Disinfection by-product formation and toxicity evaluation for chlorination with powered activated carbon

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A B S T R A C T

With the deterioration of source water quality, pre-chlorination and pre-addition of powdered activated carbon (PAC) have been widely applied to improve water treatment efficiency, which would lead to PAC exposure to chlorine. Although previous studies reported that some emerging carbon materials (e.g., graphene) could potentially act as disinfection by-product (DBP) precursors, there were few studies paying attention to the interaction between chlorine and the most commonly used carbon material-PAC on the DBP formation. In this study, the DBPs formed by chlorination with and without PAC were investigated, and the DBP toxicities in different systems were evaluated. The results showed that the PAC could react with chlorine and form tri-halomethanes (THMs) and haloacetic acids (HAAs). The amount of surface oxygen groups of the PAC increased during the chlorination, with these oxygen groups, especially the *meta*-positioned –OH groups, facilitating the formation of THMs and HAAs. In the presence of NOM, lower concentrations of THMs and HAAs were observed in the systems with PAC than in those without PAC, demonstrating the critical role of PAC adsorption towards DBP control. The cytotoxicity evaluation indicated that more toxic reaction products between PAC and chlorine were formed besides conventional DBPs. Moreover, the PAC with higher BET surface area and more lactonic function groups formed less toxic DBPs during chlorination, which might reduce health risk for treatment processes with pre-chlorination.

1. Introduction

Pre-chlorination has become a commonly used drinking water treatment technology to enhance algae control (Ma et al., 2012) as well as remove iron and manganese (Khadse et al., 2015) due to its low cost and persistent oxidizing ability (Daly et al., 2007). However, many groups of disinfection by-products (DBPs) were produced due to the chlorination of the organic matter, including halogenated salicylic acid, halogenated phenol, halogenated nitrophenol (Dong et al., 2021; Yang et al., 2019), of which some are highly toxic (Golea et al., 2017; Goslan et al., 2017). Among them, trihalomethanes (THMs) and haloacetic acids (HAAs) have already been regulated in many countries, such as the U.S. and China (Dong et al., 2021). In addition, powdered activated carbon (PAC) has been extensively applied to control the micro-pollutants such as taste & odor (T&O) compounds, pharmaceutical compounds and pesticides etc. (Lucas et al., 2021; Srinivasan and Sorial, 2011). For example, to solve the T&O problem, at least 39–55 mg

L^{-1} PAC was required at four water treatment plants in Adelaide, South Australia (Cook et al., 2001). Due to the negative influence of the co-agulants on the PAC adsorption (Seckler et al., 2013), PAC can be added at the intake of the source water, before coagulation (Srinivasan and Sorial, 2011; Yu et al., 2007). Thus, in cases of prechlorination, PAC could potentially form DBPs. Till now most of the DBP formation studies were focused on the chlorination of the natural organic matter and micro-pollutants (Golea et al., 2017; Hebert et al., 2018). The chlorination of PAC itself and the effects of the PAC on the formation of DBPs during chlorination still require further investigation.

Some other carbon materials except PAC, such as nC_{60} and graphene oxide (GO), which may release into the drinking water sources, can act like the organic matters as DBP precursors during the chlorination (Alpatova et al., 2013; Du et al., 2017, 2016; Wang et al., 2012). Du et al. (2016) investigated the formation of THMs by five types of carbon nanotubes, GO and reduced GO, and found that all these carbon materials could act as the precursors of THMs in aqueous phase. They also

suggested that the carbon atoms at the middle of two *meta*-positioned —OH groups on the benzene ring were more active and might prefer to form THMs with chlorine oxidation. However, limited studies pay attention to the DBP formation with the presence of the carbon materials that commonly used: activated carbon (AC). Only Voudrias et al. (1987) reported that additional products were formed when free chlorine reacted with phenols adsorbed on granular AC (GAC), including chlorohydroxybiphenyls (hydroxylated PCBs) rather than producing the mono-, di, or tri- chloro derivatives which were supposed to be formed by chlorine with phenol in solution. They speculated that surface free radicals were produced from the oxidation of GAC with aqueous HOCl. Our previous study also suggested that the PAC could catalyze chlorine to generate free radicals (Huang et al., 2021). In addition, the AC has also been widely used to control the DBP precursors and DBPs. Utku et al. (2020) revealed that the adsorption of halogenated DBP precursors mostly occurred in the mesoporous region. Babi et al. (2007) also proved that the GAC post-filter contributed lot to the adsorption of already formed THMs and HAAs. Therefore, the effects of PAC could be rather complicated on the DBP formation because it could act as the DBP precursors, adsorb the DBPs precursors and the formed DBPs, and may also produce other by-products by the free radical chain reaction. However, to date little is known about the regulated DBPs such as the THMs and HAAs formed by the PAC during chlorination, and the effects of PAC on the NOM reaction with chlorine and the toxicity of the products need further understanding.

Therefore, this study was designed to investigate the impacts of PAC on the DBP formation during chlorination with and without NOM. The cytotoxicity of their products was comparatively observed using the normal rat kidney (NRK) cell. Finally, the effects of PAC properties including surface area, pore size, pore volume and surface functional groups on the products toxicity were evaluated.

2. Materials and methods

2.1. Reagents and materials

The standards of DBPs used in this study, namely, trichloromethane (TCM), trichloroacetic acid (TCAA), dichloroacetic acid (DCAA) and chloroacetic acid (CAA) were obtained from AccuStandard, Inc. (New Haven, CT, USA). Anhydrous sodium sulfate (Na_2SO_4) and sodium thiosulfate ($Na_2S_2O_3$) were obtained from Sinopharm Chemical Reagent Company (Shanghai, China). Methyl tert-butyl ether (MTBE) was purchased from J&K (China). Sodium hypochlorite (chemically pure) was used for the preparation of the chlorine stock solution with a concentration of 1.0 g L^{-1} (as Cl_2), which was kept at 4 °C until use. Humic acid (HA) was obtained from Sigma-Aldrich. All of the reagents used in this research were of analytical grade unless otherwise noted.

PACs were obtained from Ningxia Guanghua Co. Ltd (China) and their abbreviation and basic information are provided in Table S1 and Table S2, respectively. PAC was washed by deionized water until the pH of filtrate was near to 7.0. The PAC was then dried in an oven at 115 °C for 12 h.

2.2. Characterization of PAC

The surface area and pore size distribution of PAC samples were characterized using an AUTOSORB (Quantachrome, USA) computer-controlled surface analyzer. To further understand the reaction between chlorine and PAC, the PAC after chlorination was collected and freeze-dried for characterization by Fourier Transform Infrared Spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) using a NEXUS 670 FTIR spectrophotometer (Nicolet, USA) and Kratos AXIS SUPRA (Shimadzu, Japan), respectively. The XPS data was analyzed by the Avantage. The C1s spectra of the carbons generally comprised three peaks with differentiated binding energy values via deconvolution corresponding to: (C-I) C—C and C—H (graphitic carbon) at 284.8 eV, (C-II)

C—O (phenolic, alcohol and ether) at 285.5 eV and (C-III) $O = C$—O (carboxyl and ester) at 288.5 eV (Liu et al., 2013a). The O 1 s spectra of the carbons comprised three peaks with differentiated binding energy values via deconvolution corresponding to: (O-I) $C = O$ groups (ketone, lactone, ester and carboxyl) at 531.10 eV, (O-II) C—OH or C—O-C groups at 533.07 eV and (O-III) chemisorbed oxygen at 535.10 eV (Liu et al., 2013a, 2013b).

2.3. Experiment procedures

The pH of all solutions was adjusted to 7.5 by using a 10 mM phosphate buffer solution before the chlorination. The concentration of PAC used in the experiments was 10 mg L^{-1} to amplify the possible reactions during water treatment. Based on previous studies on DBP formation potential (Doederer et al., 2014; Sanchís et al., 2020), relatively high chlorine dose of 7.5 mg L^{-1} as Cl_2 was selected to maintain a sufficient chlorine residual. To investigate DBP formation from PAC under practical conditions, three PACs (PAC2, PAC5 and PAC-initial) with similar iodine value were also evaluated using lower doses of chlorine (1 mg L^{-1} and 3 mg L^{-1} as Cl_2). The chlorine was first mixed with 10 mg L^{-1} PAC alone, which was denoted as PAC—Cl, to distinguish the DBPs formed only by the PAC. The effect of PAC on the DBP formation with the NOM was compared by the reaction between chlorine (7.5 mg L^{-1}) and HA (10 mg L^{-1}) with and without 10 mg L^{-1} PAC, denoted as NOM-Cl and PAC—NOM-Cl, respectively. Water samples were collected and filtered by the 0.45 μm membrane to remove PAC at determined intervals for the DBP detection and other measurements. Na_2SO_4 (6.0 g) and $Na_2S_2O_3$ (1:1.2) were added to 30 mL water sample followed by rapid extraction with MTBE (U.S.EPA, 1995, 2003).

2.4. Analytical methods

Four DBPs, namely, TCM, TCAA, DCAA and CAA were measured in this study according to EPA 551.1 method using gas chromatography (Agilent 7890, Santa Clara, CA, USA) equipped with an electron capture detector (Agilent Technologies, Santa Clara, CA, USA) (Yu et al., 2019). The column used for detection was an HP-5 fused silica capillary column (30 mm × 0.25 mm I.D. with film thickness of 0.25 mm). The pH of the water samples was measured by using a pH meter (HACH HQ 40d, Loveland Colorado, USA) after calibration with standard solutions prior to use. The N,N-diethyl-p-phenylenediamine (DPD) method was used to measure residual free chlorine in the solution, with result presented in mg/L as Cl_2 (HACH Pocket Colorimeter II, Loveland Colorado, USA). Measurement of molecular weight (Mw) was conducted by HPSEC consisting of a high-performance liquid chromatography system (Waters 1525, Waters, Milford, Massachusetts, USA) and a size exclusion chromatography column (TSKgel G3000SWXL, Tosoh, Yamaguchi, Japan). Ultra-high-performance liquid tandem chromatography quadrupole time-of-flight mass spectrometry (UHPLC-QTOF-MS, ACQUILITY UPLC/Xevo G2 Q TOF, Waters, Milford, Massachusetts, USA) was applied to further investigate DBP formation, capturing other DBPs than the target compounds.

2.5. Cytotoxicity evaluation

The cytotoxicity test was selected to assess the overall toxic effect from the products. The NRK 52[E] cell line derived from rat proximal tubule epithelium was obtained from the Cell Bank of the Chinese Academy of Sciences (Shanghai, China). NRK 52[E] cells were grown in 25 cm[2] petri dish (Nunc, Denmark) in Dulbecco's modified Eagle Medium containing 5% (v/v) fetal bovine serum, and maintained at 37 °C in a 5% CO_2/air incubator. The colorimetric MTT assay has been used to evaluate the DBPs chronic cytotoxicity in NRK 52[E] cells, respectively (Muellner et al., 2008; Yang et al., 2014). The culture medium was removed after 24 h and 48 h. A 0.5 mg ml^{-1} MTT solution (200 μl) was added to each well. After incubation, the medium was removed, and the
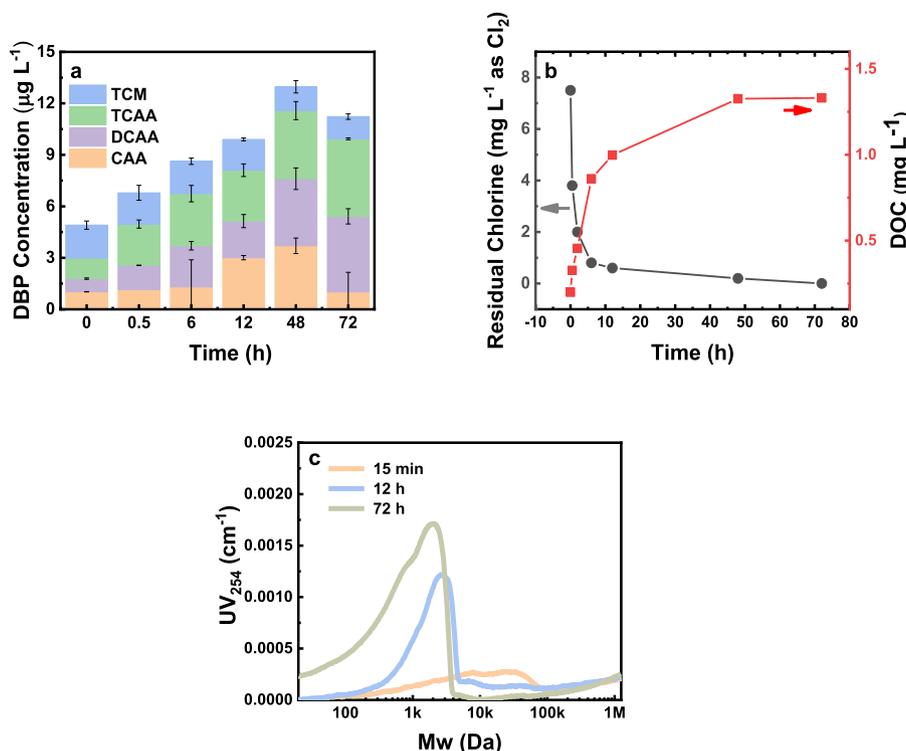
Fig. 1. a. Formation of TCM and HAAs from chlorination of PAC alone; b. Residual chlorine and DOC concentration during chlorination of PAC; c. the organics Mw in the solution released from the chlorination of PAC alone.

formazan crystal was solubilized by a 10 min treatment with 150 μL of isopropanol in the incubator. The absorbance of each well was measured on a microplate reader (EPOCH2T, Biotek) at 570 nm. The relative cell viability was calculated by conducting 3 duplicate experiments and taking the mean value.

3. Results and discussion

3.1. The reaction between chlorine and PAC

3.1.1. The DBPs formed by PAC with chlorine

As illustrated in Fig. 1a, the chlorine reacted with PAC alone and formed the common DBPs, such as THMs and HAAs. As for THMs, only TCM without bromine was determined in this study. The total concentration of DBPs first increased and then decreased after 48 h. Particularly, the concentrations of DCAA and TCAA increased persistently in 72 h, while the concentrations of TCM and CAA first increased and then decreased, which might be due to the PAC adsorption. The reduction for the DBP concentrations after 48 h, might result from the exhaustion of

Fig. 2. FTIR spectra of the initial PAC and PAC after chlorination (PAC—Cl).

chlorine. The residual chlorine at 48 h was only 0.2 mg L^{-1} as shown in Fig. 1b. When the chlorine completely reacted with carbon, the concentration of DBPs reached the maximum in the solution. In addition, the DBP concentrations formed by PACs under relatively lower concentration of chlorine (1 mg L^{-1} and 3 mg L^{-1} as Cl_2), which might be more approached to actual application are shown in Fig. S1. Different from the results at 7.5 mg L^{-1} chlorine, the DBP concentrations all decreased with time, which might be due to the relatively lower chlorine concentration as shown in Fig.S2. PAC5 with the highest chlorine decay rate formed the maximum amount of DBPs at the 0.5 h, but the PAC-initial with medium chlorine decay rate exhibited the least DBP concentration, which might be due to its superior adsorption capacity resulting from the abundant micropore volume. The adsorption ability for THMs and HAAs with small Mw based on the micropore volume could also explain the lower DBP concentration of PAC5 compared with PAC2 after 2 h. Babi et al. (2007) proved that the THMs and HAAs could be removed by the GAC adsorption. Therefore, due to the excellent adsorption capacity of PAC, the total concentration of DBPs formed by the reaction between chlorine and PAC should be higher than the detected amount in the solution.

The collected PAC was re-dispersed into 1 L pure water under ultrasound. After 2 h ultrasound, the DBP concentrations in the solution were measured and the results are shown in Fig. S3 (left bar). It could be noted that an approximate total concentration of 20 μg L^{-1} THMs and HAAs was detected in the solution. Therefore, it suggested that the DBPs formed by the PAC and chlorine was more than the examined concentration as shown in Fig. 1, some of which were trapped by the PAC adsorption and did not released to the solution.

The DOC concentration and the Mw of the released organics were measured as shown in Fig. 1b and c, which could also prove that the chlorine surely reacted with the PAC. It could be noted that the DOC concentration significantly increased with time, especially within the first 12 h, after that the DOC concentration almost remained stable, which might be due to the low residual chlorine concentration. The Mw of the released organics was relatively large ranged from 100 to 100,000
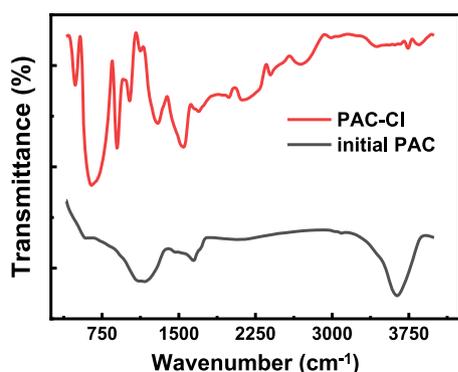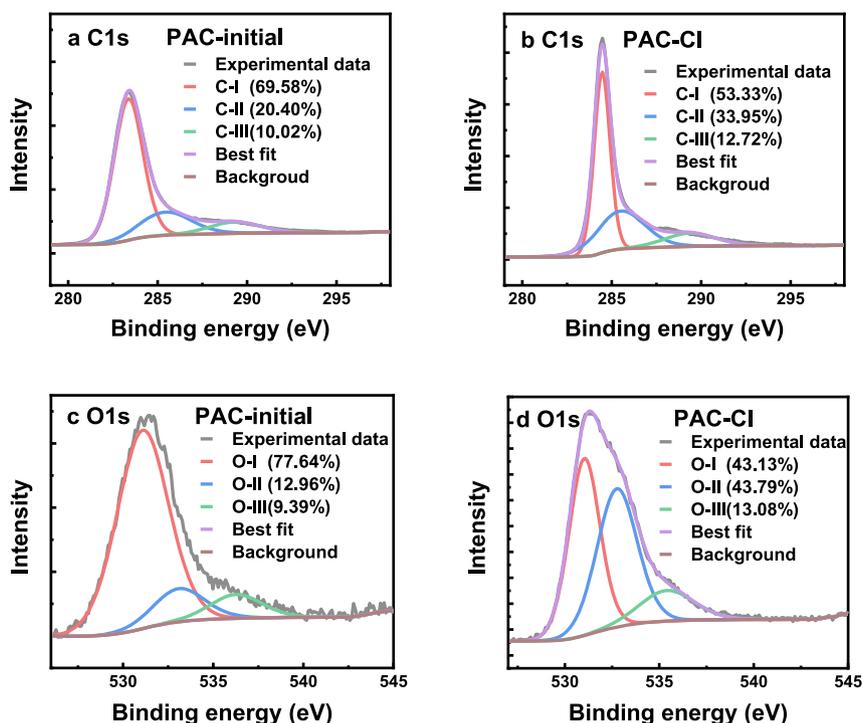
Fig. 3. XPS spectra of initial PAC (PAC-initial) and PAC after chlorination (PAC—Cl) with peaks of C 1 s (a-b) and O 1 s (c-d).

Table 1
The surface C/O/N/Cl contents of PACs.

	C (%)	O (%)	N (%)	Cl (%)
PAC-initial	90.64	8.42	0.79	0.15
PAC—Cl	83.45	15.32	0.64	0.60

Table 2
FTIR spectra bond assignments of PAC-initial and PAC—Cl.

	Wavenumber (cm^{-1})	Assignments	Reference
PAC-initial	3350	O–H stretching by the hydroxylic group and chemisorbed water	(Pradhan and Sandle, 1999)
	3050	C-H stretching in aromatic compounds	(Yang et al., 2021)
	1120	C–O stretching in acids, alcohols, phenols, ethers, and/or esters groups	(Boehm, 1971; Torrellas et al., 2015)
PAC—Cl	1650–1900	residual water vapor	(Torrellas et al., 2015)
	1550	combination of carboxyl C=O stretching of non-aromatic carboxylic acid and lactone structures	(Du et al., 2016)
	1200–900	C–O stretching in acids, alcohols, phenols, ethers, and/or esters groups	(Boehm, 1971; Torrellas et al., 2015)
	646	C–Cl stretching	(Du et al., 2016; Wang et al., 2012)

Da, while after 12 h, the Mw of the organics decreased to 100–4000 Da and most was mainly distributed below 1000 Da. Previous study has reported that the average Mw of high Mw DBPs formed by chlorination of HA was around 2000 Da (Zhang and Minear, 2002), which was similar with the product Mw after 72 h. In addition, the released organics also indicated that the chlorine would result in the destruction of the carbon structure. Previous studies by Vinke et al. (1994) and Yang

et al. (Yang et al., 2010) also demonstrated the chlorine could change the carbon surface. Thus, it could be inferred that the chlorine destructed the structure of the carbon and released some large Mw compounds into the solution and then leading to transformations into smaller molecules and DBPs. Therefore, it required further understanding of the usage of PAC and the pre-chlorine at the same time.

3.1.2. Characterization of PAC after chlorination

As shown in Fig. 2 and 3, the surface functional groups of PAC after chlorination (PAC—Cl) were more abundant than those of PAC-initial. The principal band and their corresponding functional groups obtained from FTIR spectrum are compared in Table 2. The XPS also indicated that the surface oxygen content was increased after chlorination as shown in Table 1. The surface chlorine content slightly increased from the 0.16% to 0.60%, which also proved that the chlorine might react with the carbon. The Cl2s peak was too small to be deconvoluted and therefore only the C1s and O1s peaks of these PACs and their deconvolution are presented in Fig. 3. After reaction with chlorine, the proportions of C-II/C-III group and O-II/O-III group increased, especially C-II and O-II groups, which was in agreement with the FTIR results. Thus, it could be inferred that on the carbon surface, the phenolic, alcohol and ether group which contained the C—OH and C-O-C bond increased after chlorination.

Though the precise structure of the PAC is still unknow, the functional groups at the edges could be deduced through different analytical method. Previous studies have proved PAC was comprised of carbon platelets, and several functional groups on the surface (Bhatnagar et al., 2013; Wang et al., 2020). The surface functional groups were similar with the NOM, mainly contained oxygen and hydrogen. Thus, the formation of THMs and HAAs with PAC and NOM might be analogous. The meta-positioned –OH groups could play significant roles in the production of THMs and HAAs (Dynamics, 2008; Johannes and Rook, 1977. The proposed degradation pathways of PAC and formation of TCM and HAAs are shown in Fig. 4. In addition, it could be noted that after the chlorination, the -OH might bind with the carbon surface, which was consistent with the FTIR and XPS results.
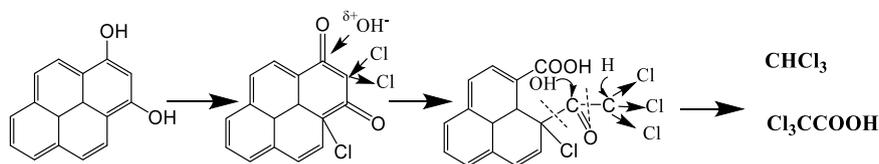
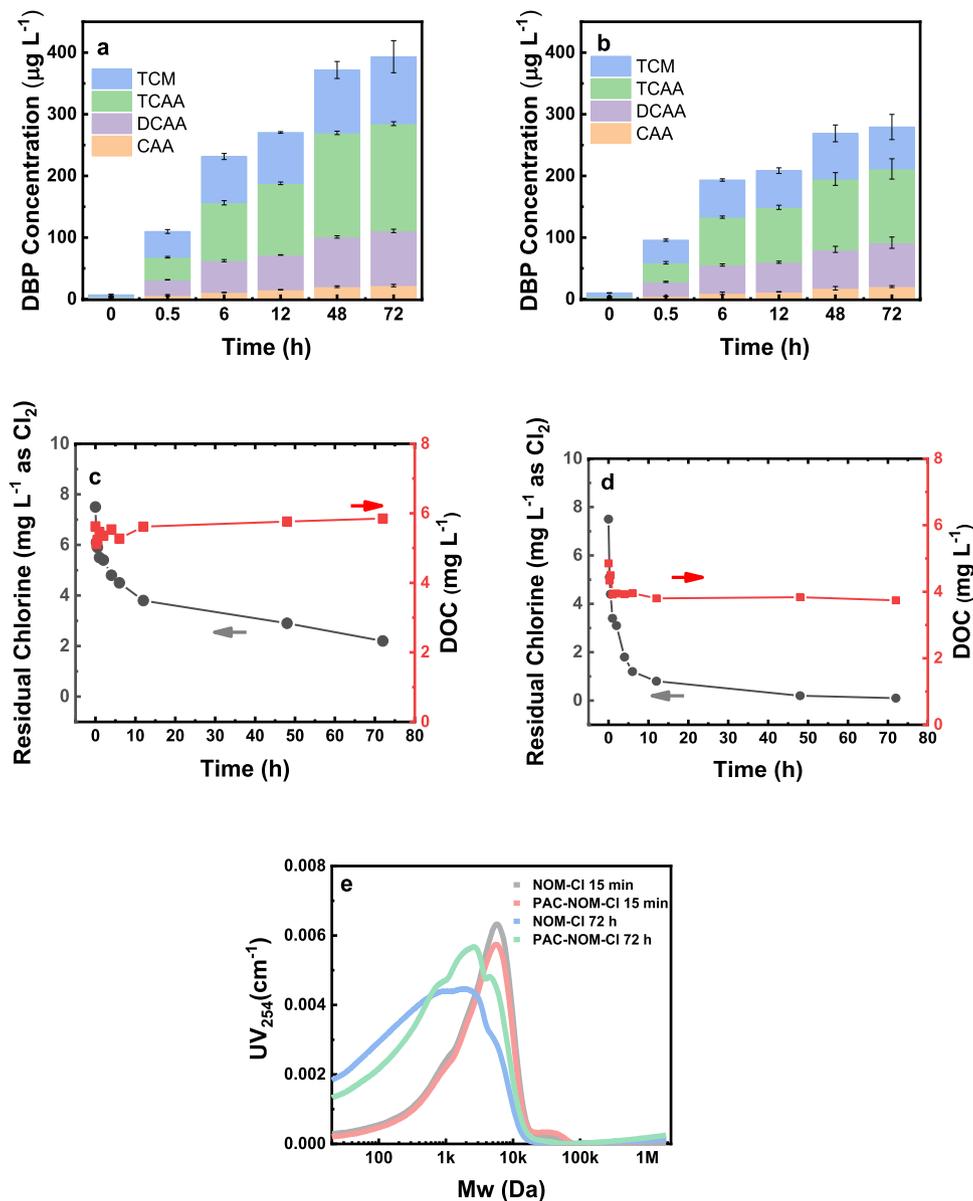**Fig. 4.** Scheme of DBP formation with PAC.

Fig. 5. a-b. Formation potential of TCM and HAAs from chlorination of NOM without (a) and with (b) PAC; c-d. Residual chlorine and DOC concentration during chlorination of NOM without (c) and with (d) PAC; e. the organics Mw in the solution released from the chlorination of NOM with and without PAC.

3.2. DBPs formed by NOM with and without PAC

The DBP formation with and without PAC in HA water was compared as shown in Fig. 5. It could be noted that for the chlorine decay rate with the presence of PAC was more rapid than that without PAC. However, though the consumption of chlorine was more rapid and PAC itself could act as the DBP precursors, the DBPs concentration in the solution with the presence of PAC was lower. One possible reason might be that the formed DBPs were adsorbed by the PAC. As shown in Fig. S3, after ultrasound, the adsorbed DBPs were released from PAC and the

concentrations of TCM and HAAs on PAC were calculated to be approximately 12 and 4 μg g^{-1}. However, even after combining the amount of DBPs on the PAC surface, the total amount of DBPs with PAC was still less than that without PAC. Therefore, it could be inferred that the consumption of chlorine might lead to other products rather than the commonly known DBPs such as TCM and HAAs, which also had been proved by the previous studies (Voudrias et al., 1987, 1985), and they found that with the presence of PAC, a series of free radical chain reactions were occurred. This phenomenon had also been proved by the electron spin-resonance spectroscopy results as shown in Fig. S4. It could
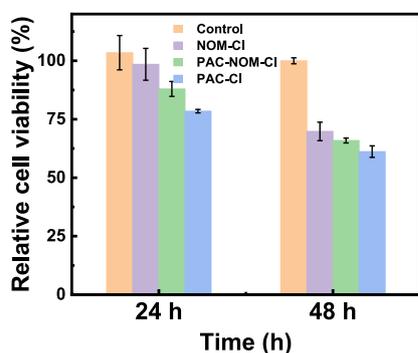
Fig. 6. The relative cell viability of NRK 52[E] cells exposed to NOM-Cl, PAC—NOM-Cl and PAC—Cl solution for 24 h and 48 h.

be noted that with the presence of PAC, the free radical was much stronger than chlorine with NOM alone. In addition, as shown in Fig. S5, the chromatograms corresponding to the two systems were obviously different, which could confirm that different by-products were formed by the chlorination of PAC.

The DOC concentration without the PAC was kept almost stable around 6 mg L^{-1}, while the HA was adsorbed by the PAC in the PAC—NOM-Cl system with a reduction of DOC concentration. As for the Mw of the organics in the solution, at the first 15 min, the Mw was almost the same for NOM-Cl and PAC—NOM-Cl. At 12 h, the Mw of the organics was slightly different. The compounds in the NOM-Cl exhibited smaller Mw compared with those in the PAC—NOM-Cl, which might be because the smaller organics were more easily adsorbed by the PAC, or different products were formed in these two different situations.

3.3. Toxicity of DBPs with and without PAC

Though the generation of known DBPs including THMs andHAAs was fewer, other unknown products could be generated with the presence of PAC, and their toxicity should be more concerned by the public. Therefore, the MTT assay was used to measure the toxicity of different substances produced by the PAC alone with chlorine, and the NOM chlorination with and without PAC.

As shown in Fig. 6, for the acute toxicity in 24 h and 48 h, the products formed by PAC alone with chlorine demonstrate the highest cytotoxicity with a cell viability reduction of 30%, followed by PAC—NOM-Cl and the NOM-Cl. It could also be deduced that the new products formed by the PAC alone and chlorine was more toxic than the common DBPs formed by chlorine and NOM. Thus, the PAC alone with chlorine presented the highest toxicity, and PAC—NOM-Cl also contained certain amount of such new substance formed by the PAC and chlorine, exhibiting the median toxicity.

In addition, another study by Cuthbertson et al. (2019) has proved that the combination of pre-chlorination and GAC filtration was effective in DBPs and toxicity control. In that study, the pre-added chlorine should already be depleted by coagulation/flocculation-sedimentation-sand filtration process and when reaching the GAC filter, the residual chlorine concentration was negligible. They found that the GAC was more effective in removing chlorinated-NOM rather than the original NOM and less toxic DBPs were formed after GAC adsorbed the DBP precursor. In our study, the chlorine was directly contacted and reacted with PAC, and more toxic products were formed by the free radical reaction catalyzed by PAC (Huang et al., 2021). As suggested by McCreary et al. (1982), the activated carbon promoted the reaction of free chlorine with phenolic acids to produce a variety of oxidized products, such as polyphenols and quinones, which were not produced by simple aqueous phase reaction between chlorine and phenolic acids in the absence of carbon. Voudrias et al. (1987, 1985) also reported that free chlorine reacted with phenols adsorbed on GAC, many additional products including chlorohydroxybiphenyls (hydroxylated
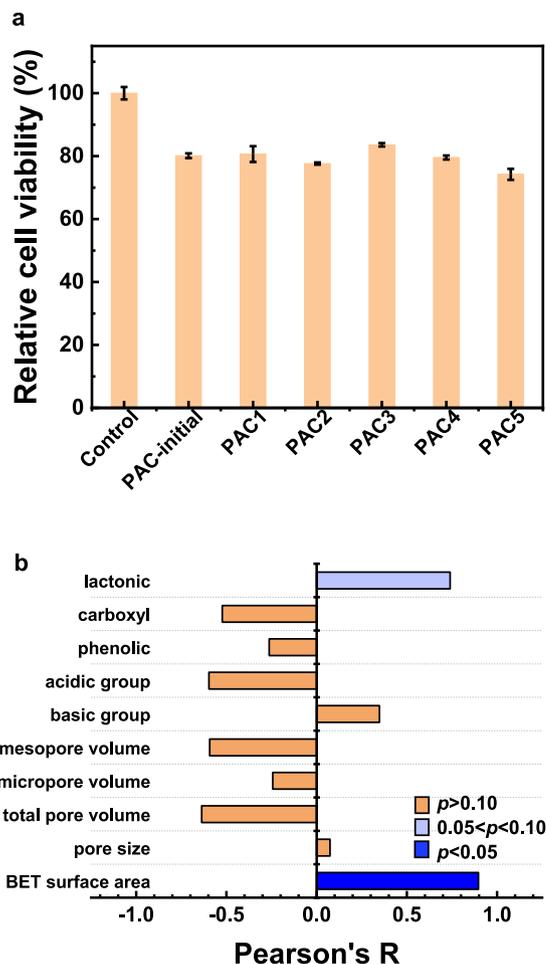

Fig. 7. a. The relative cell viability of NRK 52[E] cells exposed to products of chlorination of various PACs; b. the correlations between relative cell viability and PAC properties.

PCBs) were formed, which were not detected in the direct reaction between chlorine and dilute phenols solution. As indicated by the toxicity test the additional by-products formed through the free radical reaction between PAC and chlorine were more toxic. Thus, it is better to apply pre-chlorination before PAC adsorption for the sake of toxic DBP control.

3.4. The effect of PAC properties on the by-products toxicity

As mentioned above, the chlorine reaction with PAC was somewhat different from its reaction with NOM because there were free radical chain reactions between the PAC and chlorine. The toxicity effects of by-products in the presence of various PACs and the correlations between PAC properties and the toxicity were evaluated as shown in Fig. 7. The chlorine decay rates with the presence of various PACs were also compared as shown in Fig. S6. It could be noted that the physical properties, such as the pore size and pore volume did not exhibit any significant correlations with the relative cell viability, and only the BET surface area was positively correlated with the relative cell viability with significance at the $p = 0.05$ level. As for the different surface functional groups, there was only positive correlation between lactones and the relative cell viability ($p = 0.10$). Other PAC surface functional groups including basic groups, acidic groups, phenolic hydroxyl group and carboxyl group do not show any significant correlations with relative cell viability.

The toxicity of the DBPs formed by PAC chlorination might be influenced by two factors: one was the DBP adsorption capacity of PAC, which might impede the releasing of DBPs; the other one was the PAC

surface functional groups which might impact the formation of DBPs. Therefore, the carbon with higher BET surface area might adsorb the products more easily and resulted in releasing less toxic products. The carbon with more lactonic group might be less active to the chlorine than that with more phenolic hydroxyl and carboxyl groups (Deborde and von Gunten, 2008). Therefore, it could be deduced that the carbon with higher surface area and more lactonic group released less toxic by-products.

4. Conclusion

This study investigated the DBP formation and toxicity by the reaction between PAC and chlorine. The PAC itself could act as DBP precursor and react with chlorine to form DBPs including THMs and HAAs and other variants. The released THMs and HAAs were also reduced by the PAC adsorption, and thus when NOM reacted with chlorine, the detected THMs and HAAs in the solution with PAC were less than those without PAC. However, though PAC could adsorb DBPs and control their release in the solution, the different reaction products resulted from free radical reaction with the presence of PAC were more toxic than those without PAC. In addition, the products formed by PAC with higher surface area and more lactonic groups were less toxic. Above all, this study can provide guidance for selecting appropriate PAC type to reduce toxic effects from DBPs for treatment plants using pre-chlorination.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.watres.2021.117660.

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