

# Particle capture models: Comparison with experimental data

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## Abstract

Sand filtration is becoming a widely used technique for the treatment of urban run off water, particularly for the capture of particulate metal pollutants. Currently the design rules for such systems are focussed on the civil engineering and hydrological aspects, whilst metal removals are typically quoted as broad percentages. The present study is the first step in developing a new design method for such systems, by comparing an established particle capture model consisting of two partial differential equations, one for particle capture and one for loading. The particle capture model was fitted to the outlet concentrations of several metal species, assuming that all particles of a particular metal are identical and have the same probability of capture. Particle loading through the column was then used as a check on the model. Whilst the particle loading results near the surface of the sand

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filter are typically of the right order of magnitude, the model tended to over predict loading of the particles in the mid section of the sand filter. Modelling is presented showing that the assumption of particle uniformity may be the cause of this over prediction. An example is presented where the model fails to predict the loading, highlighting the need to include dissolution and washing in future models.

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## 1 Introduction

The problems of the pollution of urban run off water are known worldwide, and research has shown that Sydney Harbour is no exception [3]. This pollution includes a large amount of particulate metals arising from modern life and perhaps from previous industrial activity. Birch and McCreedy [4] summarised the state of Iron Cove, an embayment on the southern side of the harbour, fed by a number of canals from the inner western suburbs of the city [4]. *With increasing population, housing density and transport infrastructure has come enhanced contaminant generation in the catchment*

Table 1: Metal removals of sand filters stated by various design manuals.

design manual	metal removal
Clayton and Schueler (1996) [8]	40–80%
CCSMPC (2002) [7]	50%
ARC (2003) [1]	75%
UPRCT (2004) [14]	30–50%

and increased supply of heavy metals to the adjacent receiving basin. Water and sediment quality has declined in the adjoining estuary, primary contact (swimming) has ceased, fishing is not recommended and marine flora and fauna are degraded. A vision to restore Iron Cove estuary to a condition where it can be socio-economically, recreationally and ecologically viable is lacking [4]. The pollutants enter the harbour during periods of low flow or as a first flush via stormwater canal systems, and are deposited near the entry of the canals to the harbour [2]. In contrast high flows are more dilute and pollutants are carried further into the main channel of the harbour by the fast flowing lower density fresh water [2]

Sand filters are structural stormwater controls employed to capture, temporarily store and treat runoff [9]. There are several design manuals used in Australia [14, 1] as well as overseas, where the majority are published in the USA [8, 13, 7]. These manuals outline different planning practices and best management practices for dealing with urban run off. Clogging and the civil engineering aspects of the design of such devices are a major focus of these manuals. Authors present and utilise a range of parameters when sizing sand filters; for example, UPRCT [14] suggests a range of operating velocities between one to five metres/day [14]. Filters are designed to operate between six months [14, 1] and five years [7] before the sand bed must be replaced. There is a wide variation in metal removals reported both with and between the different handbooks, which is summarised in Table 1. In this work we seek to examine whether particle capture filtration models could prove useful in improving the prediction and performance of such systems. To completely

model the sand filter will require models for all the processes which occur when water is run through sand columns. These include:

- flow of water through an unsaturated or saturated bed of inhomogeneous materials;
- capture of particulate pollutants;
- dissolution or precipitation of materials either pollutant or bed constituents;
- washing of small particles from the sand which may erroneously be reported as dissolved species due to the finite pore size  $0.2\ \mu\text{m}$  used to separate the dissolved and particulate species.

This article focuses on particle capture models as a first step to understanding the behaviour of such systems, due to much of the metal pollution being particulate. An upcoming article will consider the interactions between dissolved ions and captured particles. However, we are not trying to deduce the exact nature of the physical interactions occurring in the filter from the macroscopic measurements, as previous authors, notably Herzig et al. [16], have noted the difficulty of this.

## 2 Experimental methods

Particle capture experiments were conducted using two PVC columns (1400 mm tall and 150 mm diameter). The height is imposed by the geography/tidal limit of the possible sand filter site [5] and the large diameter is used to eliminate wall effects. Two different types of sand were tested, one in each column, namely Sydney and Nepean sands which were purchased from a commercial nursery. The sands differ in size and composition. Nepean is a slightly coarser sand with a mean particle size greater than  $500\ \mu\text{m}$ , compared to Sydney with a mean particle size of less than  $500\ \mu\text{m}$ . Nepean sand is predominately silica with some iron coating providing the distinct orange

colour, whilst Sydney sand is termed calciferous due to the large amount of calcium.

The experiment was run for 17 days (408 hrs) with one batch of water collected from the Dobroyd Canal, which enters Iron Cove. The columns were operated at a flow rate of  $0.5 \text{ m day}^{-1}$ . Measurements were taken of the outlet dissolved and particulate metal concentrations over time, and averages of five samples were used to estimate the percentage removal of each metal. At the end of the experiment the metal concentration loaded onto the sand in the column was measured for the upper 400 mm and lower 400 mm of the column. Particulate metal concentrations were determined by filtration ( $0.2 \mu\text{m}$ ), sulphuric acid digestion and Inductively Coupled Plasma Atomic Emission Spectroscopy analysis. Sand loading concentration samples were dried overnight in an oven set at  $200^\circ\text{C}$ , then 0.5 g of the dried sample was digested in aqua regia, before analysis by Inductively Coupled Plasma Atomic Emission Spectroscopy.

### 3 Particle capture models

There are many sand filtration models available, most based on the work of Herzig et al. [16]; for example, the model of Gitis et al. [10]. The modification of Herzig's model [16] by Gitis et al. [10] was chosen to test the proposed solution method, due the availability of a full set of parameters and that it had been validated against some experimental data [10]. The Gitis model [10] consists of a set of equations. The overall mass balance is written as

$$\frac{\partial \varepsilon C}{\partial t} + \frac{\partial \sigma}{\partial t} = \frac{\partial j}{\partial z}, \quad (1)$$

which includes the changes in porosity ( $\varepsilon$ ), concentration ( $C$ ) and particle loading ( $\sigma$ ) with time ( $t$ ) and the change in flux ( $J$ ) with vertical distance ( $z$ ). The flux of particles

$$j = uC - \varepsilon D \frac{\partial C}{\partial z}, \quad (2)$$

consists of a convection term, the product of the concentration and the superficial velocity in the  $z$ -direction ( $\mathbf{u}$ ) and a diffusion term. The diffusivity ( $\mathbf{D}$ ) is estimated by

$$\mathbf{D} = \alpha_L \mathbf{u}, \quad (3)$$

to be the product of the length scale of the sand particles,  $\alpha_L$ , and the liquid superficial velocity.

Gitis [10] divides the filtration process into three stages. The initial stage of the filtration process is filter ripening, when the particles have relatively low retention. This stage lasts until the upstream surface of media grains become coated with single particles, and the capture of particles is modelled by

$$\frac{\partial \sigma^{\text{def}}}{\partial t} = K_r \mathbf{u} C \quad \text{where} \quad 0 < \sigma < \sigma_r. \quad (4)$$

This initial stage lasts until the upstream surface of media grains become coated with single particles. The second stage of filtration starts when the particles flowing in to the sand filter interact primarily with the already deposited particles, rather than bare grains, and the retention efficiency of the particles increases. The potential for the loss of particles is also considered by Gitis to be

$$\frac{\partial \sigma^{\text{def}}}{\partial t} = K_a \mathbf{u} C - K_d \sigma \quad \text{where} \quad \sigma_r < \sigma < \sigma_u. \quad (5)$$

Gitis assumes the attachment and detachment are independent of velocity, and only compares to data obtained at two velocities (20 and 25 m day<sup>-1</sup>). The third and final stage of the Gitis model is when there is no more particle accumulation on the filter medium then

$$\frac{\partial \sigma^{\text{def}}}{\partial t} = 0 \quad \text{where} \quad \sigma = \sigma_u. \quad (6)$$

From this moment on, any suspended particles are only transferred along the transport channel formed in the bed; that is, the section of the sand filter has reached its life time. This is essentially a special case of Stage 2 where the

Table 2: Parameters used to validate the coding of the Gitis model [10].

variable	description	value	unit
$\alpha_L$	coefficient of longitudinal dispersivity	0.001	m
$\varepsilon$	porosity	0.4	-
$C$	particle concentration in the liquid	0.01	$\text{kg m}^{-3}$
$u$	liquid superficial velocity	10	$\text{m h}^{-1}$
$D$	diffusivity	0.00002	$\text{m}^2\text{h}^{-1}$
$z$	vertical direction	1	m
$K_a$	ripening stage attachment parameter	1	$\text{m}^{-1}$
$K_d$	attachment parameter	7	$\text{m}^{-1}$
$K_r$	detachment parameter	0.001	$\text{h}^{-1}$
$\sigma_r$	loading at the end of ripening	0.2	$\text{mg cm}^{-3}$
$\sigma_u$	maximum loading achievable	15	$\text{mg cm}^{-3}$

filter has become saturated with particles. The combination of Equations (1) and (2) gives

$$\frac{\partial C}{\partial t} = -\frac{1}{\varepsilon} \left[ -\left( u \frac{\partial C}{\partial D} - \varepsilon D \frac{\partial^2 C}{\partial z^2} \right) - \frac{\partial \sigma}{\partial t} \right]. \quad (7)$$

Equations (2) to (7) were solved numerically; both the concentration  $\frac{\partial C}{\partial t}$  and the loading of particles  $\frac{\partial \sigma}{\partial t}$  were solved using the inbuilt `ode15s` solver to integrate both the concentration and specific deposit over time at up to 100 discrete points (slices) along the reactor. Discrete approximations were used for the first and second derivatives of concentration with distance; that is, the spatial derivatives  $\frac{\partial C}{\partial z}$  and  $\frac{\partial^2 C}{\partial z^2}$  were solved using simpler methods, which were written directly into the Simulink model. Forward, backwards and central derivatives produced nearly identical results.

The boundary conditions used in the model were  $C = C_0$  at  $z = 0$ ,  $t > 0$ , which assumes a specific, constant concentration in the feed at the entrance of the column, whereas  $\frac{\partial C}{\partial z} = 0$  at  $z = L$ ,  $t > 0$ , which assumes that there is no concentration change at the exit of the filter. Initial conditions used

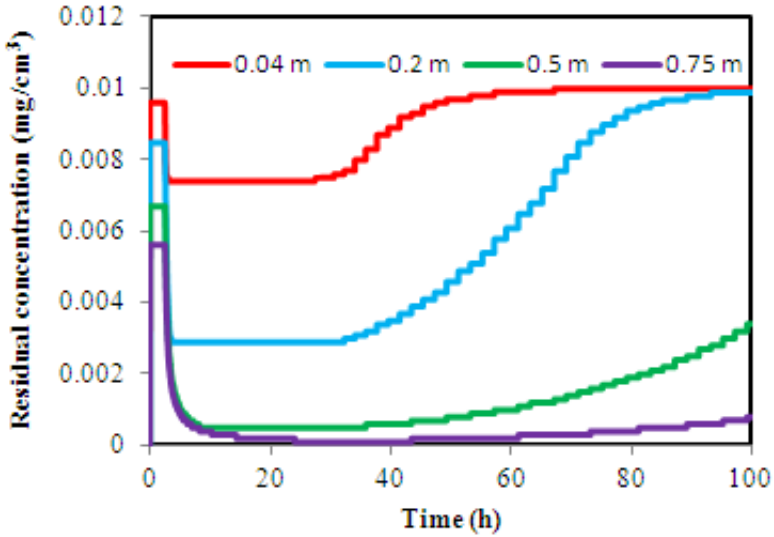


Figure 1: Specific loading calculated using Gitis parameters using Simulink model [10].

in the model were  $C(z, 0) = 0$  and  $\sigma(z, 0) = 0$ , and the values for Gitis [10] parameters are given in Table 2. The results from running this simulation are shown in Figures 1 and 2, which agree well with Figures 3 and 4 of Gitis et al. [10]. Hence indicating that the model has been correctly coded and is solving satisfactorily with 100 steps.

## 4 Comparison to experimental data

The outlet particulate metal concentration data, obtained by Carrasco [6], was used to estimate the capture parameters for a range of metals [6]. Due to the relatively short length of the experiment and the low flowrate used, approximately  $0.5 \text{ m day}^{-1}$ , the detachment parameter ( $K_d$ ) was set to zero. The



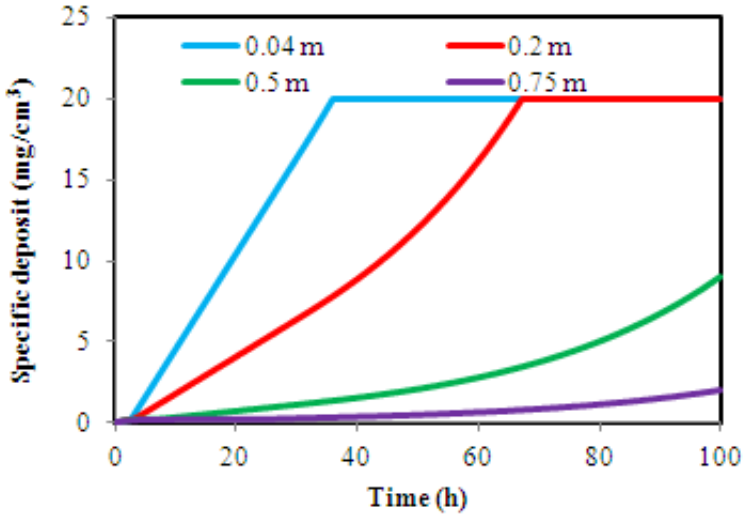


Figure 2: Specific deposit calculated using the Gitis model [10].

change in porosity has been neglected in this work as the actual concentration of particulates is very low in the urban run off system being studied. Although the inclusion of changes in porosity will be necessary when modelling large scale systems and their design life span, for such situations unsaturated flow equations also need to be included. The attachment parameter ( $K_a$ ) was varied from 0.1 to 3, and simulations were run for 408 hrs, giving a range of simulated removals of 13 to 98%. A simple exponential relationship was found to fit the value of the attachment parameter ( $K_a$ ) from the removal:

$$K_a = 0.0812 \times e^{0.0348 \times \text{removal}} \quad (8)$$

Table 3 gives the removal and attachment parameters for selected species for the three sands. Note the similar nature of the parameter values for most of the metal species in both Nepean and Sydney sands. Calcium stands out as an exception due to its high concentration in Sydney sand. Given

Table 3: Experimental removal and estimated attachment parameters for various metals, with standard deviations.

	Al	Ca	Cu	Fe	Mn	P	Zn
inlet concentration ( $\text{mg L}^{-1}$ )	0.41	0.18	0.01	0.67	0.02	0.05	0.02
	removal (%)						
Sydney	$94 \pm 6$	$52 \pm 12$	$95 \pm 4$	$94 \pm 9$	$95 \pm 10$	$72 \pm 10$	$91 \pm 6$
Nepean	$95 \pm 3$	$90 \pm 6$	$95 \pm 12$	$96 \pm 5$	$98 \pm 1$	$76 \pm 7$	$85 \pm 24$
	$K_a$ ( $\text{mm}^{-1}$ )						
Sydney	2.13	0.50	2.19	2.17	2.23	0.98	1.95
Nepean	2.21	1.85	2.19	2.28	2.49	1.14	1.55

Table 4: Simulation parameters for simulations.

sand	metal	inlet conc. ( $\text{mg L}^{-1}$ )	attachment para. ( $K_a \text{ mm}^{-1}$ )	initial loading ( $\sigma \text{ mg cm}^{-3}$ )
Sydney	Al	0.41	2.13	0.31
Sydney	Fe	0.67	2.17	0.31
Sydney	Ca	0.18	0.5	4.81
Nepean	Al	0.41	2.21	0.50
Nepean	Fe	0.67	2.28	1.44
Nepean	Ca	0.18	1.85	0.03

Calcium's relatively high solubility, it is likely that a model consisting of only particle capture may not represent this process well. A series of six simulations were run to simulate the removal and capture of Aluminium, Iron and Calcium using Sydney and Nepean sands. All simulations were run at a velocity of  $0.5 \text{ m day}^{-1}$  and other details for these simulations are given in Table 4. Initial loadings in Table 4 were determined by Carrasco [6] and were converted from  $\text{mg g}^{-1}$  to  $\text{g cm}^{-3}$  by division by the bulk density of sand ( $1600 \text{ kg m}^{-3}$  or  $1.6 \text{ g cm}^{-3}$ ) [6]. Predictions for Aluminium and Iron, given in

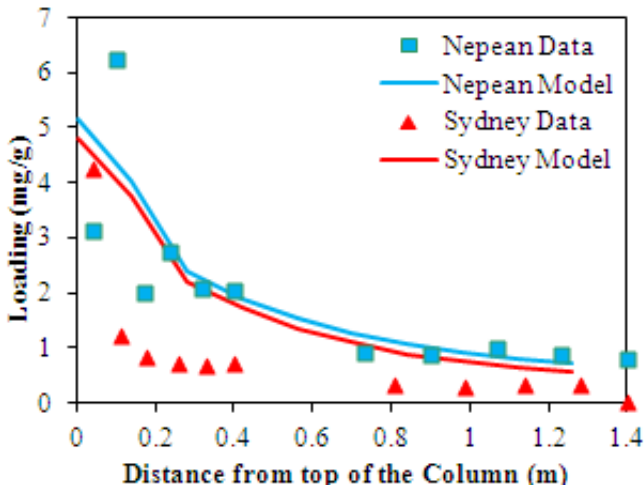


Figure 3: Prediction of aluminium.

Figures 3 and 4, respectively are reasonable in that the model predicts the magnitude of the loading in the upper section of the column and the lower section of the column. Further, the tendency of the sand filter to capture the majority of the pollutants in the upper section is clearly shown and hence this type of modelling is beneficial in explaining experimental results.

However, there is a tendency to over predict loading in the middle section of the column, seen here in all cases except for Aluminium with Nepean sand. This over prediction was also seen with other metals, which are not graphed here. A plausible cause for this over prediction of the column loading is that the model assumes that all particles are equally likely to be captured. In reality the particles not all are the same size, [11, 12] and hence are not all equally likely to be captured.

This possibility was tested simply with the model by comparing two scenarios, where a metal removal of approximately 88% is achieved. The first supposes that all particles are the same ( $K_a = 1.8 \text{ m}^{-1}$ ,  $C_i = 1 \text{ kg m}^{-3}$ ), the second

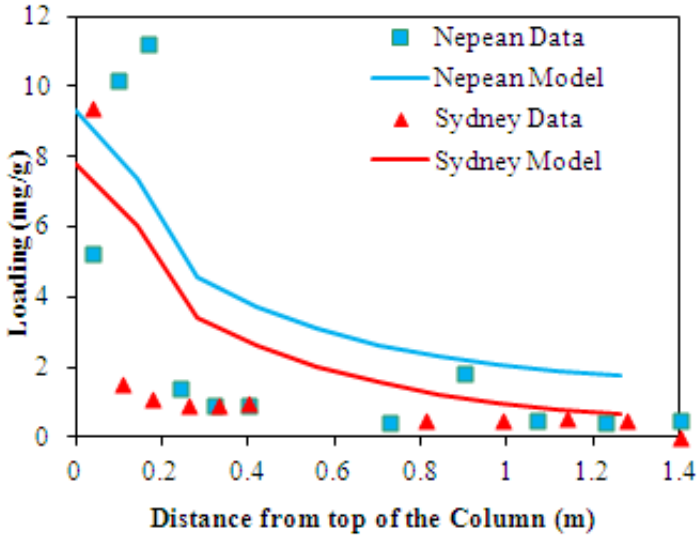


Figure 4: Prediction of iron loading.

supposes that there are two populations of particles, 80% of particles belonging to a group where the capture is close to 100% ( $K_a = 3 \text{ m}^{-1}$ ,  $C_i = 0.2 \text{ kg m}^{-3}$ ), the other 20% belonging to a group where the capture is 50% ( $K_a = 0.5 \text{ m}^{-1}$ ,  $C_i = 0.8 \text{ kg m}^{-3}$ ). A comparison of the loading predicted in such cases is shown in Figure 5, which shows the loading predicted for the two particle class case is higher at the early stages of the column, and decreases slightly faster as towards centre of the column. Qualitatively, the shape of this loading curve is a better fit to the loading data obtained experimentally. However, more experimental and modelling work would be required to justify this extra complication.

However, the use of a model consisting of only a particle capture model fails to predict the loading of Calcium throughout the sand filters. This is due in large part to the fact that the model does not include any representation of the equilibrium chemistry involved in the dissolution, or precipitation of

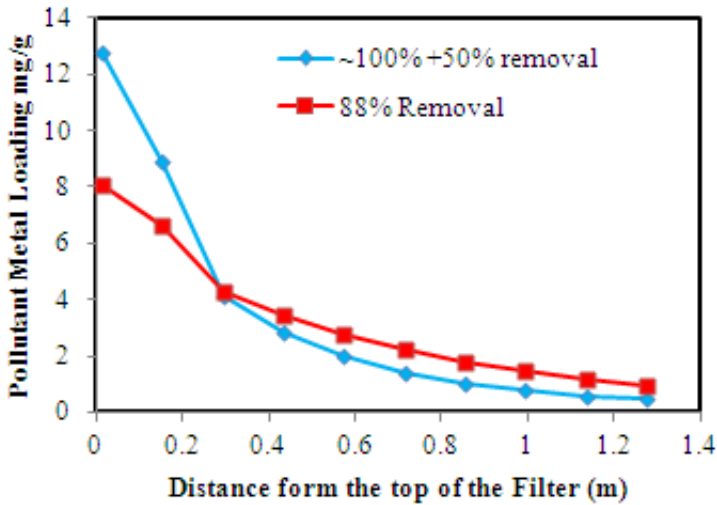


Figure 5: Comparison of two simulated sand filters achieving 88% removal.

chemistry. Even adjusting for the initial Calcium loading, the agreement remains poor in both cases.

## 5 Conclusion and future work

Particle capture models give insights into the processes occurring when urban run off containing particulate metals are filtered. The model currently provides a reasonable estimation of the loading of particles within the bed in most cases where the solubility of the metal oxide or hydroxide is not high. The models tendency to over predict the loading and the migration of particles is an area that needs further study to confirm if it is due to the inlet particles not being uniform.

Such a model may be a useful method for determining the attachment

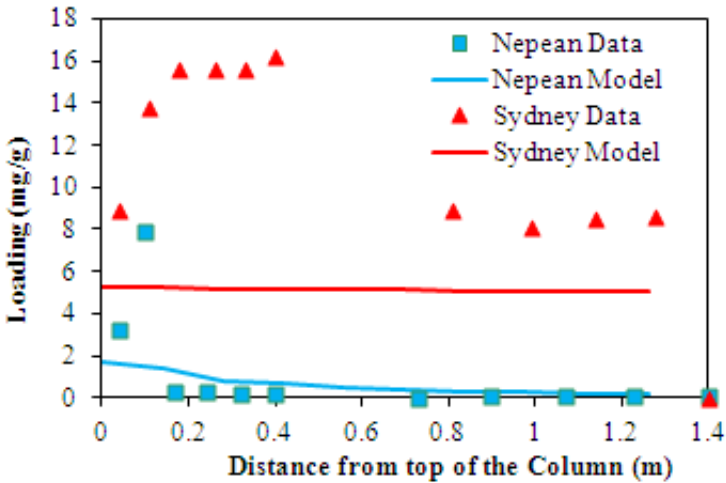


Figure 6: Prediction of calcium loading.

parameters for sand filter experiments conducted by different authors, using different sands and conducting experiments over different lengths of time. It may prove to be a better and more useful method than simply using percentage removal, as such a figure is often too broad to be useful being dependent on both the length of the sand filter and the time for which the experiment is run. The dependence of the capture parameter on velocity would be a useful further study, with Zamani and Maini [15] finding that the attachment parameter is generally inversely proportional to velocity. Such models may also prove to be more useful than the large percentage bands currently used in design manuals.

Any model is only as good as its assumptions, neglecting metal solubility is a limitation, which is obvious for relatively soluble metals such as Calcium. It is also likely to be important for many other metals as the relevant discharge specifications are comparable to the solubility of the metals. Hence future

work will need to incorporate the solubility of metals.

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