Practical Paper

Development and implementation of the software *mEnCo*© to predict coagulant doses for DOC removal at full-scale WTPs in South Australia

J. van Leeuwen, M. Holmes, U. Kaeding, R. Daly and D. Bursill

ABSTRACT

Conventional surface water treatment plants (WTPs) rely on optimised coagulation for effective clarification, filtration and chlorination performance. WTPs operated at sub-optimal coagulation conditions are at risk from failing treated water microbial, disinfection by-product, chemical and aesthetic quality goals as well as incurring excessive sludge production and treatment cost. This is especially important when treating water that contains a high concentration of natural organic matter (NOM). Removal of NOM by coagulation can be enhanced by optimising the inorganic coagulant dose and coagulation pH. This paper describes the development and implementation of a software model *mEnCo*© (referring to modelling enhanced coagulation) that enables WTP operators to rapidly determine coagulation chemicals. Implementation was carried out in a four-stage process comprising model evaluation by (1) jar tests and pilot-scale studies, (2) comparison of *mEnCo*© predictions with historical water quality and coagulant dose trends at Adelaide metropolitan WTPs, (3) parallel studies where *mEnCo*© predictions were compared with the usual methods applied by operators for chemical dose determination and (4) application of *mEnCo*© for dose determination and review. United Water International (UWI) began using *mEnCo*© in July 2003 for prediction of chemical doses for coagulation control and have used the model from July 2004 to adjust coagulant doses.

Key words | coagulation, DOC, model, optimization, software, water treatment

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INTRODUCTION

Commonly used metal-based coagulants at WTPs include alum and ferric chloride and both are able to remove high percentages of colour and turbidity and various percentages of natural organic matter (NOM), depending on its character. It is important to control the concentration of dissolved organic carbon (DOC) in finished water as it has a major impact on water quality and the performance of downstream treatment processes. It is the precursor to disinfection by-products including trihalomethanes (THMs); it imparts a chlorine demand; it provides nutrients for heterotrophic bacterial re-growth; it reduces

the effectiveness of activated carbon and it leads to fouling of membranes.

DOC removal using metal coagulants is dependent upon its concentration and character as well as the coagulant type and dose, and the coagulation pH (Edzwald 1992). The DOC that is removed by coagulation is the coagulable fraction and the DOC that is recalcitrant to coagulation can be referred to as being non-coagulable (van Leeuwen *et al.* 2005). These fractions, in the case of alum- and ferric-based coagulants, are pH-dependent. The coagulable DOC comprises organics that are hydrophobic,

charged, high in molecular weight and absorb light in the UV and visible wavelength spectrum. The relative levels of UV254 nm (SUVA) and colour (specific colour) in raw water indicate the DOC removal potential using metal coagulants (Chow *et al.* 1999).

Both alum and ferric coagulants are acidic and will lower the pH of raw water. The coagulation pH can be modified by the addition of acid or base and requires control to minimize soluble metal residuals in the treated water. For example, aluminium solubility increases sharply at a pH less than 5.7 and, allowing a margin of safety, the optimum pH for alum is 6.0 and slightly lower for ferric coagulants (Letterman *et al.* 1999).

In practice, a number of factors should be considered when optimizing coagulation for DOC removal, including treatment cost, sludge production and water quality (Heidenreich *et al.* 2002). Water quality goals may include turbidity and particle removal (Budd *et al.* 2004), residual metal coagulant concentration and water quality at the customer tap (THMs, chlorine residual, microbiological parameters). Optimum coagulant dose rates can be determined in a number of ways, including operator experience, jar tests, zeta meter and streaming current detector. In this paper we describe the development and application of models and software (*mEnCo©*) for coagulant dose determination at six major water treatment plants in metropolitan Adelaide, South Australia.

MATERIALS AND METHODS

Water supply and treatment in Adelaide

Adelaide's raw water is supplied from local catchments and the River Murray. River Murray water can be high in turbidity and may exceed 100 nephelometric turbidity units (NTU), while raw water from local catchments has a high NOM content, resulting in high DOC and colour (peak values can exceed 14 mg/L and 80 Hazen Units, HU, respectively). Myponga WTP is the only plant that relies solely on local catchment, the other plants (Anstey Hill, Barossa, Little Para, Hope Valley and Happy Valley) can be supplied using various combinations of catchment and River Murray water. Surface water is treated at the six WTPs using alum coagulation, clarification, filtration and chlorination.

The individual WTPs and their respective water distribution systems (WDSs) are operated by UWI as combined systems to meet water demand and quality goals at the customer tap. Alum and chlorine doses are adjusted according to raw water quality, current WTP and WDS performance, and previous trends in seasonal behaviour of the WDS to meet water quality targets for THMs, microbial parameters and chlorine residual at the customer tap and to minimise cost of treatment. All six WTPs are optimised for DOC removal to varying degrees.

Water quality in the WDSs is monitored at key locations and performance is assessed on a daily basis to ensure compliance with contractual requirements and Australian Drinking Water Guidelines 2004. A number of key raw water quality parameters are measured including UV absorbance at 254 nm (UV254), colour, turbidity and alkalinity, all of which are input parameters for the newly developed software, *mEnCo©*.

mEnCo© software

This software was designed to enable WTP operators to rapidly determine the coagulation pH and chemical dose rates required to remove DOC (van Leeuwen *et al.* 2003, 2005; Kastl *et al.* 2004; Daly *et al.* 2007). A key feature of the model is that water quality inputs (turbidity, colour at 456 nm and UV absorbance at 254 nm) can be easily and rapidly determined at the WTP by operators. Raw water UV254 and colour are determined after filtration using a 0.45 μm filter. UV254 is measured at 254 nm using a quartz cuvette and colour is measured at 456 nm using a glass cuvette. Curvettes were zeroed against high purity water (e.g. Milli-Q Plus) and read against air. For colour measurement, an optical density reading of ~ 0.070 nm correlates directly to 50 HU. Turbidity (in NTU) was measured by turbidimeters.

mEnCo© has two complementary functions:

1. A generic function intended for a wide range of raw waters, that allows prediction of required chemical doses (coagulant and for pH control) for near-maximum or target NOM removal.

2. A specific function to accurately predict the concentration of residual DOC in treated water. This function requires calibration through limited jar testing (Kastl *et al.* 2004).

Since 2002, the generic function has been routinely used at six major WTPs in metropolitan Adelaide, South Australia. The generic function was developed by undertaking a large number of jar tests using raw surface waters widely ranging in water quality (DOC concentration and character, turbidity, alkalinity and a peak conductivity of ~1000 (S/cm) obtained from various locations in Australia (van Leeuwen *et al.* 2001). From this data, a series of mathematical equations were developed to relate coagulant (alum or ferric chloride, dose and pH) to raw water DOC, UV254, colour (Col), turbidity and alkalinity and these have been previously reported (van Leeuwen *et al.* 2001, 2005). Examples of the mathematical relationships between DOC (as measured and characterised by UV at 254 nm/cm and colour) and coagulant dose required for enhanced coagulation are given below:

$$\text{Dose (mg/L)} = A_1 + B_1 \ (\text{UV254})^{0.5} + C_1 e^{(-\text{UV254})} \tag{1}$$

$$\text{Dose (mg/L)} = A_2 + B_2 \ (\text{UVCol})^{0.5} + C_2 e^{(-\text{UVCol})} \tag{2}$$

where A_1, B_1, C_1, A_2, B_2 and C_2 are constants and UVCol is UV254 × log(colour × 10).

Separate mathematical relations have been developed that relate raw water turbidity to coagulant dose and these have been previously reported (van Leeuwen *et al.* 2001, 2003). Once the dose is calculated it is then added to the dose determined to be required based on the DOC concentration and character. Hence, the two parameters of DOC and turbidity are treated as independent variables. Although it is likely that there is some interdependence of the two variables on the coagulant dose, the application of these as independent variables has been found to be practically applicable based on jar test and pilot plant data (2001 and 2007) and in the prediction of doses for full-scale treatment.

Equations relating raw water quality parameters to estimate coagulant dose for target percentage removals of DOC (50–90%) have also been developed and reported (van Leeuwen *et al.* 2003).

Coagulant dose prediction for turbidity removal using *mEnCo*$^©$ was established from jar tests of turbid waters from the River Murray and Bendora Reservoir, Australian Capital Territory (van Leeuwen *et al.* 2005).

The generic function in *mEnCo*$^©$ is intended to enable rapid prediction of:

- the alum or ferric chloride dose rate required to achieve a user-specified reduction in coagulable DOC in the range 50–90% without pH control;
- the alum or ferric chloride dose rate required to achieve enhanced coagulation without pH control;
- the alum or ferric chloride dose rate plus acid or alkali dose required to achieve a given percentage removal of DOC or enhanced coagulation condition for a specified coagulation pH; and
- the acid or alkali dose for pH control including coagulation pH and post-coagulation correction.

The enhanced coagulation dose is defined in *mEnCo*$^©$ as the coagulant dose where a reduction of 0.15 mg/L DOC occurs with an increase of 10 mg/L coagulant (van Leeuwen *et al.* 2005). The addition of coagulant above this would result in a negligible increase in DOC removal. The model can also be used to estimate the acid or alkali (sodium hydroxide) dose required to achieve a target coagulation/post-coagulation pH. This is based on the raw water alkalinity, coagulant acidity, a model of the pH titration curve, selection of suitable pH control reagents and selection of a coagulation or post-coagulation pH. The alkalinity of the raw water can be entered directly if known (as $CaCO_3$) or determined by measuring the volume of a standard acid or coagulant (alum) needed to lower the raw water pH to 5.5, or through standard laboratory analysis for measuring alkalinity (van Leeuwen *et al.* 2003).

The user can select either a percentage of the coagulable DOC to be removed (50–90% in 1% intervals) or the dose required to achieve enhanced coagulation conditions (Enh). The coagulant type (ferric chloride or alum) can be selected along with the method of expressing concentration, for example $Al_2(SO_4)_3.18H_2O$ for alum. Once entered, the user is able to obtain a predicted coagulant dose (mg/L) without pH control. The user can also obtain a prediction of the coagulation pH that would result from the addition of

the predicted coagulant, provided the alkalinity of the raw water is entered.

An estimate of the coagulation pH after coagulant addition may also be made by entering a user-specified coagulant dose together with the raw water alkalinity (mg/L as CaCO₃). Target pH conditions may require acid as well as coagulant to be dosed and either sulfuric acid or hydrochloric acid dose rates can be predicted (mg/L). Target conditions that require a higher pH require base addition and sodium hydroxide dose rates can also be predicted. Implementation of *mEnCo*© into UWI operations was carried out in a four-stage process comprising of: (1) model evaluation by jar tests and pilot-scale studies, (2) comparison of *mEnCo*© predictions with historical water quality and coagulant dose trends at Adelaide metropolitan WTPs, (3) parallel studies where *mEnCo*© predictions were compared with the usual methods applied by operators for chemical dose determination, i.e. jar testing, and (4) application of *mEnCo*© for chemical dose determination and review.

Model validation trials

Pilot plant trials using flat bed clarifiers, ranging in capacity from 800 L/h to 3700 L/h, were undertaken to validate *mEnCo*© predictions at Happy Valley, Anstey Hill and Middle River WTPs in South Australia and at the Googong WTP, ACT. The results of these trials have been previously reported (Holmes *et al.* 2006).

RESULTS AND DISCUSSION

Evaluation of *mEnCo*© historical data

A desktop study was also undertaken by UWI to assess the appropriateness of *mEnCo*© as an operational tool. The main aim of the study was to retrospectively compare the actual alum dose used at each metropolitan Adelaide WTP with the model-predicted dose (MPD) for alum to achieve 60, 70, 80, 85 and 90% removal of the coagulable DOC, as well as the dose required to achieve enhanced coagulation with and without pH control. Historic water quality data (raw water UV254, colour, turbidity and

alkalinity) for a two-year period (January 2002–December 2003) was used as input data for *mEnCo*©. Results from this study revealed several findings. It was apparent that the alum dose rates predicted by *mEnCo*© were in the range used at the WTPs. The study also indicated periods when the WTPs had been operated with a lower or higher alum dose as compared to the *mEnCo*© enhanced coagulation predicted alum dose. This study did suggest that the application of *mEnCo*© could lead to opportunities for savings in chemical costs as well as improved water quality. Jar tests were used during this period to assist operators establish alum dose rates at a frequency of one every two months, or sooner if sudden changes in raw water quality were experienced. The study also investigated the performance of the model in predicting coagulation pH. In general *mEnCo*© gave a reasonably accurate prediction of the coagulation pH (range in difference 0–0.25 pH).

Implementation of *mEnCo*© into operations

UWI began using *mEnCo*© in July 2003 to predict the required alum dose to achieve 80% and 90% coagulable DOC removal and enhanced coagulation. Figure 1 shows the actual alum doses at the Barossa and Happy Valley WTPs for the period from July 2003 to December 2007 and the *mEnCo*© predicted doses at those times. From July 2004 *mEnCo*© outputs have been used routinely to adjust WTP coagulant doses.

Enhanced coagulation is applied at Barossa and Myponga WTPs where coagulation pH is optimised at pH 6.1. *mEnCo*© MPDs for these plants therefore reflect the alum dose required for maximising DOC removal. The other four Adelaide WTPs, including Happy Valley (Figure 1(b)), are operated using alum doses that achieve between 80% and 90% coagulable DOC removal, as predicted by *mEnCo*©. Prior to the introduction of *mEnCo*© significant over- or under-dosing of alum coagulant was possible due to the subjective nature of jar testing, and the fact that DOC analyses were not undertaken in conjunction with the jar tests. This was despite the plants being run by experienced operators. Figure 1(a) demonstrates how UWI adopted *mEnCo*© predicted results to achieve near-maximal removal of DOC at Barossa WTP from July 2004 to 2006. This shows that the use of *mEnCo*© can lead, at various times, to cost
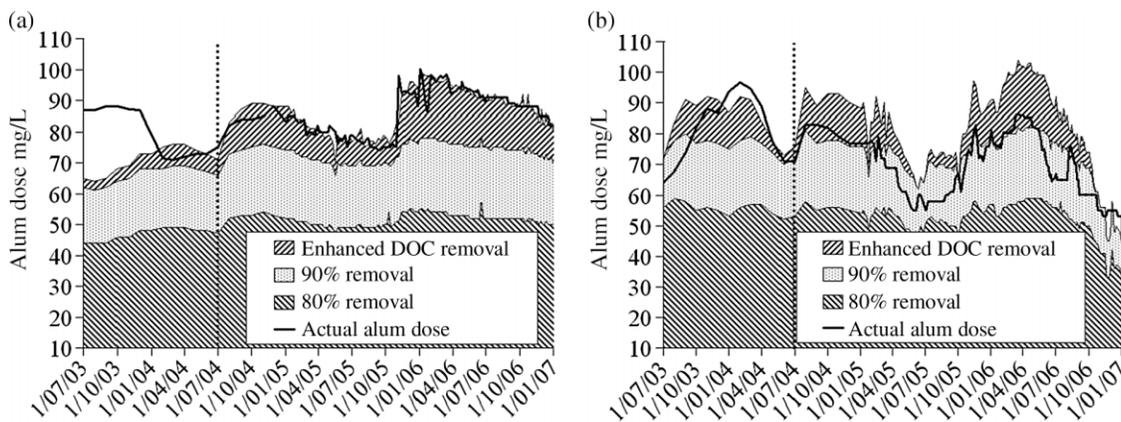
Figure 1 | Actual and *mEnCo*© predicted alum doses at (a) Barossa WTP (targeting enhanced coagulation) and (b) Happy Valley WTP (targeting 80% to 90% coagulable DOC removal), July 2003 to June 2006.

savings, by preventing coagulant over-dosing, and improved water quality compliance, by preventing coagulant under-dosing. Similarly, Figure 1(b) also shows how the alum dose targeted to remove 80–90% of the coagulable DOC has been more closely achieved at Happy Valley WTP, with chemical cost savings, since the adoption of *mEnCo*© in July 2004.

Anstey Hill WTP can treat raw water from two different sources: the River Murray and catchment water from the Millbrook Reservoir. These two waters can be of significantly differing quality, with the River Murray water generally being low in DOC but high in turbidity and the Millbrook water generally being high in DOC and low in turbidity.

The source water to the WTP may be changed from one source to another at very little notice and it may not be

possible to obtain a sample of the new raw water in time to undertake a jar test prior to the new water reaching the plant. Under these circumstances application of *mEnCo*© predicted alum doses has resulted in water quality remaining within specification during the change in source water (Figure 2(a)).

Coagulant and chlorine dose rates are applied at the water treatment plants to achieve water quality guidelines (Australian Drinking Water Guidelines [ADWG] 2004) and license requirements from the South Australian Water Corporation for coliforms, THMs and free-chlorine residual at the customer tap. WTPs are also operated to achieve low filtered water turbidity (<0.1 NTU) and low aluminium residual (<0.2 mg/L) (Holmes & Oemcke 2002). Prior to implementation of *mEnCo*©, jar tests were used as a tool to select alum dose rates at metropolitan Adelaide WTPs.
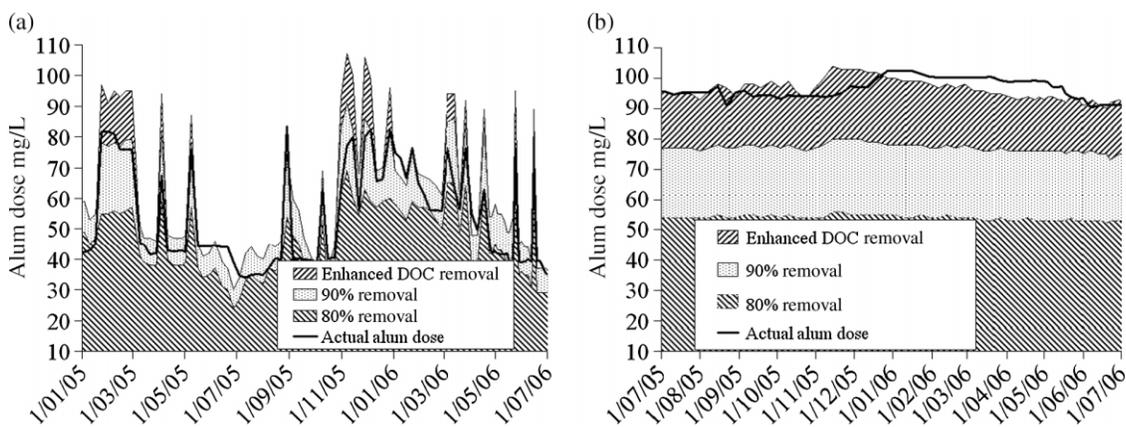

Figure 2 | Actual and *mEnCo*© predicted alum doses at (a) Anstey Hill WTP, January 2005 to June 2006 (targeting 80% to 90% coagulable DOC removal) and (b) Myponga WTP, July 2005 to June 2006 (targeting near maximum DOC removal).

During this time water quality was fully compliant with contractual and ADWG requirements at the WTPs and in the network. Full compliance has also been achieved using *mEnCo*©.

However, reliance on *mEnCo*© alone is not appropriate for controlling coagulant dosing at these plants. The optimal coagulant dose for DOC removal may, for instance, not be the optimal dose for particle removal, where particle removals and residuals form treatment and treated water quality requirements. Depending on plant design and hydraulics, the application of *mEnCo*© may lead to insufficient development of flocs needed for effective clarification. At times it has been necessary for an individual plant to use an alum dose in excess of that predicted by *mEnCo*© due to poor floc formation at the MPD. An example is the Myponga WTP during the late summer and autumn of 2006 (Figure 2(b)). The water treated by the Myponga WTP is very high in DOC but low in turbidity and, due to both water quality and plant design, the floc produced was small, weak and difficult to remove through the flotation process. At this time the flotation process was not operating effectively when alum was dosed at the MPD. The dose was therefore increased above the MPD for a six-month period until raw water quality had changed to the extent that the MPD again produced a treatable floc. The exact reason is unknown. This highlights the importance of maintaining vigilance at the WTP and continuing to monitor parameters such as settled/floated water and filtered water turbidity to ensure that the plant is operating as required at the MPD. Similar vigilance must be maintained to monitor key performance indicators in the WDS.

Recently published work (Budd *et al.* 2004; Holmes *et al.* 2004) has also shown that maximum removal of particles through a WTP may require higher coagulant doses than are required for optimum DOC removal. *mEnCo*© has also been assessed for use at two UWI operated WTPs in Ballarat, Victoria, Australia. These plants have a contractual requirement to produce filtered water with a particle count of less than 100 particles per mL in the 2–15μm size range. Experience at these plants has indicated that, if the plant were operated at the coagulant doses predicted by *mEnCo*© for maximum DOC removal, then the particle counts may at times exceed that contractual limit. Higher alum doses are required to ensure that the particle count target is achieved. Therefore the *mEnCo*© predicted results require interpretation when fine-tuning the operation of WTPs. Actual coagulant doses may be required to be higher than *mEnCo*© predicted doses to compensate for inadequate WTP design that may give rise to poor mixing, inappropriate contact times and short circuiting.

Prediction of pH correction chemical dose

Barossa WTP is the only metropolitan Adelaide WTP with the capacity to dose sulfuric acid in order to obtain an optimum coagulation pH. Therefore the plant has the capacity to reduce alum dose and increase sulfuric acid dose while maintaining the optimum coagulation pH. This facility is useful as this plant has limited sludge treatment facilities and lower alum doses result in reduced sludge production. *mEnCo*© can be used to determine the additional acid dose required to achieve the target coagulation pH (6.1) for a range in alum dose rates (Figure 3).

Use of *mEnCo*© as a design tool

With the confidence gained from its application at the six WTPs, *mEnCo*© has been used as a design tool to determine potential coagulant and pH correction chemical doses for a proposed new WTP in South Australia. UWI was contracted to determine the design parameters for a proposed WTP to treat water from Wirrina Reservoir, a privately owned and operated water supply in South Australia. The existing WTP does not use coagulation and no jar test or historical water quality data was available to determine either treatability of the water or potential required coagulant doses. A 12-month monitoring programme was initiated to provide raw water quality data, including colour, turbidity, UV254 and alkalinity. This data was used in conjunction with *mEnCo*© to predict the alum and ferric doses for a range of different DOC removals (Figure 4(a)), as well as the doses of pH correction chemical needed to obtain the required coagulation pH (Figure 4(b)). This allowed an estimation of the required chemical storage and dosing requirements for the proposed new plant as well as an economic comparison of the different coagulants.
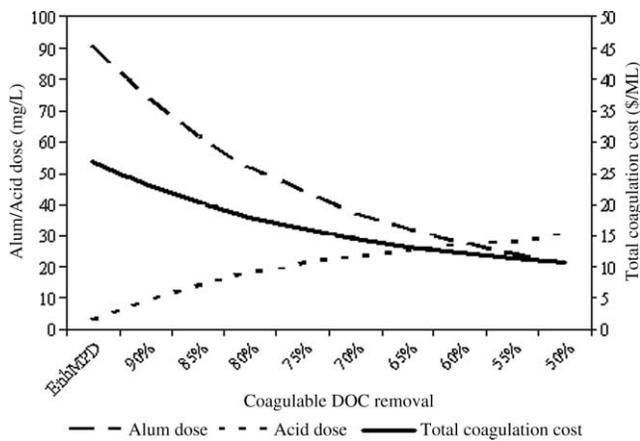
Figure 3 │ mEnCo© predicted alum and acid doses and coagulation costs to achieve a coagulation pH of 6.1 for water from Barossa Reservoir, 3 July 2006.

Comparison of the *mEnCo*© outputs to the results of a jar test undertaken on one of the samples indicated that the point of diminishing returns for DOC removal in the jar test compared closely with the near-maximum (or enhanced) model predicted dose (EnhMPD) predicted by *mEnCo*©.

mEnCo© has also been used for sizing additional lime slaker capacity for pH correction at the Happy Valley WTP and determining the financial implications, in terms of cost of additional pH correction chemicals, of increasing the contractual pH set point at United Water operated WTPs in the town of Ballarat, Victoria, Australia.

The development of the models and software was primarily designed for conventional treatment (coagulation,

flocculation, sedimentation/DAF and filtration) of water sources such those of South Australia where the DOC can be up to ∼14 mg/L, turbidity to ∼600 NTU and conductivity to ∼1000 μS/cm. Objectives in treating these types of raw waters are to maximise or achieve target removal of DOC while still meeting drinking water guidelines (e.g. Australia Drinking Water Guidelines 2004) for colour, turbidity and other parameters. With input of alkalinity to the software, changes in pH with the addition of alum (or ferric chloride) can be predicted for waters and water conditions found in South Australia. Where the key objectives of treating water for drinking purposes are different to that designed, such as for manganese and arsenic removal, or where pre-chlorination is performed, then the models are no longer suitable for application. Application of any model needs to be assessed on the basis of achieving the required treated water quality and this varies between countries and potentially between their states and territories. Hence, application requires assessment for suitability and potentially modification according to site-specific water quality conditions and treatment systems that exist. As detailed in this paper, application of models and software involves testing for suitability to assess the reliability and accuracy of dose predictions. The benefits are that, once established, they can provide significant labour, cost and time savings by removing the need for frequent jar testing, and enable rapid response to source water quality changes.
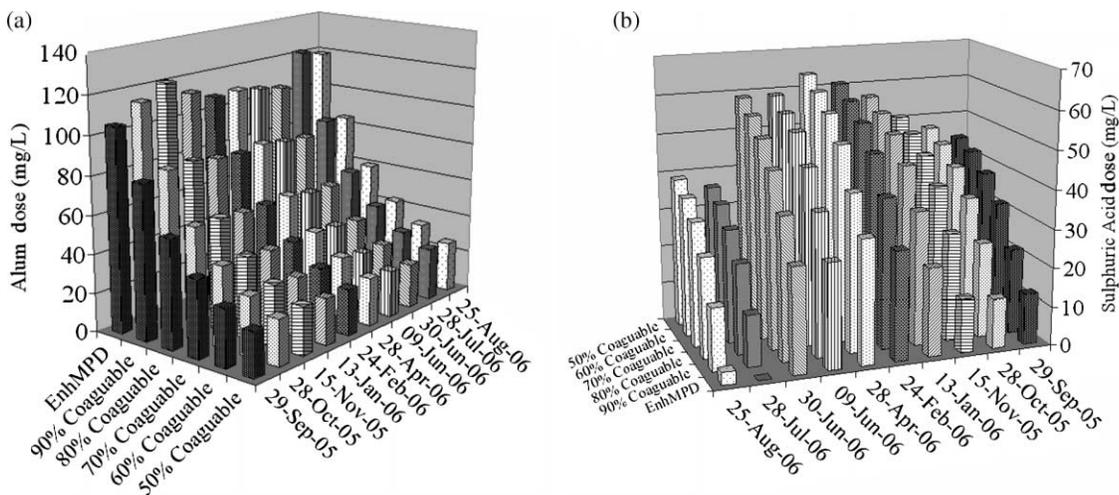

Figure 4 │ mEnCo© predicted doses at Wirrina Reservoir for samples taken between September 2005 and August 2006 for (a) alum EnhMPD and (b) sulfuric acid to achieve a coagulation pH of 6.1.

CONCLUSION

mEnCo© has been applied to predict chemical doses at six major WTPs in metropolitan Adelaide since July 2004. The software is viewed as a valuable tool for improved management of water treatment operations in Adelaide, and is particularly valuable under conditions of rapidly changing water quality. It has reduced the need to undertake jar tests and has enabled coagulation processes to be optimised for both DOC removal and chemical cost. This has allowed for water supply of improved quality to customers in Adelaide that is cost effective. *mEnCo*© has also been used as a design tool and has proved to be particularly valuable when designing new coagulation and pH correction dosing facilities.

ACKNOWLEDGEMENTS

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