretching vibrations of C-H bonds and C=C/C-O groups [40,41], respectively. Moreover, the weak peaks observed at 1401 cm⁻¹ and 1060 cm⁻¹ were ascribed to the vibrational modes of -CN/C=N and P-O bending, which indicated the successful doping of N and P into the porous carbon. Meanwhile, due to the rich phosphate groups of phytic acid, it can be covalently modified on the surface of carbon materials through condensation reactions, thereby promoting the formation of C-O-P bonds. Therefore, the introduction of P doping appeared to facilitate the formation of functional groups containing C-O-P bonds within the carbon structure [42]. Compared to NPPC-700-2 and NPPC-900-2, the FTIR peak intensity of the NPPC-800-2 sample was higher, which may be due to the fact that 800 °C was the optimal activation temperature and promotes the production of N and P functional groups [43].



Figure 4. FT-IR spectra of the samples.

The surface chemical properties and configurations of N, P co-doped atoms in NPPCs were investigated by XPS analysis, and the results are listed in Table 1. It can be observed that the NPPC-800-2 exhibited a N content of 4.17% and P content of 0.62%, indicating that the integration of N and P elements was induced successfully within the carbon matrix. The N1s and P2p spectra measurements of NPPC-800-2 are presented in Figure 5a,b. Among them, the N1s spectrum presented four distinct sub-peaks at 398.5 eV, 400.4 eV, 401.6 eV, and 406.5 eV, corresponding to pyridine-N, pyrrole-N, graphite-N, and oxidized-N species,

respectively [44]. Meanwhile, the P2p spectrum displayed two discernible sub-peaks at 133.4 eV and 134.3 eV, which was attributed to C-P-O and C-O-P functional groups, respectively. In terms of the N species, the pyrrole-N content was larger than other N species' content. And for P species, the C-O-P bond content was larger than C-P-O bond content. Figure 5c,d illustrate the spectra of N1s for NPC-800-2 and P2p for PPC-800-2; it was concluded that the formation of the same relatively high content of pyrrole-N and C-O-P was observed. Compared to single doping, the method of N, P co-doping induces the reaction of melamine and phytic acid at high temperatures, and it a greater propensity towards the formation of comprehensive functional groups is preferred, which is consistent with the FTIR spectra [45,46]. Additionally, the content of the N and P functional groups is further calculated in Figure 5e; it can be deduced that the number of functional groups on the surface of carbon materials can be increased to form strong chemisorption with N₂O, meaning that the incorporation of N and P could alter the electronic structure of the carbon material to make an augmentation in surface active sites and is conductive to the abundance of micropores and mesopores structure being generated, enhancing the interaction between NPPCs and N₂O.



Figure 5. The N1s spectra of (**a**) NPPC-800-2, and (**c**) NPC-800-2; the P2p spectra of (**b**) NPPC-800-2, and (**d**) PPC-800-2; (**e**) functional group contents of the sample.

	Element Con	ntent (wt.%)	
С	0	Ν	Р
83.96	9.15	4.17	0.62
81.36	12.51	1.52	-
85.01	10.69	-	0.98
84.39	11.89	-	-
	C 83.96 81.36 85.01 84.39	Element Cor C O 83.96 9.15 81.36 12.51 85.01 10.69 84.39 11.89	Element Content (wt.%) C O N 83.96 9.15 4.17 81.36 12.51 1.52 85.01 10.69 - 84.39 11.89 -

Table 1. The element content in NPPCs.

The morphology and elemental distribution of N, P co-doped porous carbons were further investigated using scanning electron microscopy (SEM). Figure 6a,b illustrate a distinct pore structure, which is predominantly composed of micropores. The results show that doping N and P changed the morphology and structure of carbon through the activation process [47]. Meanwhile, P doping resulted in a more regular pore size compared with N doping, as shown in Figure 6c,d. Additionally, the elemental mapping image of NPPC-800-2 can be seen in Figure 6e, where it has been demonstrated that the N and P elements were evenly distributed on the surface of NPPC-800-2, meaning that the N and P are successfully doped onto the carbon skeleton, which is also consistent with the FTIR and XPS spectra.



Figure 6. SEM images of NPPCs: (a,b) NPPC-800-2; (c) NPC-800-2, (d) PPC-800-2. Elemental mappings: (e) NPPC-800-2.

Figure 7 presents the N₂ adsorption and desorption isotherms and pore size distribution curves obtained for the NPPCs. According to the IUPAC classification, the N₂ adsorption–desorption isotherms for the NPPCs exhibited characteristic type I behavior, indicating that a porous carbon material was dominated by micropores [48,49]. When the relative pressure (P/P_0) approached 0, the observed vertical linear region could be attributed to the monolayer adsorption of N₂ in the microporous. When the P/P_0 was

over 0.2, these samples exhibited an adsorption hysteresis of the ring-shaped adsorption isotherms, indicating the presence of a certain number of mesopores. Additionally, there is a slight increase in the adsorption isotherms at higher relative pressures $(P/P_0 = 0.9-1.0)$, suggesting the existence of a small amount of macropores. The findings demonstrated that the introduction of N and P doping exerts a significant influence on the pore structure. Furthermore, the pore size distribution curve is displayed in Figure 7b, and the surface texture of NPPCs is presented in Table 2. These results unequivocally validated the prevalence of a highly abundant microporous structure (<2 nm) within NPPCs. The N-doped samples showed an enhanced specific surface area and a more pronounced micropore structure, whereas the P-doped samples demonstrated a more intricate pore structure [50]. Meanwhile, the average pore diameters of NPPCs were distributed around 0.8 nm, and the NPPC-800-2 had lower diameters, suggesting that co-doping N, P promoted the formation of micropores. Additionally, the BET specific surface area and total pore volume (V_T) of the NPPCs showed a significant improvement, with the activation temperature increasing, which might enhance the activation degree. Generally, the N doping enhanced the surface polarity of carbon to modify the pore structure, while P doping induced a change in the carbon structural orientation. It was inferred that the addition of KOH at high temperatures could significantly enhance the pore size structure of carbon, leading to an increased formation of micropores. Simultaneously, the incorporation of phytic acid might facilitate melamine in generating a greater number of active sites, resulting in a more suitable micropore volume.



Figure 7. N₂ adsorption–desorption isothermal curves at 77 K (**a**) and pore size distribution of the samples (**b**).

Samples	S_{BET} (m ² ·g ⁻¹)	S_{mic} (m ² ·g ⁻¹)	V_{T} (cm ³ ·g ⁻¹)	V_{mic} (cm ³ ·g ⁻¹)	V_{mes} (cm ³ ·g ⁻¹)	d (nm)
NPPC-700-2	761	666	0.35	0.25	0.09	1.87
NPPC-800-2	1038	810	0.48	0.31	0.13	1.85
NPPC-900-2	1116	969	0.52	0.38	0.13	1.87
NPC-800-2	2223	1945	1.05	0.82	0.32	1.85
PPC-800-2	535	453	0.28	0.17	0.09	2.09
PC-800-2	1852	1705	0.79	0.686	0.10	1.69

Table 2. Surface texture properties of the samples.

3.2. N₂O Adsorption Evaluation

3.2.1. Adsorption Performance

 N_2O adsorption tests were conducted to investigate the adsorption performance of NPPCs. Figure 8a–c illustrate the adsorption breakthrough curves of N_2O on the NPPCs at a temperature of 25 °C. With an initial concentration of 500 ppm, the adsorption capacity of NPPCs for N_2O increased initially and then decreased with the rise in carbonization activation temperature. It seems that the sample of NPPC-800-2 achieved an optimal value. Additionally, with the increase in mass ratio between KOH and pre-carbonized carbon, the

adsorption capacity and breakthrough time of N₂O by NPPCs was firstly increased and then decreased. It was inferred that this was due to the significant influence of temperature and KOH ratio on the adsorption behavior of N₂O by NPPCs because the temperature variation and the ratio of KOH had a great impact on the generation of pore structure and surface functional groups of biomass-derived porous carbon, thereby synergistically affecting the N_2O adsorption performance. Specifically, the porous carbon, which was prepared with an appropriate KOH dosage at a ratio of 1:2 and an activation temperature of 800 °C, displayed a maximum N₂O adsorption capacity. Among them, the sample of NPPC-800-2 presented superior performance in terms of N₂O adsorption with a maximum capacity (0.839 mmol \cdot g⁻¹). Compared to PC-800-2, NPC-800-2 and PPC-800-2 exhibited a certain degree of enhancement in N2O adsorption. Considering the action strength of N and P in N₂O adsorption, along with specific surface area and XPS analysis, P doping promoted the formation of C-O-P groups and pyrrole, and then more active sites were generated, while N doping aimed to improve the specific surface area and pore structure of porous carbon, thereby increasing the N₂O adsorption capacity. Moreover, it can be found that the P-doped samples exhibited superior adsorption performance than the N-doped samples at identical conditions. This enhancement can be attributed to the massive generation of active pyridine-N and pyrrole-N species within the presence of phytic acid, thereby providing an increased availability of alkaline active sites for N₂O adsorption. During the heating treatment process, the melamine would thermally polymerize to form N-doped carbon frameworks ($g-C_3N_4$). And then phytic acid can be used simultaneously as a phosphorus source, which can be chemically cross-linked with $g-C_3N_4$ to form a N, P co-doped carbon framework [51]. Therefore, it was concluded that N, P co-doped carbon could effectively modify the pore structure, generate a greater number of functional groups and active sites, thereby improving the N₂O adsorption performance of NPPCs.



Figure 8. (a) Adsorption penetration curves of NPPCs at different activation temperature. (b) Adsorption penetration curves of NPPCs at different KOH ratio. (c) Adsorption penetration curves of NPPCs with different N and P doping. (d) Linear relationship between adsorption capacity at different temperatures and N functional groups in NPPCs samples. (e) Linear relationship between adsorption capacity at different temperatures and P functional groups in NPPC samples. (f) Adsorption cycle performance test of NPPC-800-2.

To further investigate the impact of surface N and P functional groups on N₂O adsorption performance, the N₂O adsorption capacity (Q) was normalized by specific surface area (S_{BET}), yielding the normalized adsorption capacity (Q/S_{BET}) as a representation of N₂O adsorption per unit specific surface area. As depicted in Figure 8d,e, the R^2 between the normalized N₂O adsorption capacity of NPPCs and P-containing functional groups was

0.9349, which was larger than that of N-containing functional groups. These findings indicated that the N₂O adsorption performance of as-prepared porous carbon was primarily influenced by P-containing functional groups, while the N-containing functional groups could further enhance the adsorption effect via the pore structure improvement, which served as a secondary factor.

Additionally, the recycling capability of the adsorbent on N₂O uptake was also analyzed, and the cyclic adsorption performance of the NPPC-800-2 is shown in Figure 8f. Compared with the first adsorption, it was illustrated that the NPPC-800-2 maintained a consistent adsorption performance, which retained approximately 80% of its initial adsorption capacity even after 10 cycles of adsorption and desorption. These findings prove that N, P co-doped porous carbon (NPPC-800-2) not only presents efficient and rapid separation of N₂O within a short duration of adsorption but also shows the excellent reusability of multiple cycles.

3.2.2. Fitting of Dynamic Adsorption Model

The fitted adsorption breakthrough curves of N₂O on NPPCs are exhibited in Figure 9a–c, and the experimental results and Yoon–Nelson fitting parameters are summarized in Table 3. As an easy semiempirical model, the Yoon–Nelson model does not require detailed information about the properties of the adsorbate, adsorbent, and adsorption bed to investigate the dynamic adsorption process. It could be seen that the Yoon-Nelson model demonstrated good fit for the adsorption breakthrough curve of N_2O on NPPCs, and NPPC-800-2 attained a correlation coefficient (R^2) exceeding 0.9994. The observed results demonstrate that the temperature increment significantly enhanced both K_{YN} and R^2 , thereby establishing temperature as the primary determinant to determine dynamic adsorption in the Yoon–Nelson model. Meanwhile, the au value was calculated and corresponded closely to the experimental $t_{0.5}$ value, implying that the Yoon–Nelson model effectively simulated the adsorption behavior of N₂O on NPPCs. The adsorption rate constant (K_{YN}) of N_2O decreased with the increased carbonization temperature, indicating a gradual reduction in mass transfer resistance. This observation also suggested that the increase in micropore volume, which was caused by the higher activation temperatures, might contribute to the decrease in mass transfer resistance, thereby illuminating the relationship between mass transfer resistance and potential micropore distribution.

		Yoon–Nelson Fitting Parameters			Thomas Fitting Parameters			
NPPCs	$\ln \frac{C_t}{C_0 - C_t} = F$	$ln \frac{C_t}{C_0 - C_t} = K_{YN}t - \tau K_{YN}$			$\ln\left(\frac{C_0}{C_t}-1\right) = \frac{K_{Th}q_0m}{V} - K_{Th}C_0t$		a (Experiment)/	
	K _{YN} /min ⁻¹	τ (Theory)/min	(Experiment)/ min	R ²	$\frac{K_{Th}\times 10^{-5}}{m^3\cdot min^{-1}\cdot mg^{-1}}$	q ₀ (Theory)/ mmol·g ⁻¹	mmol·g ⁻¹	R ²
NPPC-700-2	0.3401	11.94	11.65	0.9893	0.4119	0.5397	0.576	0.9846
NPPC-800-2	0.5148	17.96	17.81	0.9994	0.5999	0.8337	0.839	0.9965
NPPC-900-2	1.1157	8.993	8.422	0.9972	1.3631	0.4225	0.414	0.9923
NPPC-800-0	0.9548	4.083	3.502	0.9732	1.2802	0.1935	0.241	0.9827
NPPC-800-1	0.3986	5.391	4.705	0.9541	0.5280	0.2292	0.282	0.9613
NPPC-800-3	0.8984	9.411	8.956	0.9982	1.3661	0.4475	0.442	0.9845
NPC-800-2	0.7639	9.652	9.404	0.9978	1.2268	0.4558	0.459	0.9934
PPC-800-2	0.3608	11.82	11.83	0.9869	0.4342	0.5349	0.571	0.9864
PC-800-2	1.3544	6.701	7.326	0.9994	1.3559	0.3182	0.319	0.9901

Table 3. Yoon–Nelson and Thomas fitting parameters of N₂O on NPPCs.

Yoon–Nelson: where K_{YN} is the adsorption rate constant of Yoon–Nelson model, min⁻¹; τ is the time required for adsorption to reach 50% of the penetration point, min. Thomas: where K_{Th} is the adsorption rate constant of Thomas model, m³·min⁻¹·mg⁻¹; q is dynamic adsorption capacity, mmol·g⁻¹.

The Thomas model is an idealized representation based on the Langmuir model and assumes no axial diffusion, enabling estimation of the equilibrium adsorption capacity of the adsorbate. Consequently, it can be effectively employed in this dynamic adsorption investigation. The N₂O adsorption penetration curve of the NPPCs was also fitted to the Thomas model, as depicted in Figure 9d–f, and the corresponding fitting parameters are presented in Table 3. It is also evident that the Thomas model exhibits a strong cor-

relation with the N₂O adsorption penetration curve, with a correlation coefficient (R^2) exceeding 0.9965 for the NPPC-800-2. The theoretical adsorption capacity of N₂O for each sample was individually calculated, and the obtained results closely matched the actual adsorption capacity, thereby demonstrating the excellent capability of the Thomas model in simulating dynamic N₂O adsorption. The theoretical and experimental adsorption values exhibit a close correlation across different temperatures and various N and P doping levels, highlighting the significant influence of temperature and N, P dopants on the adsorption capacity. However, when considering NPPCs with different KOH ratios, there are some discrepancies observed between NPPC-800-0 and NPPC-800-1 fittings, suggesting that an appropriate KOH ratio is a crucial factor affecting the adsorption capacity [52].



Figure 9. Yoon–Nelson model: (**a**) fitting curve of N_2O adsorption breakthrough on NPPCs at different activation temperatures; (**b**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratios; (**c**) fitting curve of N_2O adsorption breakthrough on NPPCs at different N and P doping. Thomas model: (**d**) fitting curve of N_2O adsorption breakthrough on NPPCs at different activation temperature; (**e**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different KOH ratio; (**f**) fitting curve of N_2O adsorption breakthrough on NPPCs at different N and P doping.

3.2.3. Adsorption Mechanism

Numerous reports have demonstrated that the doping of heteroatoms can improve the gas adsorption capacity. Notably, the adsorption results indicated that the N_2O adsorption capacity of the prepared carbon was affected by the heteroatom doping on the porous carbon. To further demonstrate the influence of N and P functional groups on N₂O adsorption, all spin-polarized DFT calculations were performed by using the DMol³ package included in the Material Studio 17.1 software [53,54]. The electronic properties of both N and P functional groups and N₂O adsorption systems were optimized and computed, which employed the generalized gradient approximation (GGA) along with Perdew-Burke-Ernzerh (PBE) exchange-correlation functions. The N functional groups on NPPCs were composed of pyridine-N, pyrrole-N, graphite-N, oxidized-N, etc., of which a greater content of pyrrole-N was observed. In terms of the P functional groups of NPPCs, C-O-P represented the predominant functional group, wherein $(CO)_2$ -P(O)(OH) was particularly prevalent. The configuration of the N, P functional groups and the optimized adsorption site for the N₂O adsorption are presented in Figure 10, following geometric optimization. It can be observed that the pyrrole-N and (CO)₂-P(O)(OH) were more likely to interact with oxygen atoms, which showed that the oxygen site could be the dominant adsorption in the N₂O adsorption process. Moreover, the adsorption energy of various adsorption systems was further calculated by optimizing the adsorption sites. As presented in Table 4, the adsorption energy of pristine graphene was determined to be $-0.87 \text{ kJ} \cdot \text{mol}^{-1}$. The absolute values of the adsorption energies for pyrrole-N and (CO)₂-P(O)(OH) were both calculated to exceed 1 kJ·mol⁻¹, suggesting that the N, P co-doped functional groups possessed a higher affinity for N₂O adsorption compared to monolayer graphene configurations. It was also concluded that the synergistic effect of (CO)₂-P(O)(OH) and pyrrole-N demonstrated the maximum pronounced performance of N₂O adsorption (adsorption energy: -3.39 kJ·mol⁻¹), implying that N, P co-doped carbon was found to be more effective for enhancing N₂O adsorption. Another crucial parameter explaining N₂O's absorption performance is equilibrium distance (d_e), which represents the stable equilibrium stage of adsorption between absorbent and absorbate at their closest proximity. According to the calculation results from Table 3, d_e values of three functional groups were measured to be 1.809 Å, 1.786 Å, and 1.623 Å, respectively, which were both shorter than the d_e value of pristine graphene (2.479 Å). It was concluded that the N, P co-doped functional groups presented superior affinity towards graphene, indicating that the incorporation of different N, P co-doped functional groups promoted a meaningful interaction between graphene configurations and N₂O molecules and then improved the N₂O adsorption on the NPPCs.



Figure 10. Adsorption system configuration of nitrogen and phosphorus functional groups containing nitrogen (C: gray, H: white, O: red, N: blue, P: pink).

System	Ead (kJ·mol ⁻¹)	de (Å)
Graphene	-0.87	2.479
Pyrrole	-1.35	1.809
(CO) ₂ -P(O)(OH)	-2.51	1.786
Pyrrole and (CO) ₂ -P(O)(OH)	-3.39	1.623

Table 4. Adsorption energy and adsorption equilibrium distance of different functional groups.

4. Conclusions

In this work, the N, P co-doped porous carbon was successfully prepared through the one-step method of carbonization and activation. By optimizing the ratio of KOH and activation temperature, the N, P co-doped biomass-derived porous carbon achieved an abundance of microporous structures and heteroatom functional groups, which presented the exceptional adsorption performance of N₂O. The sample of NPPC-800-2 demonstrated a high specific surface area (1038.48 cm²·g⁻¹), abundant micropores (0.31 cm³·g⁻¹), and enriched content of N and P (N, 4.17 wt.% and P, 0.62 wt.%). It also displayed a remarkable N₂O adsorption capacity of 0.839 mmol·g⁻¹ under the conditions of 1 bar and 25 °C. The Yoon–Nelson and Thomas model were found to effectively describe the dynamic adsorption behavior on NPPCs, and the calculated adsorption energy and equilibrium distance of the molecular simulation also fully validated the impact of N, P functional groups on N_2O adsorption. It was concluded that the N_2O adsorption capacity of NPPCs was affected by the co-doping of N and P, which modified the functional groups and microporous structure of as-prepared carbon. This work not only highlights the introduction of N and P elements co-doped for the enhancement of N_2O adsorption but also proposes a promising way of low-cost and effective capture of N_2O with the waste biomass resources.

This work will also promote the sustainable development of two aspects. From the view of the principles of the circular economy, the research findings propose an environmentally friendly solution for dealing with the large amount of fast-growing eucalyptus waste in the rural region of Guangxi, China, and for achieving high-value utilization of agricultural waste. On the other hand, a reasonable application of effective N_2O adsorption and greenhouse gas reductions with eucalyptus bark-based porous carbon will be possible.

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