The prediction of solute transport in surcharged manholes using CFD

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Abstract Solute transport processes occur within a wide range of water engineering structures, and urban drainage engineers increasingly rely on modelling tools to represent the transport of dissolved materials. The models take as input representative travel time and dispersion characteristics for key system components, and these generally have to be identified via field or laboratory measurements. Computational Fluid Dynamics (CFD) has the potential to reveal the underlying hydraulic processes that control solute transport, and to provide a generic means of identifying relevant parameter values. This paper reports on a study that has been undertaken to evaluate the feasibility of utilising a CFD-based approach to modelling solute transport. Discrete phase modelling has been adopted, as this is computationally efficient and robust when compared with the time-dependent solution of the advection–dispersion equation. Simulation results are compared with published laboratory data characterising the dispersion effects of surcharged manholes, focusing specifically on an 800 mm diameter laboratory manhole for a flowrate of 0.002 m^3/s and a range of surcharge depths. Preliminary indications are that the CFD results adequately replicate the measured downstream temporal concentration profiles, and that a threshold surcharge depth, corresponding to a change in hydraulic regime within the manhole, can also be identified.

Keywords Computational Fluid Dynamics (CFD); dispersion; hydraulic regime; manhole; sewer; solute transport; surcharge

Introduction

Solute transport processes affect the performance of a wide range of water engineering structures, including water supply reservoirs, stormwater retention ponds, sewage treatment wetlands and combined sewage overflows. In the context of urban drainage, future legislation is likely to increasingly focus on the effects of dissolved pollutants. The behaviour of dissolved materials within urban drainage systems is determined by the two main solute transport processes, advection and dispersion. Dispersion effects may act to reduce or eliminate first foul flush effects or to moderate peak concentrations associated with intermittent discharges. Dispersion also implies that pollutant materials may be present a long time before and after predictions based on mean travel time would suggest. Urban drainage network models that predict the transport of dissolved substances are increasingly used. Some of the models transport the pollutants by advection only, while others (e.g. MOUSETRAP) also account for the effects of dispersion. Dispersion in sewer pipes may be straightforward to estimate, as it is a function of friction and shear effects (Guymer *et al.*, 2005). However, knowledge regarding these processes in ancillary structures – including manholes – is limited. In some instances laboratory or field measurements have been conducted (see e.g. Guymer *et al.*, 2005), but these are time consuming and case specific. It is clear that a versatile and generic approach for determining the dispersive effects of urban drainage structures would be of benefit.

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Computational Fluid Dynamics (CFD)-based software tools enable engineers to simulate flow patterns and associated pollutant transport mechanisms within both natural and engineered hydraulic structures. Grimm (2004) undertook detailed analysis of two CFD-based approaches to modelling solute transport in a pipe. The approaches used were: a species model, in which the solute was modelled as a second species with identical physical properties to water; and a discrete phase (or particle tracking) approach, in which the solute was modelled by tracking large numbers of very small neutrally-buoyant particles through the flow field. Of the two, the discrete phase modelling approach was found to be more computationally efficient, with comparable predictive ability to the species model. The present paper therefore adopts the particle tracking approach to consider the effects of a surcharged manhole on solute dispersion characteristics.

Guymer *et al.* (2005) presented comprehensive data from laboratory experiments on the travel times and dispersion associated with a solute pulse passing through a surcharged manhole. Four manhole diameters were considered over a broad range of flow-rates and surcharge depths. Of particular interest in this work was the identification of a threshold surcharge level at which the solute transport characteristics indicated a sharp transition between pre- and post-threshold conditions; at surcharge levels below the threshold the travel times varied linearly with discharge, whilst above the threshold travel times dropped to a low and constant level. This behaviour has been interpreted as reflecting two distinct hydraulic regimes; pre-threshold the incoming flow mixes throughout the manhole volume, whilst post-threshold the upper volume of fluid within the manhole appears to be cut-off, forming a dead zone which incoming flow passes beneath. This data clearly represents an interesting test for a CFD model, and this paper presents the preliminary results of a study aimed at reproducing and extending this data set. The preliminary study focuses on one manhole configuration (800 mm diameter), under one flow rate (0.002 m^3/s), with surcharge depths ranging from 15 to 300 mm. Direct validation of the CFD flow field prediction was not performed, as appropriate laboratory data were not available. The retention time distributions (RTD) and calculated travel times, however, may be seen to provide a useful indirect means of validation.

Model configuration

Physical manhole model

The 800 mm diameter manhole considered was a circular manhole structure with no benching, as shown in Figure 1. The centreline of the inlet and outlet pipes passed through the vertical axis of the manhole. The study was performed under steady state conditions using Fluorometry. Two modified Series 10 Turner Design fluorometers were

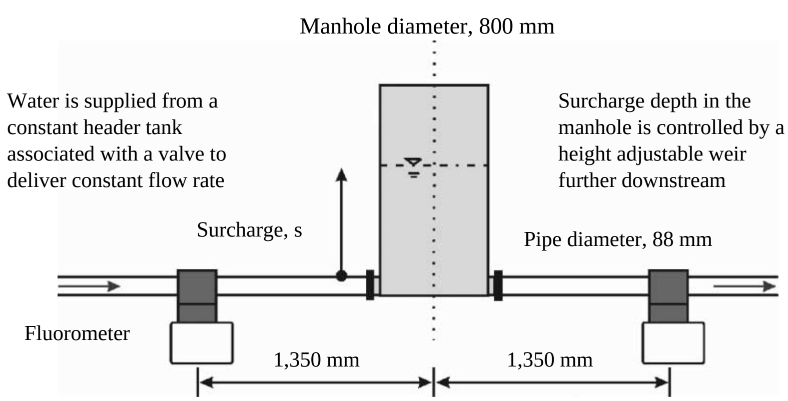

Figure 1 Experimental configuration (after Guymer *et al.*, 2005)

fixed at 1.35 m from the manhole centrelines on both sides to monitor temporal concentration distributions of the injected dye, Rhodamine WT. In order to ensure that the dye was fully mixed before reaching the fluorometers, the injection was made 10 m upstream.

CFD manhole model

The simulations were undertaken using the Gambit (version 2) pre-processor software for generation of the computational mesh, and the Fluent (version 6) CFD software for numerical analysis. To minimise computational time and effort, the CFD model inlet and outlet corresponded to the positions of the two fluorometers, with a total longitudinal distance of 2.7 m. The complex geometry of a circular manhole prohibits the use of a 2 dimensional model for representation. A previous CFD manhole study (Asztely and Lyngfelt, 1996) attempted to predict head loss in a surcharged manhole using a 3 dimensional symmetrical model, i.e. only half of the manhole was simulated in 3 dimensions. Results at high 'surcharge to pipe diameter' ratio were in good agreement with experimental findings. However, at lower surcharge levels the CFD predictions deviated noticeably because the symmetry of the model was unable to reproduce observed non-symmetrical flow patterns, which relate to the head loss mechanisms in a manhole. As a result, it was decided to model the entire study section in 3 dimensions. The 3 dimensional model was predominantly mapped with hexahedral cells with the total number of cells ranging from 55,000 to 130,000, depending on surcharge depth.

Numerical models

Flow field simulation. The Renormalized Group (RNG) k-ϵ turbulence model, developed by Yakhot and Orszag (1986), was chosen for flow field simulations. The selection of this model was based on its enhanced ability to deal with swirling flow (Fluent, 2001) and the research group's previous experience. Dennis (2000) documented five possible flow regimes occurring in a surcharged manhole, some of which included surface swirling and internal recirculatory flows. Consideration was given to the most suitable method for representing the manhole free-surface. Although algorithms such as the Volume of Fluid (VOF) model (Fluent, 2001) allow the position of the air–water interface to be determined from the flow boundary conditions, such multiphase approaches are computationally expensive. For this reason the free surface was represented using a 'rigid lid' approximation. Other boundary conditions were defined as follows: the inlet boundary was defined as a velocity inlet, using a fully developed velocity profile generated from a 10 m length of straight pipe; the outlet was defined as a pressure outlet; and non-equilibrium wall functions were employed to solve the near wall flow field. It was thought that the effect of wall roughness on the global flow field prediction would be negligible, and a roughness height of 8×10^{-5} m was assumed (Grimm, 2004).

Solute transport modelling. Two CFD modelling architectures, Lagrangian and Eulerian, are available for solute transport modelling. The one considered in this paper is a Lagrangian approach, the Discrete Phase Model, which models the solute phase as a large number of discrete particles. The model predicts particle trajectories using a force balance equation, i.e. equating the particle inertia with the forces exerted on the particle. The local turbulence eddy characteristics of a particle are simulated via a stochastic modelling process, in which the local turbulence properties link to the time-averaged turbulent kinetic energy and a Gaussian probability distribution (Fluent, 2001). Stochastic modelling implies that a large number of realisations (or particles) are required to attain statistically meaningful results. Grimm (2004) suggested that 60,000 individual particles should be sufficient. Since the travel time of a solute was of interest, the properties of the particles were set identical to water and had a diameter of 1 μm (based on the recommendation of Grimm, 2004). This eliminates the effects of buoyancy and sedimentation due to differential density of the fluid and particle phases. The simultaneous injection of 64,000 neutrally buoyant particles was undertaken evenly across the model inlet. The travel time of a particle was defined as the time taken for it to pass from model inlet to outlet.

Solute transport prediction

Output manipulation and model validation

Fluent reports the solute transport predictions in the form of individual travel times for 64,000 particles. These individual times were assimilated into a Retention Time Distribution (RTD) using a histogram process. However, the RTD curve obtained from an instantaneous injection cannot be compared directly with the laboratory observations, as the laboratory inlet profiles are usually Gaussian or skewed. A comparable outlet trace was therefore generated through the superposition of outlet profiles in accordance with the measured inlet profile. Figures 2a and 2b present examples of the routed RTD profiles, normalised with the total number of injected particles. In the same figures, for comparative purposes, the corresponding laboratory observations have been normalised with the total area under the curve. It should be noted that the examples shown in Figures 2a and 2b were randomly chosen for the purpose of presentation. There may be cases where the goodness of fit of the CFD profile to the recorded is worse or better than those presented.

The simulation results, shown in Figures 2a and 2b, provide some confidence in the use of CFD for the prediction of flow and solute transport in surcharged manholes. In general, the important features of the recorded profiles, such as time of peak, peak magnitude and the decaying mode of the tail, are reproduced by the simulations in a similar fashion to the laboratory observations. Guymer *et al.* (2005) identified a transition in mixing mode in the manhole as a function of surcharge. At low surcharges (e.g. 90 mm, Figure 2a), a fully mixed condition seems to occur. This is reflected in significant peak attenuation, followed by an approximately exponentially decaying tail. At high surcharges (e.g. 300 mm, Figure 2b), the transport mode appears to be dominated by advection, with comparatively limited mixing occurring in the manhole. In this preliminary study, the CFD predictions have also revealed these two distinct flow regimes. However, in both cases the CFD data clearly indicates a secondary peak in the downstream tracer profile. In the low surcharge case the laboratory data gives no indication of a secondary peak, whilst in the high surcharge case a secondary peak is evident, though it occurs sooner and the peak value is marginally higher than the CFD results suggest. The occurrence of these secondary peaks clearly warrants further investigation. However, the primary aim

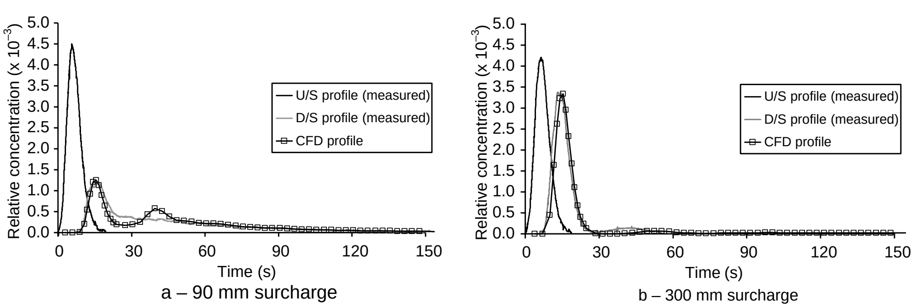

Figure 2 Comparison of the normalised laboratory observations and the routed RTD profiles

of the current study is to evaluate the effects of manhole configuration on the timing and magnitude of the peak discharge; the fits of the simulated downstream profiles to the measured data were judged acceptable for this purpose.

Mean travel time results

Figure 3 presents the variation of mean travel time with surcharge of the laboratory observations (after Guymer *et al.*, 2005) and the CFD predictions. It might be expected that the mean travel time in the physical model would be directly proportional to surcharge because of the corresponding change in storage volume. However, Figure 3 indicates that this is only the case at low levels of surcharge; beyond a threshold depth a marked reduction in travel time occurs. For surcharge levels above the threshold (about 210 mm) the mean travel times remain at a low and nearly constant level. The threshold is believed to represent the transition between the two hydraulic regimes. The raw CFD predictions (denoted as 'Entire CFD profile' in Figure 3) diverge from the monitored data. No reduction in the mean travel time at high surcharges is evident, although there is some evidence of non-linear behaviour around the threshold depth. At low surcharges, the CFD results tend to over-estimate the travel time by up to 10 s.

Discussion

Effect of extreme residence times

From the goodness of fit of the routed and measured profiles shown in Figure 2b, it is not immediately obvious why the differences between measured and simulated travel times at high surcharge levels should be so pronounced. Although there are disagreements between the profiles, such as the shape of the falling limb and a slight delay of the peak arrival, the important characteristics of the routed CFD profile show good agreement with the observed distributions.

One explanation that can be offered for this anomaly may relate to mass recovery of the injected particle/solute. One of the important features of the Discrete Phase Model is that it guarantees a high particle recovery, usually 100%. As a consequence, the model would not lose track of any particles moving through a flow domain, even a particle that might have been trapped in a dead zone or boundary layer for a significant length of

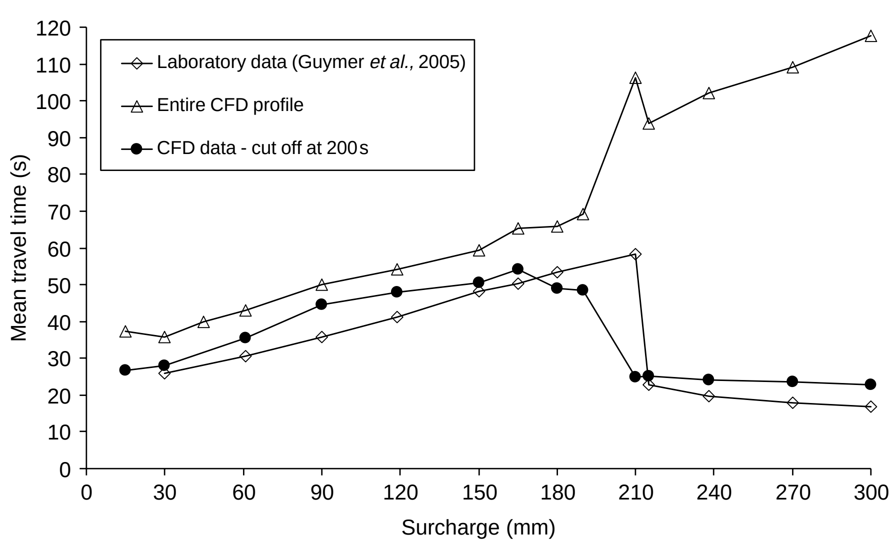

Figure 3 Variation of mean travel time with surcharge

time. The inclusion of such 'super-retained' particles in the mean time calculation may increase its value quite considerably. For example, in Figure 2b the mean residence time recorded is 117.7 s. However, the maximum residence time of the last escaped particle is recorded at 2,540.3 s, which is more than 20 times higher than the mean residence time. In practice, these extreme values are usually non-measurable in the laboratory due to limitations in instrument sensitivity. The effects of 'super-retained' particles on mean travel time were studied via a profile truncation process. A cut-off point of 200 s was selected; this was observed to be close to the last data point of the measured concentration profile. The revised mean travel time results for this truncated downstream profile are also displayed in Figure 3. A sharp transition in the mean travel time is evident at approximately 210 mm surcharge, and the revised CFD travel times provide a good match to the measured laboratory data. Importantly, the CFD results identify the threshold surcharge depth (transition from fully-mixed to cut-off volume) to within 5% of the laboratory observations. One limitation of this subjective approach to the elimination of 'super-retained' particles is the potential impact on mass recovery. In fact, at low surcharges, a high mass recovery (around 97%) was still attained. For high surcharge cases, mass recovery dropped to around 82%. Further investigation is required to define a more robust scientific approach that will enable fair comparisons to be made between travel time and dispersion characteristics obtained from laboratory measurements and CFD output.

The relationship between flow field and solute transport

One of the strengths of CFD is its ability to demonstrate the flow field for any specified plane in a flow domain. Such information can enhance the understanding of the mixing process in the manhole, as solute transport is the consequence of fluid motion. Due to page length constraints, only two scenarios, 90 mm and 300 mm surcharge, are covered. Two flow planes, the central vertical plane and the horizontal plane centred on the pipes, are presented in each case.

Central vertical plane. The flow fields for the two cases on the central vertical plane are shown in Figure 4. The first noticeable dissimilarity may be spotted in the behaviour of the submerged jets. At the low surcharge, the jet appears to expand and experience a high rate of energy exchange, which can be observed in the decay of maximum jet velocity. Whereas, at the high surcharge, the jet spreading is minimal, leaving a horizontal jet propagating straight through the manhole with much less mixing with the fluid in the structure. The flow regime appears to segregate into two regions, developing a dead zone above the boundary of the jet and the surcharge volume and a straight through section underneath. Compared with the low surcharge case, in the high surcharge case the jet core velocity reduces less with distance travelled.

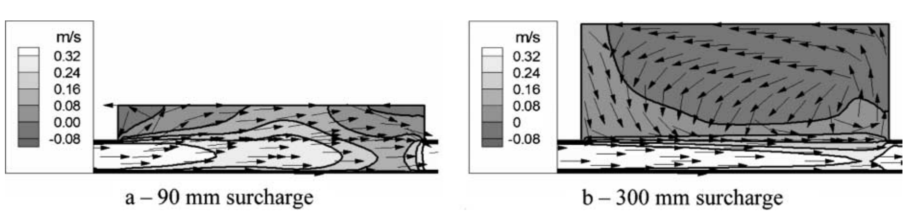

Figure 4 Longitudinal velocity contours with velocity vectors in the 800 mm diameter manhole on the central vertical plane (flow direction – left to right)

Horizontal plane at mid pipe depth. An interesting flow pattern is shown in the low surcharge case. The geometry of the CFD manhole model generated was totally symmetrical in shape and a fully-developed velocity profile was specified at the model inlet. However, the CFD model predicted an asymmetrical flow field, as shown in Figure 5a. A vortex is formed in the manhole adjacent to the impinging jet which tends to drag the jet towards the swirling centre. As a result, the jet shape is distorted. The chaotic and swirling motion of the flow field suggests that the solute is likely to approach fully mixed condition within the manhole. Figure 5b displays the flow pattern on the horizontal plane of the high surcharge case. It is evident that the asymmetrical flow pattern is replaced with a symmetrical flow field. The impinging jet tends to extend transversely as it travels downstream, but ceases to spread in proximity to the manhole outlet. This may be attributed to the combined effects of the space constraints due to the manhole wall and the dragging force induced by the exiting flow. Near the manhole outlet, because of the wall boundary, water is forced to re-circulate back towards the centre of the manhole. Comparing the degree of jet spreading in Figure 4a (vertical) and 4b (horizontal), the jet seems to extend more widely in the transverse direction.

Correlation of the flow field and the mean travel time prediction. At pre-threshold depths the flow profiles can be characterised by an asymmetrical flow in association with a swirling motion. This hydraulic regime appears to promote a fully mixed condition in the manhole structure. As a result, the effective mixing volume in the structure increases with the surcharge volume; and hence mean travel time exhibits a linear relationship with surcharge. In addition, the arrival time of the peak in Figure 2a is later than that in post-threshold. This is because of the high decay rate of the maximum velocity in the core.

The flow regime at post-threshold depths can be regarded as two separated regions, a surcharge volume situated above a straight through section. In the straight through section, a low degree of jet spreading significantly reduces the number of particles dispersing into the dead zone. Figure 2b suggests that approximately 70% (the Gaussian shaped portion of the distribution) of the total particles experience short-circuiting, i.e. without any mixing in the manhole. It was found that increasing the surcharge depth led to an increase in the recirculation volume but with no effects on solute transport within the straight through section. This portion of the solute (70%) is dominated by advective transport, and is essentially independent of surcharge depth. Therefore only 30% of the total particles would be influenced by depth variations at post-threshold depths. Differences in the surcharge volume are evident in the form of the secondary peak and the tail of the distribution. This may also explain the noticeable effects on the mean travel time when the cut-off scheme was applied.

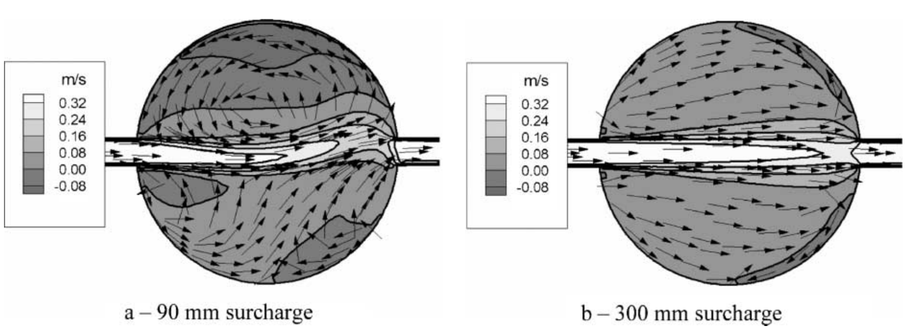

Figure 5 Longitudinal velocity contours with velocity vectors in the 800 mm diameter manhole on the horizontal plane at mid pipe depth (flow direction – left to right)

Transferability

Guymer *et al.* (2005) presented experimental results that showed that the threshold depth was independent of discharge, but varied as a function of manhole diameter. The present paper forms part of a project aimed at utilising both experimental and CFD modelling approaches to identify generic scaling laws for solute transport in manholes. Similar approaches have also been utilised to identify the solute transport characteristics of storage tanks (Stovin and Grimm, submitted).

Conclusions

This paper conducted a study to evaluate the feasibility of utilising a CFD-based approach to modelling solute transport in a surcharged manhole. The study focused on an 800 mm diameter manhole operated at one flow rate, 0.002 m^3/s. Simulations were undertaken using the RNG k-ε turbulence model for the flow field and with the Discrete Phase Model for solute transport simulation. Validation of the CFD predictions was carried out by means of retention time distributions (RTD) comparison, an indirect means of validation. Although there was some disagreement between the simulated and observed recession limbs, good representations of the first peak arrival time and magnitude were observed.

Considering the mean travel time results, the raw CFD predictions deviated significantly from the measured data. A transition in the mean travel time, i.e. a sudden reduction in the mean time at high surcharges, was not identified and an over-prediction of the mean time up to 10 s at low surcharges was observed. When a cut-off was applied to the 'tail' of the simulated concentration profile, the revised mean travel time provided a good match to the observed laboratory data. Importantly, the threshold depth was established to within 5% of the laboratory observations.

Examples of flow fields at pre- and post-threshold surcharges were shown. At pre-threshold, the chaotic and swirling motion appeared to promote a fully-mixed condition in the manhole. Under this condition, travel time has a direct relationship with surcharge. At post-threshold, the flow regime was found to be detached, forming a straight through section underneath a dead zone. Varying surcharge changes the mixing conditions of the dead zone but does not affect the straight through section. As the advection process is dominant in post-threshold mixing, i.e. mixing is reliant upon the conditions of the straight through section, travel time appears to be independent of surcharge volume.

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