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Modelling both the continual erosion and regeneration of discolouration material in drinking water distribution systems

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Abstract

The erosion of the cohesive layers of particulate matter that causes discolouration in water distribution system mains has previously been modelled using the Prediction of Discolouration in Distribution Systems (PODDS) model. When first proposed, PODDS featured an unvalidated means by which material regeneration on pipe walls could be simulated. Field and laboratory studies of material regeneration have yielded data that suggest that the PODDS formulations incorrectly model these processes. A new model is proposed to overcome this shortcoming. It tracks the relative amount of discolouration material that is bound to the pipe wall over time at each of a number of shear strengths. The model formulations and a mass transport model have been encoded as software, which has been used to verify the model's constructs and undertake sensitivity analyses. The new formulations for regeneration are conceptually consistent with field and laboratory observed data and have potential value in the proactive management of water distribution systems, such as evaluating change in discolouration risk and planning timely interventions.

Keywords Discolouration, distribution networks, water quality modelling

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Introduction

The occurrence of discoloured water in drinking water distribution systems (DWDS) is often attributable to particulate matter, detected as turbidity, that had been attached to pipe walls but, following the onset of anomalous hydraulic conditions (e.g. flow increases), becomes entrained in the bulk flow. Discolouration can be associated with aesthetic, chemical and/or microbiological water quality failures (Vreeburg and Boxall, 2007).

In recent years an interest has developed in modelling the relationship between water main condition and the turbidity generated as a result of material erosion from the pipe wall (Boxall et al., 2001; Vreeburg, 2007; Ryan et al., 2008). Such discolouration modelling can potentially offer:

- an estimation of the quantity of discolouration material within a length of main and the ease with which it could be mobilised (e.g. from a burst or controlled flow increase such as from flushing);
- predictions of the turbidity or suspended solids concentration that would result from increasing flows in a main (given a calibrated discolouration model);
- a means for designing the hydrant flushing operations that are often used for cleaning distribution mains so as to decrease discolouration risk to a satisfactory level.

It was originally thought that discolouration was due to the re-suspension of sediments but Boxall et al. (2001) calculated that the size and density distributions of discolouration material do not usually allow for gravitational settling. They proposed the Prediction of Discolouration in Distribution Systems (PODDS) model under which material (organic and inorganic matter) instead ubiquitously and continually binds to the pipe wall around its circumference as cohesive layers with a single 'shear strength' τ_c [Pa]. PODDS was primarily developed to model the material erosion process and increases in bulk water turbidity. Its erosion mechanism is as follows:

- 1. An increase in pipe flow causes an increase in the shear stress τ_a [Pa] at the wall.
- 2. Material then erodes from the wall and becomes entrained in the bulk flow at a rate that is a function of $\tau_a \tau_c$ if $\tau_a > \tau_c$.
- 3. As a result, the amount of material at the wall decreases but its shear strength τ_c increases.

It is therefore possible to 'flow condition' a main by increasing τ_a above prevailing conditions to remove all material weaker than a 'target' τ_a .

An inverse linear relationship between the amount of material at the wall and τ_c simulates layers being eroded from weakest to strongest upon an increase in τ_a ; this approach to modelling erosion events has been validated using field data (Boxall and Saul, 2005; Boxall and Prince, 2006). When PODDS was originally developed, functionality was included to allow for the regeneration of cohesive layers (following layer erosion then a decrease in τ_a) as the reverse of mobilisation, i.e. from strongest to weakest. This was not based on any observations or data, rather that it was readily implemented at the time of encapsulating the model within a modified version of the EPANET DWDS modelling software (Boxall and Saul, 2005; USEPA, 2008).

An understanding of discolouration risk and material regeneration processes is particularly important in trunk mains due to the large populations supplied. Flow conditioning is now being used as a management strategy for (a) the non-disruptive cleaning of trunks that have been linked to discolouration complaints and (b) improving the condition of trunks to allow them to be operated at higher flows (Husband et al., 2011). Precise flow adjustments are made to mobilise discolouration material in a controlled, predictable way; this material then typically passes through the DWDS to consumers at acceptably low concentrations. Flow conditioning can be difficult due to the range and granularity of flow control needed and the infeasibility of flushing to waste in the majority of cases. However, it can be much cheaper than asset replacement or refurbishment (98% in Husband et al. (2011)). Ideally, conditioning operations would be designed and assessed using discolouration models that can track the amount of material at the wall of a main (discolouration potential) over multi-month or multi-year periods and can be used to calculate the optimal frequency and magnitude of controlled flow increases.

Discolouration material regeneration processes have been investigated during several field studies. This is typically achieved by first flushing a main once whilst measuring flow Q(t) and turbidity T(t) at the downstream end. The relationship between turbidity and total suspended solids (TSS) at the levels seen in DWDS is approximately linear (Boxall et al., 2003), allowing turbidity to be treated as a concentration. The amount of material that is mobilised during the flush is therefore $\int_{flush_start}^{flush_end} T(t) \cdot Q(t) dt$ (assuming the water entering the main has negligible turbidity). The main is then flushed again several months later and the same calculation performed. A coarse relative regeneration rate can be calculated from the ratio of the two material quantities and the duration of the 'regeneration period'.

In the Netherlands, Blokker et al. (2011, Table 2) flushed 12.3 km of mains of different diameters and materials ($\emptyset = 63 - 300 \, mm$; asbestos cement and PVC) within distribution area 'site A' on three occasions. Decreasing material quantities were mobilised with each flush but the material regeneration rate across flushes 1–2 and 2–3 was constant, indicating that regeneration is a continuous, potentially linear process. In England, Husband and Boxall (2008) undertook repeated distribution main flushing. They found evidence of regeneration being a linear process that continues until the material at the pipe wall reaches a steady state, with that state being dictated by prevailing hydraulic forces.

Discolouration potential and material regeneration rates have been detected and quantified for a variety of pipe diameters, pipe materials and source water types (Blokker et al., 2011; Husband and Boxall, 2011). Husband and Boxall (2011) calculated the relative annual material regeneration and the average regenerated turbidity between flushes for 67 pipes in England. Results highlight the effect that material supply from the pipe wall (iron corrosion) and bulk water (organic-rich surface water sources) can have on relative regeneration rates. The background water quality does not however appear to correlate with discolouration potential (see Figure 9 in that article). Overall, Husband and Boxall (2011) observed that regeneration rates in networks that do not contain iron mains are largely driven by the bulk water quality. Further, Vreeburg et al. (2008) showed that the installation of $0.1 \,\mu m$ filtering in distribution systems significantly reduces regeneration rates but regeneration still occurs.

During their field studies, Husband and Boxall (2011) increased the flow (and therefore shear stress) during each flush in steps to assess the relationships between discolouration potential and shear strength. As can be seen from fig. 1, the initial flush of each main generated more turbidity than the subsequent flushes, implying that the cohesive material layers had not fully regenerated (reached a steady state) over the intervening period(s). However, a turbidity response can be seen during later flushes for each increase in shear stress, indicating that all strengths of cohesive layers are regenerating simultaneously. This contradicts the assumption made during the development of the PODDS model that as discolouration material erodes from weakest to strongest-bound layers that the inverse may be true for regeneration.





(a) Groundwater, internal diameter (ID) = 100 mm, unlined cast iron.

(b) Surface water, ID = 73 mm, unlined cast iron.



polyethylene.

Figure 1: Turbidity data from the repeated flushing of distribution mains. Flush 1 data shown in sub-figure a previously published in Husband and Boxall (2010). Sub-figure b previously published in Husband et al. (2010).

The findings of these field studies concur with those of laboratory experiments. Sharpe et al. (2010) connected three parallel pipe loops (high-density polyethylene; 203 m long; internal diameter of 79.3 mm) to a tank with a 24 h system residence time. The tank was fed with treated moorland run-off via a cast iron trunk main. After being cleaned using high flushing flows and superchlorination, the pipes were subjected to a 28-day material accumulation phase during which a different steady boundary shear stress was imposed per pipe. During a subsequent material mobilisation phase, the flow (and τ_a) was maintained for a duration of three pipe turnovers at each of several discrete levels. Turbidity was monitored at the downstream ends of each pipe loop and was normalised by the background turbidity prior to the mobilisation phase. The entire experiment was undertaken at 8 then $16^{\circ}C$. Fig. 2 shows that the discolouration material accumulates a variety of shear strengths simultaneously, rather than stronger-bound material binding to the wall before weaker-bound material.



Figure 2: Results of laboratory studies into discolouration material regeneration (previously unpublished). Material layers were developed over 28 days under a steady boundary shear stress of $0.1 \text{ Pa} (0.2 \text{ L} \cdot \text{s}^{-1})$ at 8°C and 16°C. These layers were then eroded through imposing a series of discrete increases in shear stress.

At present PODDS can only model material erosion and not regeneration as its formulations cannot permit all layer strengths to regenerate simultaneously: the scalar τ_c can only decrease during erosion and increase during regeneration. A new model that is not subject to this limitation is presented in the following section.

Methods

The simultaneous regeneration of discolouration material over a range of shear strengths could be modelled if the amount of material at the wall is tracked over time for an array of discrete shear strengths. In contrast, the PODDS model assumes that there is a simple, linear relationship between the scalar shear strength and the discolouration potential.

Let the material condition function $\varphi(\tau, t)$ be the relative amount of discolouration material bound to the wall of a pipe p with shear strength τPa at time t. Here τ is a vector and should not be confused with the scalar τ_c in the PODDS model. Let $\varphi(\tau, t) \in [0, 1]$ where 0 corresponds to complete depletion (no material) and 1 to maximum accumulation/regeneration (maximal material). Let $\tau \in [0, \tau_{max}]$, where τ_{max} equals the maximum shear stress that the wall of pipe p is anticipated to experience. The applied hydraulic shear stress at the wall at time t is $\tau_a Pa$.

Under eroding conditions ($\tau_a > \tau$), the rate of change of condition is driven by the 'excess shear stress' ($\tau_a - \tau$) (as per the PODDS model) to ensure that weaker layers erode quicker than stronger ones (eq. 1). The lack of an equivalent term in eq. 1 for regenerating conditions ($\tau_a < \tau$) reflects the fact that regeneration is not necessarily primarily driven by hydraulic forces. This distinction can be seen in the units of the erosion rate coefficient $\beta_e = [Pa^{-1} \cdot s^{-1}]$ and regeneration rate coefficient $\beta_r = [s^{-1}]$. These units ensure that $\varphi(\tau, t)$ is unitless and so can be 'clipped' to [0, 1].

$$\frac{\partial \varphi(\tau, t)}{\partial t} = \begin{cases} -\beta_e \cdot (\tau_a - \tau) & \tau_a \ge \tau \land 0 < \varphi < 1\\ \beta_r & \tau_a < \tau \land 0 < \varphi < 1\\ 0 & \varphi \le 0 \lor \varphi \ge 1 \end{cases}$$
(1)

The clipping mandates that the model be evaluated numerically over a mesh bounded by $\tau \in [0, \tau_{max}]$ and $t \in [0, t_{max}]$. The change in condition of material with discrete strength τ_i is calculated iteratively over discrete time steps as per eq. 2.

$$\varphi(\tau_{i,},t) = \varphi(\tau_{i,},t-\Delta t) + \left(\frac{d\varphi(\tau,t)}{dt} \cdot \Delta t\right)$$
(2)

In a similar manner to PODDS, the material flux rate from a unit area of pipe wall to the bulk water (eq. 3) is a function of the change of material condition discretely integrated over the range of eroding material strengths. It is hypothesised that the material flux of material from the

bulk water to the wall is negligible relative to the flux of material to the bulk so the former is not modelled directly in eq. 3, only via the regeneration rate parameter β_r .

$$\frac{dN(t)}{dt} = -\alpha \sum_{i} \left(\varphi(\tau_i, t) - \varphi(\tau_i, t - \Delta t)\right) d\tau \text{ for } \tau_a \ge \tau_i$$
(3)

If turbidity is proportional to TSS and is therefore a concentration of discolouration material then it is proposed that material quantity be measured in Turbidity Pseudo-Mass Units (TPMU) where $1 TPMU = 1 NTU \cdot m^3$ (Nephelometric Turbidity Unit). So in eq. 3 the material release rate from a unit area of pipe wall, dN(t)/dt, and the material release coefficient α have units of $TPMU \cdot m^{-2} \cdot s^{-1}$ and $TPMU \cdot Pa^{-1} \cdot m^{-2}$ respectively¹.

A reference implementation of this model has been coded using Python's scientific computing functionality (Oliphant, 2007). A Lagrangian, time-driven mass transport model (Rossman and Boulos, 1996) has been included to model the advection and mixing of turbid water and for calculating the turbidity at DWDS points of supply. The mass transport model tracks the concentration and volume of a number of discrete water plugs as they move through each pipe. It assumes complete and instantaneous mixing. The reference implementation can presently model only a single pipe.

Results and discussion

The model constructs were initially verified through supplying the reference implementation with artificial data. Figure 3 demonstrates the functionality of the model using a simple shear stress profile. Although the condition of 250 layers was tracked during the execution of the simulation the changing condition of just three layers has been plotted to illustrate the presented concepts (Figure 3a–ii). All layers are eroded by the first step increase in shear with the weakest material being eroded more quickly, as can be seen in the plot of φ . Material with strengths of 0.2 and 0.3 Pa then regenerates to a maximal level when the shear drops to below 0.2 Pa. Upon a second step increase in shear stress only the strongest of the three explicitly depicted shear strengths withstands the eroding forces. All three identified strengths then subsequently regenerate when the applied shear stress drops down to 0.1 Pa. Figures 3a–ii and 3a–iv show two spikes in the mass release rate dN(t)/dt and the downstream turbidity T(t) that correspond to the erosion driven by the two step increases in shear stress. Note that the model permits different layer strengths to erode from strongest to weakest but regenerate independently.

The functionality of the proposed model was further verified through calibrating the model using the flow and turbidity data associated with three consecutive flow trials. The flow in a trunk main that links a treatment works to a service reservoir was temporarily increased for operational reasons on three separate occasions over a 72.2 day-period to atypical levels. The concrete-lined ductile iron main is $3.7 \, km$ long and has an internal diameter of 440 mm. The system configuration and the first of the flow trials are detailed in Seth et al. (2009). Discolouration issues associated with the main persisted following the upgrade of the treatment works' filters, suggesting that turbidity events were due to material mobilisation within the main.

The following data were collated for calibrating a model of the trunk main:

- Pipe flow ($\Delta t = 1 \min$ for trials 1 and 3; $\Delta t = 15 \min$ for trials 2 and between trials).
- Turbidity at the downstream end of the main ($\Delta t = 10 s$ for trials 1 and 3; $\Delta t = 5 25 min$ for trial 2; no monitoring between trials).
- Turbidity at the upstream end of the main (i.e. treatment outflow; $\Delta t = 15 min$).

The aim was to minimise the dissimilarity between the turbidity observations during the trials and the turbidity prediction generated by the model.

The trunk main was modelled as a single length as it does not feature any branches and there is little evidence for longitudinal variation in material accumulation quantities or rates. A shear stress

¹In the version of this article published as doi:10.2166/ws.2013.176, the units of dN(t)/dt were erroneously stated as $TPMU \cdot Pa^{-1} \cdot m^{-2}$ and the units of α were erroneously stated as $TPMU \cdot m^{-2} \cdot s^{-1}$.



Figure 3: A demonstration of how the proposed model generates a turbidity response at the downstream end of a single pipe. Pipe internal diameter = 75 mm; roughness= 0.1 mm; length= 20 m; $\Delta t = 0.5 s$; 250 τ bands ($\Delta \tau = 0.0026 Pa$); if $\tau_i < \tau_a (t = 0)$ then $\varphi (t = 0, \tau_i) = 0$ else $\varphi (t = 0, \tau_i) = 1$; $\beta_e = 0.1 Pa^{-1} \cdot s^{-1}$; $\beta_r = 0.005 s^{-1}$; $\alpha = 4.0 TPMU \cdot Pa^{-1} \cdot m^{-2}$; flow $Q \in [0.68, 1.75] L \cdot s^{-1}$. (a) From top to bottom: (i) a temporal shear stress profile (model input); (ii) the changing condition $\varphi (\tau, t)$ for $\tau \in \{0.2, 0.3, 0.4\}$ due to erosion and regeneration; (iii) the rate of material release dN(t)/dt due to the erosion of all layers weaker than the shear stress; (iv) the turbidity response (model output). (b) Variation in relative material condition φ with respect to time and shear strength. White indicates shear strengths that are completely depleted; black indicates maximal material at a shear strength.

time-series profile was calculated from the flow profile using a Darcy Weisbach roughness of 0.1 mm (from a calibrated hydraulic model of the main). Relative material quantities were tracked for 100 discrete shear strength bands; these bands correspond to the range of shear stresses experienced over the simulation period $(1.55 \times 10^{-11} \text{ to } 7.73 Pa)$.

Estimating the amount of material φ at each strength τ_i at t = 0 is non-trivial as the initial system state depends on the material erosion and regeneration over the months or possibly years prior to the first flow trial. Stepped flow increases during the first trial showed that significant material erosion only occurred when the shear stress was increased from approximately 3.0 to 3.3 Pa. It was therefore assumed for this first verification that $\varphi(\tau_i, t = 0) = 0$ if $\tau_i < 3.15 Pa$ otherwise $\varphi(\tau_i, t = 0) = 1$ for each strength τ_i .

The upstream turbidity profile was used as an input to the Lagrangian transport mechanism to model the influx of suspended material from upstream.

Once the model had been configured, it was calibrated by manually adjusting the model parameters to minimise the integral of squared errors (ISE) between non-zero turbidity observations and the corresponding turbidity predictions. The best achieved fit is shown in Figure 4 ($ISE = 1136 NTU^2$ and $R^2 = 0.73$ with $\beta_e = 1.66 \times 10^{-4} Pa^{-1} \cdot s^{-1}$, $\beta_r = 5.84 \times 10^{-8} s^{-1}$ and $\alpha = 1.13 TPMU \cdot Pa^{-1} \cdot m^{-2}$). The model fit over each of the three trial periods is shown in more detail in Figure 5.

Figures 4 and 5 demonstrate that the proposed model is capable of emulating material erosion and regeneration over a period that features three successive flow trials using a continuous stream of data and a constant parameter set. The strength-dependent nature of the erosion process and strength-independent regeneration process can be seen in the time-series plots of relative material for selected strength bands.

A manual exploration of the parameter space for the model instance used for validation suggested that for a given dataset there are multiple fitting optima and there is covariance between the parameters. To further complicate (and potentially increase the dimensionality) of the model fitting process, there is uncertainty in the initial system state. It may therefore be desirable if not mandatory to use a metaheuristic such as evolutionary or swarm optimisation (e.g. Kennedy et al., 2001) to efficiently explore the problem space when fitting the proposed model to a dataset. In addition, it may be possible to achieve more accurate calibrations if continuous rather than flow-trial-specific turbidity data are used.

The model is largely mesh independent i.e. the material mobilised over a simulation N_{total}



Figure 4: Details of model validation for a 3.7 km-long trunk main. (a) Boundary shear stress profile over and between three flow trials covering a 72.2 day period. (b) The variation in relative material quantity φ for three selected shear strength bands shows erosion and regeneration occurring at different strengths.



Figure 5: Model validation for 3.7 km-long trunk main. (a) Boundary shear stress profile, (b) predicted variation in relative material quantity φ for selected shear strength bands, (c) predicted material flux rate dN(t)/dt from each m^2 of pipe wall and (d) predicted and observed turbidity response at the downstream ('d/s') end of the main for each of three successive flow trials.

is relatively independent of both $\Delta \tau$ and Δt as is necessary for a numerical model. However, the accuracy of N_{total} asymptotically converges as the values of $\Delta \tau$ and Δt decrease (Figure 6), thus sensitivity analysis can be conducted to give maximum sensible values for both and limit the computational effort required for simulations. When calibrating the model for real-world systems the maximum values of $\Delta \tau$ and Δt may be limited by the accuracy and precision of the model inputs and the instrumentation used to capture that data and also by the accuracy desired by the end user.

Currently the same values of α , β_e and β_r are assumed for all shear bands i.e. the model is simpler than the four-parameter PODDS model; however the implementation of the proposed model allows the inclusion of varying values of α , β_e and β_r , allowing for more complex behaviour to be reproduced if required. It is also felt that parameters α , β_e and β_r are more physically realistic than their PODDS counterparts and relative values can be intuited for different systems. In accordance with the observations in Husband and Boxall (2010) and Husband and Boxall (2011) an unconditioned, corrodible, unlined iron pipe is expected to release much material during erosion (high α) but this process is unlikely to result in material exhaustion (low β_e). The subsequent regeneration should be relatively quick (high β_r). In polyethylene (PE) pipes β_e should be relatively high as material exhaustion can easily be achieved although the amount of material mobilised, and therefore α , will be low. Regeneration and β_r will be slower and lower than for unlined iron pipes. β_r represents different processes in unlined iron and PE pipes; it is a proxy for a variety of complex processes including iron corrosion, scale formation, slime development and biofilm growth.

The shear strength range over which material erosion and regeneration are to be discretely tracked must be decided at the start of a model run. It is computationally inefficient to simply pick a large number for τ_{max} , the upper bound of that range. For a particular simulation τ_{max} could be



Figure 6: Sensitivity of the proposed model to $\Delta \tau$. (a) dN(t)/dt and T(t) for a constant τ range but different values of $\Delta \tau$ (given a pulse increase in τ_a). (b) The accuracy of the model predictions asymptotically improves when $\Delta \tau$ decreases.

set to the shear stress above which material erosion has not been detectable in similar mains to the one being modelled. However, there is contradictory evidence for the conditions required for 'clean' pipes:

- In the Netherlands pipes are considered clean if flushed at $1.5 \, m \cdot s^{-1}$ (Vreeburg and Boxall, 2007).
- Attempts to calibrate the PODDS model for plastic mains in the UK indicated that no more material was being eroded from the wall when the shear stress exceeded $\approx 1.2 Pa$ (Husband and Boxall, 2010) yet Sharpe et al. (2010) saw material erosion at much higher shear stresses in PVC pipes under laboratory conditions.
- During hydrant flushing fieldwork Husband and Boxall (2010) did not find any evidence of there being a cleaning shear stress in unlined iron pipes.

Instead, one could attempt to measure rather than estimate the cleaning shear stress for the main(s) of interest but this may not be practical given the cost in terms of water wastage, energy, time and money and the risk to customers. It is suggested that a risk-based approach be taken and τ_{max} be based on the maximum shear stress that a main is anticipated to experience. A value can therefore be determined by the modeller by estimating the maximum flow over the simulation period. The method for calculating that flow will depend on whether the motivation for the modelling work is to study the discolouration risk that may result from a burst (in which case the orifice equation could be used to estimate flows) or from deliberately increasing the mean flow up to a target level for operational reasons.

The proposed model still requires thorough validation, primarily to explore the error in predictions made using calibrated models and continuous flow data. This should be done through testing its applicability to different systems. It is also necessary to investigate whether temporal variance in parameters such as β_r is significant and therefore needs to be modelled.

It is the intention to integrate the model within an existing hydraulic modelling package, as was done for PODDS. This will allow for the modelling of dendritic and looped multiple-pipe systems and could allow simulations to be set up and executed from a graphical environment that is familiar to the water industry and academia.

Conclusions

In this paper a new model has been proposed for tracking over time both the erosion and accumulation/regeneration of cohesive layers of discolouration material from the walls of water distribution systems. The existing PODDS model may be suitable for modelling material erosion but its formulations do not represent material regeneration processes. The proposed model is not subject to that limitation. A software implementation and a material transport model have been coded as software so as to verify the empirical, numerical model and test for mesh independence. The model's material-strength-dependent erosion and strength-independent regeneration processes have been demonstrated through manually fitting the model to continuous flow and partly continuous turbidity data from a series of trunk main flow trials. If the model can successfully be validated then it could be used to design and schedule flow conditioning operations for managing discolouration risk.

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