Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Phosphate functionalized activated carbon sachet filters for drinking water purification

Table S1: XPS test parameters for a survey and narrow scan

Test parameters	Survey scan	Narrow scan
Energy scale	Binding	Binding
Pass energy/eV	150	20
Number of scans	4	5
Dwell time/ms	10	50
Lens mode	standard	standard
Energy step size/eV	1	0.05

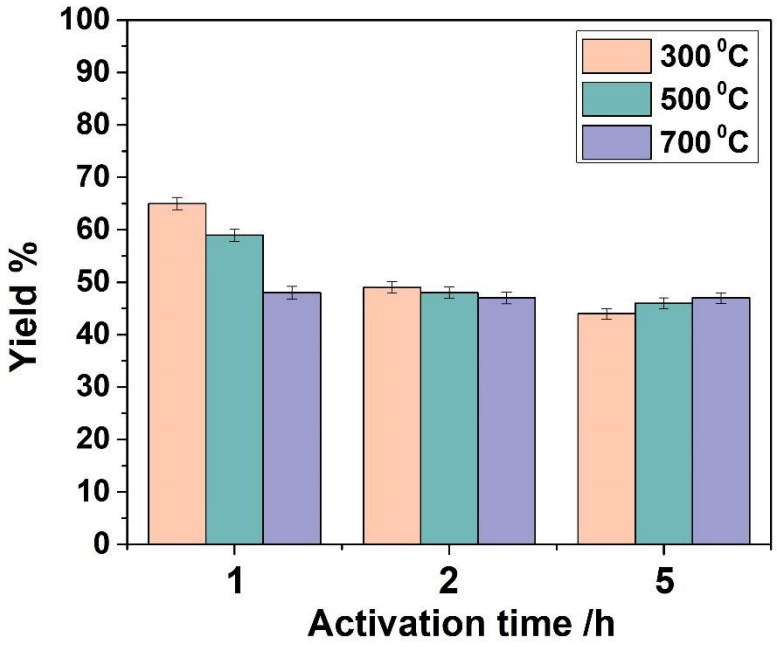

Figure S1: Percentage yield of FAC synthesized by vapor activation method at different activation time and temperatures

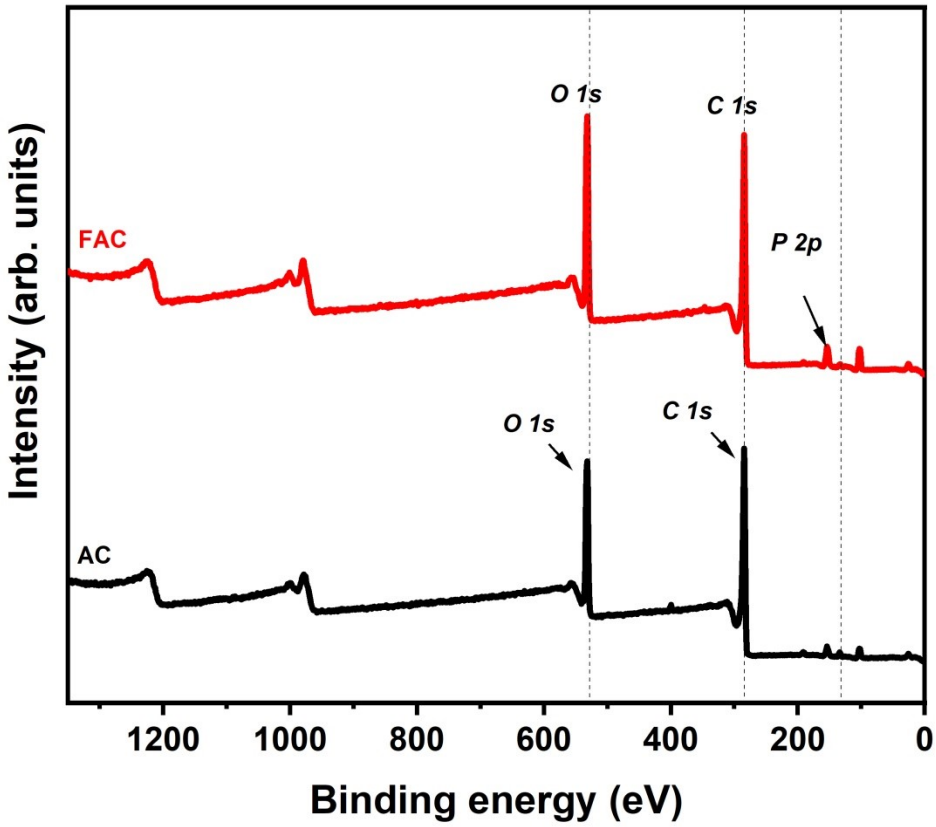

Figure S2: XPS survey spectra of AC and FAC

Table S2: FTIR functional groups with corresponding wavenumbers

Functional Groups	Wavenumber/cm^{-1}	
	AC	FAC
O-H stretching vibration	3384	3201
C–H hydroxyl groups asymmetric stretching	2923, 2860	-
C=C vibrations	1593	1575
-C=O stretching vibrations	1700	1752
C-O asymmetric stretching	1240	1195
P-O-P	-	1080

Table S3: XPS quantitative results for AC and FAC

Peak	Binding energy (eV)		Chemical state
	AC	FAC	
C 1s	286.25	286.45	carbon species in alcohol, phenols, ether groups, C-O-P and/or C-O-C linkage
C 1s	284.75	284.80	graphitic sp^2 carbon
C 1s	288.30	291.40	carbon species in carboxylic groups or esters (C-O-P and/or C-O-C bonds)
O 1s	531.85	533.25	singly bonded oxygen in C-OH, C-O-C and/or C-O-P groups
O 1s	533.40	534.80	non-carbonyl oxygen in carboxylic groups
P 2p	-	133.54	phosphates, pyrophosphates and phosphonates
P 2p	-	134.20	metaphosphates and phenyl-phosphate

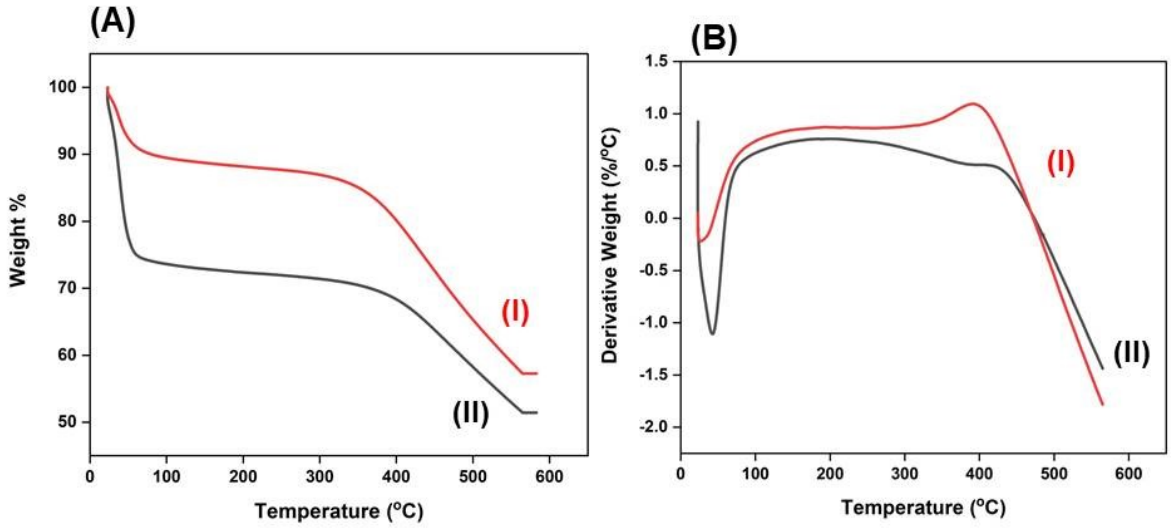

Figure S3: (A) TGA and (B) DTA curve of (I) FAC and (II) AC

Weight loss profile of FAC and AC recorded under N_2 environment with a 10 °C/min heating rate from 50 °C to 700 °C as shown in Figure S4. It can be understood from the graph that three stages of weight loss take place in both activated carbons. The primary weight loss in the range of 50–100 °C is due to moisture weight loss (7.8%). Major decomposition (46.2%) in the second stage between 100 °C and 400 °C is due to loss of chemically bound water, lignin, cellulose and hemicellulose. On further heating above 400 °C, nearly 25% weight loss due to the decomposition of the carbon compounds to volatile gases like CO and CO_2 was observed. According to DTA curves, as the temperature increases, phosphate groups are converted to several species, such as pyrophosphoric acid ($H_4P_2O_7$) and polyphosphoric acid by condensation and dehydration and eventually P_2O_5. The evaporation of P_2O_5 occurs at a temperature between 400 °C and 500 °C.

Table S4: Hardness and fluoride removal in selected sample locations after treating with activated carbon synthesized by phosphoric acid soaking method

Selected Sample Location	Latitudes and Longitudes	Hardness removal (mg/L) (±0.01)		Fluoride removal (mg/L) (±0.001)	
		Initial	Final	Initial	Final
Ipologama	8°06'03.4"N 80°30'35.0"E	413.5	269.68	0.598	0.407
Galkulama	8°16'18.5"N 80°29'54.8"E	446.22	226.34	2.430	1.5630
Mahailluppallama	8°06'10.5"N 80°28'19.0"E	556.59	327.57	1.590	0.936
Kiribathwehera	8°23'57.1"N 80°23'59.6"E	327.87	262.96	0.808	0.542
Galpalama	8°23'56.4"N 80°24'21.6"E	485.13	269.59	1.710	1.490
Alapathwewa	8°23'32.8"N 80°48'14.0"E	338.82	241.96	1.010	0.645
Hadagaswewa	8°29'42.1"N 80°11'19.9"E	295.97	212.64	1.390	1.023
Thuruwila	8°13'27.1"N 80°26'21.0"E	579.33	249.1	1.310	0.861
Kahatagasdigiliya	8°35'12.4"N 80°41'10.4"E	253.82	206.06	1.480	0.986

Table S5: XPS spectral results of FAC before and after Calcium, Magnesium and Fluoride ion adsorption

Region	Peak position/ eV			
	FAC	FAC-Ca	FAC-Mg	FAC-F
C 1s	286.45	284.85	286.25	284.80
O 1s	534.30	532.05	534.25	532.05
P 2p	135.65	134.05	136.25	133.55

Table S6: Deconvolution results of XPS spectra of FAC before and after Calcium, Magnesium and Fluoride ion adsorption

Region	Peak position/ eV				Assignment
	FAC	FAC-Ca	FAC-Mg	FAC-F	
C 1s	284.80	284.85	284.80	284.80	graphite
	286.45	286.3	286.30	286.45	R-OH, C-O-P and/or C-O-C
	288.30	289.45	288.40	288.90	COOH, -C(O)-O-C
	291.40	-	290.55	-	π-π^*
O 1s	533.25	532.00	533.60	531.20	C-OH, C-O-C and/or C-O-P
	534.80	533.75	535.05	533.00	non-carbonyl oxygen in -COOH
P 2p	133.54	132.70	-	133.55	phosphates, pyrophosphates and phosphonates
	134.20	134.05	135.95	134.70	metaphosphates and phenyl-phosphate
	-	-	136.80	-	P_2O_5

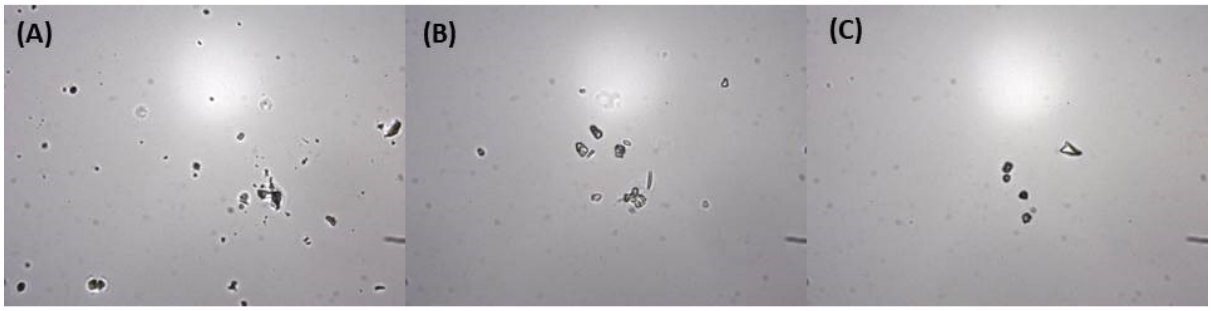

Figure S4: Light microscopic images of water (A) before treatment of FAC (B) After 20 min (C) After 24 h

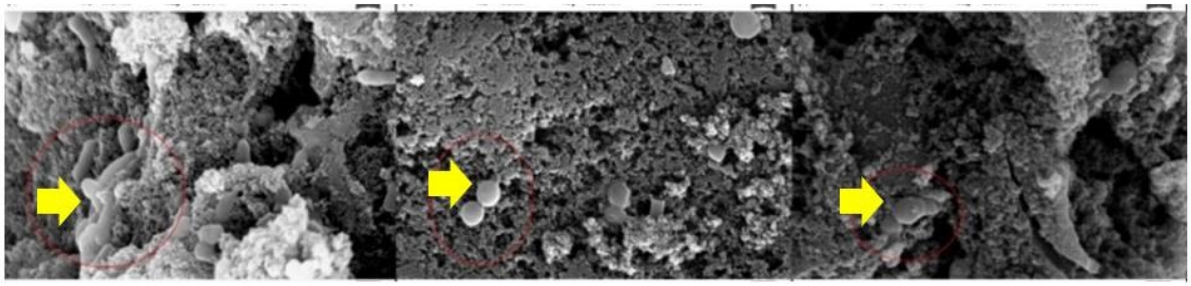

Figure S5: SEM images of water pathogens after treatment of FAC for 20 min

Table S7: Parameters of kinetic models of Calcium, Magnesium and Fluoride adsorption on FAC

Initial concentration (mg L^{-1})	$q_{e,exp}$ (mg g^{-1})	Pseudo-first-order kinetic model			Pseudo-second-order kinetic model		
		$q_{e,cal}$ (mg g^{-1})	K_1 (min^{-1})	R^2	$q_{e,cal}$ (mg/g)	K_2 (g mg^{-1} min^{-1})	R^2
Calcium							
50	7.67	2.62	0.0121	0.9610	8.01	0.0026	0.9983
100	25.802	8.50	0.0104	0.9603	25.90	0.0032	0.9916
250	29.85	13.77	0.0104	0.961	30.03	0.001	0.999
350		15.47	0.0093		33.11		

	32.60			9 0.9189		6 0.0017	4 0.9979
Magnesium 50 100 250 350	6.25 12.47 32.87 40.36	1.11 3.42 9.78 7.09	0.0094 0.0090 0.0131 0.0090	0.9637 0.9714 0.9886 0.9717	6.37 12.77 32.89 40.48	0.0026 0.0065 0.0027 0.0041	0.9978 0.9993 0.9976 0.9970
Fluoride 1 1.5 2 2.5	0.11 0.16 0.20 0.28	0.05 0.08 0.08 0.23	0.0098 0.0105 0.0094 0.0178	0.9743 0.9713 0.9629 0.9642	0.12 0.18 0.21 0.27	0.0156 0.0324 0.0441 0.0729	0.9984 0.9982 0.9972 0.9985

Table S8: Correlation coefficients (R2) and constants for the Langmuir and Freundlich isotherms for Calcium, Magnesium and Fluoride adsorption on FAC

Adsorbate	Langmuir Isotherm			Freundlich isotherm		
	Q_o (mg g^{-1})	K_L (L mg^{-1})	R^2	K_F (mg g^{-1}(L mg^{-1})$^{-1/n}$)	n	R^2
Calcium	48.26	0.01009	0.9895	1.28416	1.61	0.9989
Magnesium	518.13	0.00050	0.9969	0.36121	1.11	0.9988
Fluoride	1.43	0.17523	0.9868	0.18775	1.47	0.9980

Method S1 - Antimicrobial susceptibility testing for FAC and AC

- **Preparation of standard bacterial cell suspensions**

Stock cultures of three test strains, *E. coli* (ATCC 25922), *Salmonella typhi* (ATCC 19430) and *Shigella flexneri* (ATCC 9199) were subcultured on sterile, freshly prepared Brain Heart Infusion (BHI) agar plates and incubated at 37 ^oC for 24 h to get fresh isolated colonies. Sterile BHI broth (10 mL) was inoculated with few isolated colonies of test strains separately and incubated at 37 ^oC for another 24 h. The absorbance of resultant 24 h broth cultures was adjusted to 0.5 McFarland turbidity standards to prepare standard cell suspensions with 1.5×10^8 CFU/mL cell density.

- **Antimicrobial screening**

Screening of antimicrobial activity of the FAC was carried out using agar diffusion method against three common water pathogens, *E. coli* (ATCC 25922), *Salmonella typhi* (ATCC 19430) and *Shigella flexneri* (ATCC 9199). Briefly, Mueller-Hinton agar (MHA, OXOID) plates were inoculated with prepared standard cell suspensions using a sterile cotton swab in order to obtain a confluent bacterial growth on agar surface. Then, 1.0 mg of particles (FAC

and AC) was placed on the middle of the plates. These plates were then aerobically incubated at 37 ^{o}C for 24 h followed by visual inspection of agar surface for growth inhibition around embedded particles. Bacterial susceptibility to the relevant treatment was indicated by the presence of growth inhibition zone on agar surface (any size).

- **Minimum inhibitory concentration (MIC)**

Minimum concentration of FAC required to inhibit the planktonic bacterial population (MIC) was determined using the broth dilution method with few modifications. Briefly, doubling dilutions of nanoparticles were prepared (1.25, 2.5, 5.0, 10.0, 20.0 and 40.0 mg/mL) separately in sterile bijou bottles (1mL/bottle) in sterile BHI broth. Exactly 1 mL of standard cell suspensions of *E. coli*, *Salmonella typhi* and *Shigella flexneri* were added to corresponding bottles and incubated at 37 ^{o}C for 24 h. After incubation, bottles were visually observed for the presence or absence of turbidity of the content (bacterial growth). The minimum concentration of the treatment with no turbidity of the content was considered as the MIC point for the relevant treatment.

- **Minimum bactericidal concentration (MBC)**

Minimum concentration of treatments required to kill a bacterial population completely was defined as MBC. After visual observation of the bottles as explained in 2.8.1., 10 µL aliquot from each bottle was sub-cultured on sterile BHI agar plate and incubated at 37 ^{o}C for 24 h to detect the presence or absence of viable bacteria. Minimum concentration of the treatments with no bacterial growth on agar surface after incubation was considered as MBC.

Method S2 - Engineering design for activated carbon manufacturing pilot plant using coconut coir dust

As the final step, a pilot plant for activated carbon manufacturing was designed with a production capacity of 5 kg (FAC) per day from ground up. (Figure S6) In this regard, the scaling up of the process of synthesizing FAC is beneficial and straightforward.

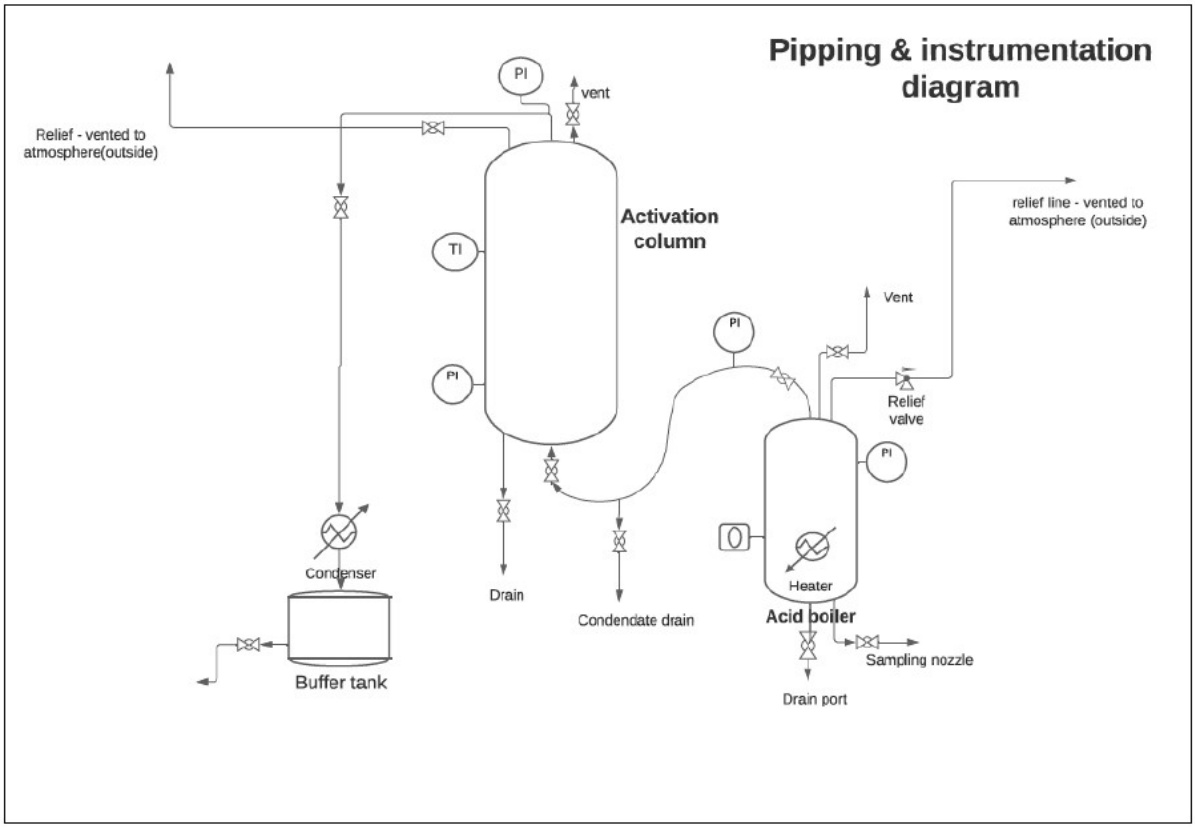

Figure S6: Piping and instrumentation diagram for the scale up design to produce functionalized activated carbon