1 **Analysis and Modelling of Powdered Activated Carbon Dosing** 2 **for Taste and Odour Removal**

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13 **Abstract:** A series of experiments were undertaken in order to
 14 understand and predict the dosage of powdered activated carbon
 15 required to remove taste and odour compounds in an Australian
 16 drinking water treatment plant. Competitive effects with organic
 17 matter removal by aluminium sulphate during coagulation were also
 18 quantified. Data on raw and finished water quality following jar tests,
 19 as well as chemical dosages and treatment performance, were
 20 statistically analysed, and a data-driven prediction model was
 21 developed. The developed powdered activated carbon dosage
 22 prediction model can be used by the plant operators for rapid dosage
 23 assessment and can increase the preparedness of the plant to sudden
 24 taste and odour events. It was also found that total organic carbon
 25 levels and properties greatly affect the ability of powdered activated
 26 carbon to remove taste and odour compounds; on the other hand,

27 total organic carbon removal is not affected by high taste and odour
28 levels, since these were still much lower than organic carbon
29 concentrations.

30 **Keywords:** Data-Driven Modelling; Powdered Activated Carbon;
31 Taste and Odour; Water Treatment Optimization

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54 **1. Introduction**

55 *1.1 Powdered Activated Carbon for Taste and Odour removal*

56 Within drinking water, there are a number of compounds that can
57 cause taste and odour (T&O) problems for water suppliers. The two
58 main compounds that are commonly associated with such T&O
59 issues are 2-methylisoborneol (MIB) and geosmin (Matsui et al.
60 2013a). In order to reduce the T&O produced by these two
61 compounds, powdered activated carbon (PAC) is typically added to
62 the raw water during the water treatment process; this is because its
63 sponge-like properties are ideal to absorb organics, including MIB
64 and geosmin (Thiel and Cullum 2007).

65
66 Generally, PAC is added at the head of the water treatment plant
67 (WTP), as this allows for the longest contact time possible before
68 other treatment chemicals are added. The effectiveness of the
69 absorbance qualities of PAC is influenced by a number of different
70 factors. These factors include the presence of natural organic matter
71 (NOM) in the raw water, PAC properties (e.g. pore structure, surface
72 area, raw material, bulk density and particle size), and water
73 treatment processes.

74
75 In terms of NOM, MIB and geosmin both have a relatively low
76 molecular weight (MW) and therefore low MW NOM could
77 effectively compete with the T&O compounds for adsorption sites. In
78 terms of PAC properties, pore structure and raw material can affect
79 its removal efficacy: optimal adsorption of T&O compounds is seen
80 with PAC having bimodal pore distribution (Newcombe et al. 2002),

81 which is generally seen in coal-based carbons (Thiel and Cullum
82 2007). PAC surface area is also important, being proportional to the
83 ability to adsorb organic contaminants (Thiel and Cullum 2007).
84 Bulk density of PAC is another critical factor; it is related to the
85 physical weight per volume of powder and it can affect the speed of
86 adsorption (Thiel and Cullum 2007). This is because PAC dosing is
87 undertaken by weight, and thus a PAC with lower bulk density would
88 be added in greater volumes. Adding a higher volume of carbon
89 would imply a larger surface area of PAC within the water, allowing
90 for higher adsorption of micro-pollutants (Thiel and Cullum 2007).

91
92 A number of research studies investigated the adsorption capacity of
93 different PACs based on a range of conditions. These are described
94 and summarized in the next sections.

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96 *1.2 Research on competitive effects of natural organic matter*

97 The study by Newcombe et al. (2002) focused on the simultaneous
98 adsorption of MIB and NOM onto activated carbon. The effects of
99 six different PACs on the removal of MIB were tested in the presence
100 of six known NOM solutions. It was found that low MW NOM
101 compounds had the highest competitive effect on the adsorption of
102 MIB onto PAC, as they directly compete with MIB for adsorption
103 sites. A number of similar studies were conducted, such as by
104 Graham et al. (2000); the experiments were run as equilibrium dual-
105 solute adsorption systems, and it was found that the adsorption of
106 both MIB and geosmin were a magnitude lower compared to the
107 adsorption in a single solute adsorption system; thus showing that the

108 presence of NOM has a significant effect on the adsorption of MIB
109 and geosmin onto PAC. In another study completed by Matsui et al.
110 (2013b), the mechanism responsible for the competitive effect
111 between NOM and MIB was investigated with respect to the
112 properties of NOM. It was concluded that NOM with a high MW and
113 a chromophoric moiety, would adsorb onto the external surface of the
114 carbon, whilst low MW and non-chromophoric NOM adsorbs onto
115 the internal surface. The NOM that competes with geosmin, as well
116 as MIB, was found to be a very low MW chromophoric NOM which
117 is also preferentially adsorbed onto the internal surface of the PAC,
118 thus competing with MIB and geosmin for adsorption sites (Matsui
119 et al. 2013b).

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121 *1.3 Research on adsorption capacity based on PAC type*

122 Thiel and Cullum (2007) evaluated the performances of 12 different
123 PACs in reducing a commercial spike of MIB and geosmin in natural
124 raw water through the use of jar tests; it was found that contact time,
125 raw water characteristics and PAC properties all had a significant
126 influence on the spike reduction. Additionally, geosmin was more
127 easily removed compared to MIB for all of the carbons that were
128 tested (Thiel and Cullum 2007), in line with findings of other studies
129 (Zoschke et al. 2011). In a study completed by Yu et al. (2007), the
130 focus was on investigating the effects of PAC surface characteristics,
131 by conducting experiments using 5 different types of PAC. It was
132 concluded that the volume of PAC micropores was an effective
133 indicator for the selection of the type of PAC to use in the removal of
134 MIB and geosmin (Yu et al. 2007). In another research study by

135 Matsui et al. (2013a), it was found that, over a given contact time,
136 T&O removal was greatly enhanced through the use of superfine
137 powdered activated carbon (SPAC), which has a smaller particle size
138 compared to PAC, but is not commercially available. Furthermore, it
139 was discovered that the required dose of PAC to achieve a certain
140 percentage of MIB or geosmin removal decreased linearly with
141 carbon particle size until a critical threshold value of D40. D40 refers
142 to a characteristic diameter through which 40% of the particles, based
143 on volume, can pass (Matsui et al. 2013a). A similar study completed
144 by Ando et al. (2010) also evaluated the adsorption capacities of both
145 SPAC and conventional PAC. Similarly to Matsui et al. (2013a), it
146 was found that there was a considerable increase in the adsorption
147 capacity for NOM using SPAC compared to conventional PAC. It
148 was concluded that this increase in adsorption capacity was due to
149 the difference in particle sizes between the two carbons. The
150 difference in adsorption capacities between SPAC and conventional
151 PAC was greater for NOM that had a higher specific UV absorbance
152 value compared to NOM with a low specific UV absorbance value.
153 Another study of a similar nature completed by Matsui et al. (2012)
154 investigated the competitive adsorption characteristics between MIB
155 and NOM on both SPAC and PAC. It was discovered that adsorption
156 competition between NOM and MIB did not increase with the
157 increased NOM uptake, because of the reduction in the particle size
158 of the carbon (Matsui et al. 2012).

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160 *1.4 Research on competitive effects due to other water treatment*
161 *processes*

Another factor affecting the adsorption of MIB and geosmin onto PAC, is the amount of coagulant used in conjunction with the PAC during the water treatment processes. For instance, a study by Seckler et al. (2013) found that the removal efficiency of MIB was higher when only PAC was added at the highest dosage, and a clear interference was noticed when the coagulant ferric sulphate was added, due to the precipitation of the coagulant during the adsorption process. This caused the coagulant to coat the surface of the PAC, thus interfering with the MIB coming into contact with the surface and pores of the PAC. The degree of interference was proportional to the ratio of coagulant mass to PAC mass (Seckler et al. 2013). Another study by Townsend (2016) investigated the coagulation kinetics and the effects of the coagulant on downstream processes, particularly on the removal of T&O using PAC. PAC was added at a number of different contact points before, during and after coagulation. It was found that the PAC most effectively removed MIB when added prior to coagulation. Whilst earlier PAC addition allows for higher MIB removal, this also requires large reactors, thus increasing the capital cost of the WTP (Townsend 2016).

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182 *1.5 Research Objectives*

Given the issues discussed in the previous sections, it can be seen that there are many interacting factors affecting the efficacy of PAC for T&O removal, and thus estimating the required dosage is as difficult as important for a drinking WTP. Therefore, the objective of this project was to determine a procedure for optimal PAC dosing estimation to remove organic contaminants (mainly T&O

189 compounds) for a drinking WTP in South-East Queensland,
190 Australia, to a standard that complies with Australian drinking water
191 (ADWG 2016). The project builds from outcomes of previous
192 research and from a number of laboratory experiments conducted and
193 discussed below; data analysis was then performed among inputs
194 (mainly raw water quality) and outputs (PAC dose, T&O removal) in
195 order to identify the most important predictors for the optimal PAC
196 dosage.

197 **2. Materials and Methods**

198 As this project involves various components, the methodological
199 approach is described below in the following sections: water
200 sampling, preliminary bench tests, jar tests, final tests, data analysis
201 and modelling.

202 *2.1 Water sampling*

203 Through collaboration between Seqwater, the main bulk water
204 supplier in South-East Queensland, and Griffith University, it was
205 possible to collect raw water samples and undertake analyses in
206 Seqwater laboratories. In order to determine the optimal PAC dose
207 required to efficiently remove MIB and geosmin, samples were
208 collected from the Capalaba WTP. This plant receives water from
209 Lake Tingalpa, bounded by Leslie Harrison dam, which is located 20
210 km south-east of Brisbane, in Queensland, Australia (Figure 1).

Figure 1. Capalaba WTP location

The raw water samples that were analysed for this project were collected from the Raw SP120 tap at Capalaba WTP on a weekly basis during the 2016/17 summer season (December-February) and the 2017 winter season (July-August). In order to complete the tests required for this project, every week 20 litres (L) of raw water were collected. This was done after letting the water run for approximately 5 minutes before filling two 10L water containers, in order to allow for the water to flush out the contaminants.

2.2 Preliminary bench tests

The quality of the raw water was tested on the same day of the undertaken sampling. Before these samples were spiked with MIB and geosmin, four different bench tests were conducted, namely: (1) pH, (2) turbidity, (3) true colour and (4) UV_{254} . The pH of the raw water was determined with a pH sensor. Turbidity was determined by using a HACH 2100N turbidimeter. A HACH DR2700 colorimeter was used to determine the true colour. To determine UV_{254} , the

HACH DR6000 UV VIS Spectrophotometer with RFID Technology was utilised. These routine tests were conducted following Seqwater procedures.

2.3 Jar tests

Throughout the course of this project, various sets of jar tests were completed, including alum tests, alum and caustic soda tests and finally PAC, alum and caustic soda tests. The purpose of these tests was to estimate the efficacy of different amounts of such chemicals in improving the quality of the raw water, with a particular focus on PAC and T&O removal. Further jar tests were also conducted during this project in order to determine the effect of different organic carbon contaminants on the removal efficiency of T&O.

2.3.1 Jar Test Set-Up

The first sets of jar tests that were completed for this project only involved alum (i.e. aluminum sulphate). The doses that were added to each of the four 2L jars were estimated based on the quality of the raw water (especially colour and turbidity) as per Capalaba WTP guidelines. A stirring speed of 150rpm for 60 seconds, followed by a stirring speed of 30rpm for 40 minutes, was used. The settling time was 30 minutes, after which, a sample was taken for analysis. Since alum causes the pH of the treated water to drop significantly, a base (i.e. caustic soda) was added in order to raise back the pH of the water.

2.3.2 PAC Addition Approach

254 A number of different types of PAC were tested to see which one
255 was the most effective in adsorbing the T&O components. The
256 different types of PAC that were used were Acticarb PS1000,
257 PS1000F and PS1300. In order to compare each of these carbons, a
258 number of jar tests were completed, using different doses of PAC
259 whilst maintaining the same alum and caustic soda doses. The
260 required dosage for the jar test was estimated based on the current
261 Capalaba WTP procedure, which relies on the amount of MIB and
262 geosmin found in the raw water. In order to complete the jar tests, the
263 stirring and timing programs described in Section 2.3.1 were applied.
264 Then the PAC, alum and caustic soda were added immediately after
265 the “auto start” button was pressed. Some jar tests were completed in
266 order to look at the effects of PAC contact time on the effectiveness
267 of T&O removal; in these cases, the same jar test methodology was
268 applied, but the contact time was changed from 5 minutes to 3 and 1
269 minute.

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271 The next set of jar tests was performed in order to test the
272 effectiveness of the selected PAC (based on results of the jar tests
273 described in the previous section) on the removal of varying levels of
274 MIB and geosmin. In the initial jar tests the dosage of MIB and
275 geosmin that was used was 100ng/L for both compounds. For the
276 following set of jar tests, the MIB and geosmin were 50ng/L,
277 150ng/L and 200ng/L.

278 Another set of jar tests was conducted to assess the effectiveness of
279 the best PAC in the removal of MIB and geosmin in the presence of
280 varying levels of organic carbon contaminants. The initial total

organic carbon (TOC) levels that were detected within the raw water were between 7 and 8mg/L. In order to increase the initial TOC levels within the raw water, potassium hydrogen phthalate (KHP) was added as an organic carbon. TOC can affect T&O removal because it is present in much higher amounts than MIB and geosmin, and because some fractions of NOM can decrease the adsorption of T&O compounds through pore blockage and/or competitive adsorption mechanisms (Ho et al. 2007).

Another set of jar tests was completed in order to evaluate the effect of different alum dosages in the presence of PAC, along with the addition of humic acid, on the T&O removal efficiency. Raw water was spiked with MIB and geosmin along with doses of humic acid of 25mg/L and 50mg/L, representing organics levels that can be recorded during heavy rainfall events in Lake Tingalpa. Once the humic acids were added to the raw water and mixed thoroughly, the UV_{254} of the water was measured. From here, the jar tests were conducted as described previously. In this case, since the alum dose was being varied for this set of jar tests, the PAC was kept the same, at a dose of 30mg/L.

A final set of jar tests was completed in order to test the competitive adsorption effect that three different types of organic carbon contaminants (namely, potassium hydrogen phthalate, quinine and tannic acid) have on the removal efficiency of MIB and geosmin by PAC. The desired amount of organic carbon contaminant that was added to each of the jars was 0mg, 5mg, 10mg, 15mg, 20mg, 30mg,

40mg and 50mg. From here, the jar tests were completed in the same manner that was described previously with consideration to the contact time of the PAC. The concentration of PAC (30 mg/L) and alum (20mg/L) were kept constant and the type of PAC used (1300) was also unchanged over the course of these experiments.

2.4 Finished water tests

In order to test the quality of the treated water, a number of bench tests, which included pH, settled and filtered turbidity, true colour and UV₂₅₄, were completed with the same procedure and equipment described previously in Section 2.2. TOC and T&O levels were also re-measured.

2.5 Data analysis and prediction modelling

The collected data from all of the completed tests were collated into an Excel spreadsheet and analysed using linear and nonlinear regression approaches, for instance with a simplified version of the algorithm proposed in Bertone et al. (2015). The removal efficiencies of MIB, geosmin, TOC, turbidity, true colour and UV₂₅₄ were calculated and correlated to the chemicals' dosages, as well as raw water quality. To visually and simultaneously inspect multivariable correlations within the full dataset, Self-Organizing Maps (SOMs) (Kohonen 1998) were developed. These types of artificial neural networks allow for dimensionality reduction by creating, through unsupervised learning training, a two-dimensional discretized representation of the input space (i.e. a map). Through the map, an increased understanding of the system can be achieved by evaluating the covariance of the variables of interest (Blokker et al. 2016).

SOMs have been previously used by the authors in similar water treatment related research problems (Bertone and O'Halloran 2016, Bertone et al. 2016), and were created through the SOM Toolbox (Vesanto et al. 1999), in a Matlab2016a (Mathworks, Natick, MA, USA) programming environment. Given the results of the data analysis, linear and nonlinear regression models were then developed, based on combinations of the most relevant inputs in order to predict target variables (e.g. PAC dose, T&O removal). In comparison to past models, which had a more targeted process-based approach (e.g. in Cook et al. (2001), predicting T&O removal rates over time based on mainly fixed PAC doses and initial T&O concentrations), the applied data-driven approach allows for checking potential correlations among several different treatment conditions/ water quality data, and in turn building the best performing prediction model by accounting for the most significant predictors only.

3. Results

3.1. Data analysis results

In Figure 2, the SOM obtained for the collected dataset is presented. The variables are divided in blocks as follows (from top to bottom): raw water, treatment, finished water, treatment efficiency. The more similar the colour patterns between different variables are, the higher the correlation and similarities between them. For instance, the map for geosmin in raw water has similar colours to the one for MIB in raw water (e.g. yellow in the top left corners, blue in the bottom right corners), meaning that for the collected data (expectedly) both these

two T&O compounds were present in proportionally similar amounts
(i.e. when geosmin was high, MIB was high, and vice versa).

Figure 2. Self-organising map of the full dataset. Abbreviations not used elsewhere: Tb=turbidity (NTU); Tcol=true colour (HU); Tw=water temperature; Max WTP PAC= maximum PAC dosing capacity for Capalaba water treatment plant (mg/L)

Although there would be no need to develop a SOM to check for such simple and expected correlation, the full SOM allow to simultaneously check for multiple correlations and to notice less expected ones. Some of the main conclusions that can be drawn from the SOM analysis are:

- Higher PAC doses corresponded to higher true color and UV_{254} readings in the raw water, and match the usage of PAC PS1000 type.
- Expectedly, the lowest levels of true colour, UV_{254} , MIB and geosmin in the finished water were achieved when the highest dosages of PAC were added to the jars.

378 • The higher the contact time, the higher the removal efficiency by
379 PAC.

380 • The rate of removal of geosmin and MIB does not seem to be
381 affected by their initial concentrations; this is in line with results of
382 previous studies (Ho et al. 2007, Zoschke et al. 2011).

383 • In contrast with previous studies (Cook et al. 2001), turbidity
384 does not seem to play a clear, significant role in T&O removal.

385 • In terms of removal efficiency, geosmin seemed to be more
386 easily removed, followed by MIB and UV_{254} , and finally TOC. The
387 higher removal of geosmin compared to MIB is in line with previous
388 research outcomes (Zoschke et al. 2011) and may be due to a flatter
389 structure and lower solubility, thus making it more prone to be
390 adsorbed by PAC (Cook et al. 2001).

391 The fact that UV_{254} and true colour are reduced better than the overall
392 organic carbon, implicitly confirms the preferential removal of
393 aromatic, humic components of NOM as confirmed by previous
394 research (Chow et al. 2008, Krasner and Amy 1995). This is also
395 confirmed by a reduction in SUVA ($= UV_{254}/DOC$), i.e. a reduction
396 in the aromaticity and average MW of NOM after treatment (Page et
397 al. 2002). As a result, it is difficult to achieve near-total TOC
398 removal, as there will be always a fraction of TOC or DOC
399 recalcitrant to coagulation (Kastl et al. 2004, Van Leeuwen et al.
400 2005).

401 • Alum and caustic soda do not have any colour variation in the
402 figure, because they had a fixed dosage for all the experiments with
403 varying PAC.

404 *3.2. Competitive effects between TOC and T&O*

405 It is important to quantify how the PAC efficacy is affected by the
 406 competitive effects between T&O and NOM with similar low MW.
 407 Figure 3 shows how the removal of TOC changes, based on different
 408 amounts of T&O in the tested raw water, and different dosages of
 409 PAC. Lighter colours represent lower PAC dosages.

410

411 **Figure 3.** TOC removal efficiency based on total T&O and PAC
 412 dosage

413

414 One would expect a decrease in TOC removal with increasing T&O
 415 concentration in raw water since, given that the alum dose is fixed,
 416 two scenarios can occur;

417 (1) if the dosed PAC is sufficient for T&O removal, then it would
 418 help remove low MW dissolved organic matter (DOM) which cannot
 419 be removed by the dosed alum;

420 (2) if instead too much T&O is present, then PAC might not be
 421 enough to even remove all T&O and help with TOC, thus less TOC
 422 removal would be achieved.

423

424 However, this trend is not present in the results. This could be
 425 justified in different ways:

(1) the fixed alum dose (20 mg/L) could be enough to remove most of the TOC of the raw water (usually less than 10 mg/L), with remaining TOC being mainly low MW, hydrophilic OM recalcitrant to removal. This is confirmed by the results of the preliminary tests with varying alum dose and no PAC addition (Figure 4). It shows how the lowest alum dose usually achieved the near maximum reduction of UV_{254} , turbidity and true colour; with little or no improvement at all for increasing coagulant concentrations, as expected from previous literature (Kastl et al. 2004, Van Leeuwen et al. 2005).

(2) there could be only a small fraction of low MW OM compared to the total TOC, thus not competing with geosmin and particularly MIB for removal by PAC; and keeping the T&O removal process by PAC, and TOC removal process by alum, distinct from each other. The two processes interfere with each other only when a very high amount of PAC is dosed (Figure 3, total T&O between 150 and 200 ng/L), leading to an excess PAC (T&O already removed) that can be used to remove low MW OM.

(3) TOC concentrations are several orders of magnitude higher than T&O levels, thus relatively small variations in T&O concentration do not have an impact in the TOC removal process.

(4) other parameters affecting the results. Further tests are necessary to collect more data and fully understand this phenomenon.

Figure 4. Removal efficiency of turbidity, UV_{254} and true colour for varying alum dose and no PAC

Figures 5 and 6 illustrate the results of the tests carried out to understand the opposite phenomenon, i.e. whether increased TOC affects the removal of T&O. In this case, the outputs seem to confirm this theory. When there was excess TOC (in the form of potassium hydrogen phthalate) added to the raw water, this had a major impact on the removal efficiency of the MIB, with an average loss in removal efficiency of 20% between best and worst initial conditions. On the other hand, it was seen from these experiments that the added TOC on average had a slightly less significant effect on the removal efficiency of geosmin (average of 15% loss in efficiency). This higher impact on MIB is in line with previous studies's results (Cook et al. 2001, Lalezary-Craig et al. 1988), showing that the competitive effect of NOM on the removal efficiency of T&O compounds has a greater impact on the removal of MIB from the raw water. While geosmin has characteristics (e.g. lower solubility and flatter structure)

468 making it more easily adsorbed by PAC, MIB is instead more prone
469 to adsorption competition with the organics.

470

471 Given the much larger concentrations of TOC in the raw water
472 compared to T&O, if such level is further increased, this will
473 inevitably lead to more PAC reacting with TOC and thus less
474 available PAC for T&O removal. It can be therefore concluded that,
475 given similar molecular characteristics and much larger
476 concentrations, TOC is prioritized in the removal process by PAC
477 and alum. Thus the WTP should be more concerned about T&O
478 removal in cases when high TOC is detected in the raw water,
479 compared to the opposite scenario of TOC removal with high T&O
480 levels. In general, it can be stated that in case of high (100 ng/L)
481 geosmin levels, the required 95% removal can be achieved within
482 PAC dosing capacity for the Capalaba WTP (30 mg/L). However, by
483 fitting regression models to the data series of Figure 5, it can be
484 estimated that, in order to achieve similar removal efficiency for
485 MIB, at least 40 mg/L of PAC would be required, which is beyond
486 the current capacity. Hence, in order to deal with high MIB levels,
487 the only options seem to be to: (1) increase the PAC dosing capacity;
488 or (2) reduce the flow to increase the concentration, with a potential
489 blend from other water sources to meet the water demand.

Figure 5. Effect of changing TOC dose rate on removal efficiency of MIB

Figure 6. Effect of changing TOC dose rate on removal efficiency of Geosmin

3.3 Effects of alum dosage and humic acids

An additional set of tests was completed to evaluate the effects of changing the alum dose rate used along with the addition of humic

acid (25 to 50 mg/L) on the removal efficiency of T&O and TOC
(Fig. 7).

Figure 7. Effect of changing alum dose on T&O and TOC removal

Noticeably, the increase in alum dosage has a relevant impact only on the removal of TOC. Given that more alum is available for coagulation, then more TOC can be removed. Unlike Figure 4, where organics removal did not seem to improve with increased alum dosage (because only the fraction recalcitrant to removal remained, even with low alum dosing), in this case a higher amount of aromatic, high MW NOM, prone to adsorption, is present due the addition of humic acids, thus a higher alum dose does lead to a higher TOC removal. However, the fact that geosmin and MIB removals are not affected by increasing alum, confirms the hypothesis that TOC is prioritized in the coagulation process and therefore the alum is used for TOC removal only.

3.4 PAC dosage prediction

By visually inspecting and analysing the collected data, it was possible to notice a nonlinear correlation between T&O removal and the ratio between PAC dose and UV_{254} of the raw water. A reason why UV_{254} is seen to have such a significant effect on the removal efficiency of T&O is because UV_{254} is usually correlated to TOC in natural waters. As it was inferred from the tests, TOC has a significant impact on the T&O removal efficiency due to the competitive effects NOM had on the adsorption capabilities of PAC. Therefore it can be concluded that, since UV_{254} is a quick approximated measure of the TOC that can be found in the raw water, it can assist with the estimation of T&O removal propensity and thus the amount of PAC required. A chart of the relationship between PAC, UV_{254} and the removal efficiency of T&O was developed from the results of the regression and this chart can be seen in Figure 8. It can be noticed how generally, given same ration between PAC and UV_{254} , the removal of MIB would be proportionally lower than geosmin; this is in line with the outcomes of previous studies (Cook et al. 2001, Thiel and Cullum 2007) and the results of this study as previously discussed.

539 **Figure 8.** Relationship between PAC, UV_{254} and removal efficiency

540 developed from regression results

541

542 From Figure 8, it is evident that, based on the UV_{254} of the raw water,
543 the effect that this parameter has on the removal efficiencies can be
544 calculated and thus the required PAC dose rate can be predicted
545 using the following method.

546 1) Measure MIB and geosmin in the raw water;

547 2) Estimate the removal efficiency to be achieved, based on
548 guidelines thresholds of 10 ng/L (ADWG 2016). This means that if
549 MIB and geosmin are, for instance, 5ng/L, then they are already
550 below guidelines values so 0% removal is required, i.e. no PAC. If
551 they are instead 20ng/L, then 50% removal is required to get below
552 threshold values. If 100 ng/L, 90% removal is required, and so on;

553 3) Measure UV_{254} of the raw water;

554 4) Using the equations from the trend lines of the chart, back-
555 calculate the PAC dosage based on measured UV_{254} and T&O. Such
556 equations can be rewritten in order to isolate the PAC terms as
557 follows:

$$558 \quad PAC_{MIB} = UV_{254} \cdot e^{\left(\frac{MIB \text{ target removal} + 0.6889}{0.2798}\right)} \quad (1)$$

$$559 \quad PAC_{Geosmin} = UV_{254} \cdot e^{\left(\frac{Geosmin \text{ target removal} - 0.1913}{0.1411}\right)} \quad (2)$$

$$560 \quad PAC_{TOC} = UV_{254} \cdot \left(\frac{TOC \text{ target removal} - 0.4935}{0.001}\right) \quad (3)$$

561

562 Such equations can be easily embedded in Excel or in a graphical
563 user interface (GUI) for ease of use.

564 The operator should safely keep the highest predicted dose out of the
565 three equations (or, at least, the first two, as TOC removal is not the
566 main goal of PAC), to ensure that all the target removals constraints
567 are satisfied.

568

569 It must be noticed that these equations do not distinguish between
570 different PAC types, as there are not enough data points (i.e. jar test
571 results) for each of them to build a significant correlation. However,
572 the recommended PAC is likely to perform better than what is
573 predicted by the regression lines, hence considering an average, such
574 as in the proposed equations, represents a safe prediction as it would
575 most likely lead to slightly higher removals. Also, most of the jar test
576 results used to develop such models are based on a fixed alum dose
577 of 20 mg/L, despite varying UV_{254} in the raw water. If the alum dose
578 is varied from this default value, it can be expected to have a slight
579 increase or decrease in the predicted TOC removal efficiency, but not
580 significant effect on T&O removal, based on the results described in
581 Section 3.3; thus this recommended PAC-optimising approach for
582 T&O removal can be considered reliable regardless of the alum dose.

583

584 *3.5 Effect of NOM character on T&O removal*

585 Another limitation of the above PAC dosage prediction approach, is
586 that the proposed equations are site-specific, since different raw
587 water quality characteristics would lead to different curves. In
588 particular, the character of the NOM would greatly affect the slopes
589 of those regression functions due to different levels of disturbance in
590 the T&O removal process by PAC. This was demonstrated through

the last set of jar tests where tannic acid (TA), quinine (Q) and potassium hydrogen phthalate (KHP) were added to the raw water; some key - features of these organic compounds are shown in Table 1.

595

Table 1 – Molecular weight and solubility of deployed organic and T&O compounds

Compound	Molecular weight [g/mol]	Solubility [g/L]
Tannic acid	1701.19	2.8
Quinine	324.42	0.5
Potassium hydrogen phthalate	204.22	80
Geosmin	182.307	0.15
MIB	168.28	0.1955

598

The TOC levels of the unspiked raw water range between 10.1 and 11.1 mg/L, while UV_{254} was between 0.479 and 0.513 cm^{-1} . Raw water was also spiked with 100 ng/L of geosmin and 100ng/L of MIB. Figures 9, 10 and 11 illustrate the different loss in removal capacity of TOC, geosmin and MIB following the gradual addition of these different organic compounds.

605

Figure 9. Effect of different NOM types on TOC removal by PAC and alum

Firstly, it can be noticed that, although adding Q and KHP led to a similar loss in TOC removal, the addition of the much higher MW TA actually improves the removal of organics, leading to higher removal rates (Fig. 9). In principle, this may be counterintuitive as higher MW, more complex organics would require more coagulant to destabilize such molecules (Divakaran and Sivasankara Pillai 2001), with other studies also achieving a better removal with lower MW organics (Chang et al. 2005); this study however was done using alum only and by varying its dose. Thus it seems that the lower MW Q and KHP are more recalcitrant to removal; while the fixed dosages of alum and PAC seemed to be able to adsorb most of the higher MW TA even at the highest concentrations (i.e. approximately 90 mg/L).

Figure 10. Effect of different NOM type on geosmin removal by PAC and alum

Figure 11. Effect of different NOM type on MIB removal by PAC and alum

With regards to T&O instead, although Q still has the worst effect in terms of reducing the ability of PAC to remove geosmin and MIB, KHP is much less impactful than with TOC removal, resulting in a lower loss in T&O removal capacity than TA. Such results are related to the solubility of these compounds: if a compound is highly soluble, it is more difficult to remove as its propensity to remain in a

liquid phase is higher; thus adding KHP affects T&O removal to a higher degree than an equivalent amount of Q. Finally, it can be noticed that in these experiments, there is not one T&O compound more impacted by TOC addition, although, similarly to previous experiments, the original (i.e. with unspiked water) removal rate was lower for MIB compared to geosmin.

3.6 Discussion

The combined results of this study seem to highlight a “TOC prioritizing mechanism”, based on which higher T&O concentrations do not affect TOC removal as much as higher TOC levels affect T&O removal. One of the most obvious reasons explaining this phenomenon is the fact TOC concentrations in the raw water were orders of magnitude higher than T&O levels. Based on this, although in Capalaba WTP PAC is mainly used for T&O removal and alum is mainly used for TOC (and turbidity) removal, those two chemicals work with, and against, each other, and thus more research work should be conducted to optimize the coagulation process as a whole, e.g. estimate both alum and PAC based on T&O, TOC, contact time, NOM character, etc. Although not significant based on SOM, larger ranges of pH could be considered to check how this affects the T&O removal efficiency. Despite not being possible for this study due to limited resources, future work should also make use of replicates to enhance the quality and reliability of the data, especially in experiments where clear trends were not present and high uncertainty and variability was noticed.

665 The fact that different removal rates are achieved based on NOM
666 signature, confirms that the proposed PAC dosage prediction model
667 must be site-specific. Preliminary work was also conducted where
668 readings with the YSI EXO fluorescent dissolved organic matter
669 (fDOM) probe were taken of samples of ultrapure water spiked with
670 Q, TA and KHP. Results show that TA and KHP are much less
671 fluorescent in the fDOM range than Q (which is used as calibration
672 standard); hence it seems that the higher losses in T&O removal
673 ability by PAC is caused by those NOM compounds more sensitive
674 to fDOM measurements. In turn, there is potential to develop a new,
675 more general, PAC prediction model based on fDOM readings as
676 well.

677

678 Recent work from the authors (Bertone and O'Halloran 2016) also
679 showed potential to predict T&O concentrations in Lake Tingalpa
680 based on remotely measured parameters (e.g. chlorophyll-a and
681 phycocyanin fluorescence probe readings); the current study, on the
682 other hand, showed potential to use T&O to in turn predict PAC and
683 optimize the coagulation process. Future work will seek to refine the
684 two models and link them to each other, in order to get on step closer
685 to the development of a fully-automated treatment optimization
686 model, largely based on remote sensors data.

687

688 **4. Conclusions**

689 In this research study, the authors combined field and laboratory
690 work with data analysis and prediction modelling approaches, in
691 order to better estimate the required PAC dosage for the Capalaba

692 WTP, based on T&O compounds present in the raw water and
693 competitive effects with organic carbon removal through coagulation.

694

695 It was seen that the removals of MIB, geosmin and TOC can vary
696 significantly under the same testing conditions. Through the
697 experiments that were completed, it was concluded that geosmin is
698 more easily removed compared to MIB and TOC. It was also
699 concluded that, by increasing the initial TOC found in the raw water,
700 this has a major impact on the removal efficiency of both geosmin
701 and MIB, with such impact being proportional to NOM solubility and
702 MW. Additional tests' results seem to highlight that a change in alum
703 dosage has a minimum impact in terms of T&O removal efficiency
704 by PAC, while a considerable change in TOC removal was recorded.

705

706 A regression approach was also used for this project as a way to
707 determine which input variables had a significant impact on the
708 removal efficiency of MIB, geosmin and TOC. Following the visual
709 identification of the most relevant variables through SOM, linear and
710 non-linear regression models were developed for the removal
711 efficiencies of MIB, geosmin and TOC by relying on the ratio
712 between PAC and UV_{254} . Based on this, a step by step approach was
713 proposed to determine the optimal PAC dose based on T&O in the
714 raw water and easily measurable UV_{254} . The developed model is
715 quick and easy to interpret for the WTP operators; as such, it can be
716 used for a rapid assessment of PAC dosage requirements, especially
717 in cases of sudden weather or water quality variations leaving limited
718 time for traditional manual estimation procedures. Therefore, it

719 provides a user-friendly decision support tool leading to increased
720 water treatment proactivity.

721

722 Nevertheless, it is currently a site-specific model, as it was also
723 demonstrated that the character of the NOM greatly affects the TOC
724 and T&O removal capacity by PAC (and alum). Despite that,
725 preliminary work showed potential to use fDOM probe readings as a
726 model correction factor, since such fluorescence probe seems to be
727 more sensitive to those organics creating the highest impediments to
728 T&O removal. Thus, future work will seek to improve the model by
729 incorporating information on DOM character through fDOM
730 readings, as well as through the development and integration of an
731 accurate DOM-based alum prediction model.

732

733

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738

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852

Highlights

- Experiments to optimise powdered activated carbon dose for taste and odour removal
- Organic matter amount and property affects taste and odour removal efficiency
- Taste and odour amount does not affect organic matter removal
- Data-driven prediction model for powdered activated carbon

■ T10 removal efficiency
 ■ Geosmin removal efficiency
 ■ TOC removal efficiency

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Analysis and Modelling of Powdered Activated Carbon Dosing for Taste and Odour Removal

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