# Release of hydrogen sulfide under intermittent flow conditions – the potential of simulation models

Natércia Matias, Rita Matos, Filipa Ferreira, Jes Vollertsen and
José Saldanha Matos

## ABSTRACT

For engineering purposes it is especially useful to be able to predict and control sewer corrosion rates and odor impacts as well as to design effective measures aiming to reduce effects related to hydrogen sulfide formation and release. Doing so, it is important to use modeling tools that are capable of assessing variations of dissolved oxygen, dissolved sulfide and hydrogen sulfide gas concentrations for a wide range of environmental scenarios. Two such models were assessed: AEROSEPT, an empirical formulation, and WATS, a conceptual and more complex approach. The models were applied to evaluate the effects of transitions between pressure mains and gravity sewers in the air–liquid mass transfer of hydrogen sulfide at the Ericeira sewer system in Portugal. This network is known to have odor and corrosion problems, especially during summer. Despite the unavoidable uncertainties due to the unsteady flow rate and the quantification of air velocity and turbulence, the simulation results obtained with both models have been shown to adequately predict the overall behavior of the system.

**Key words** | air–water mass transfer, hydrogen sulfide gas, intermittent discharges, modeling, turbulence

**Natércia Matias** (corresponding author)
**Rita Matos**
**Filipa Ferreira**
**José Saldanha Matos**
Department of Civil Engineering, Architecture and Georesources (DECivil) & Civil Engineering Research and Innovation for Sustainability (CERIS),
Instituto Superior Técnico (IST), University of Lisbon,
Avenida Rovisco Pais, 1049-001 Lisbon,
Portugal
E-mail: *natercia.matias@ist.utl.pt*

**Jes Vollertsen**
Department of Civil Engineering,
Aalborg University,
Sofiendalsvej 11, DK-9200 Aalborg SV,
Denmark

## INTRODUCTION

Intense and continuous urban expansion during the last decades has sparked many challenges to a sustainable development and to the general well-being of society. The effects of this growth have been reflected in sewer systems as well, namely in the planning, design and implementation of increasingly larger, longer and more complex systems. These lead to higher risk of problems related to hydrogen sulfide ($H_2S$) due to physical, chemical and biological changes of the wastewater while flowing along the networks. Awareness of the effects of such changes on the performance of drainage infrastructures has been increasing in the scientific community, and models aiming to forecast dissolved sulfide ($S_D$) and hydrogen sulfide gas ($H_2S_g$) concentrations are available. Nevertheless, this knowledge is not always taken into account for planning and design purposes.

$H_2S$ is one of the species of $S_D$ that, when in its gaseous form, may have important effects on urban infrastructures. These can be summarized as: building up of unpleasant odors (Talaiekhozani *et al.* 2016), creation of toxic and potentially deadly atmospheres in confined spaces, and corrosion of gravity sewers, manholes and pumping stations (Jiang *et al.* 2014; Sun *et al.* 2015), possibly leading to structural weakness and/or collapse (Matos 1992).

$H_2S$ gas, even in concentrations below 1 ppm, is corrosive to metals and, if oxidized on moist surfaces may produce sulfuric acid and attack concrete. It has a characteristic odor of 'rotten eggs', an odor threshold around 0.1 to 2 ppb, and is flammable in the range between 4.3 and 45.5%. $H_2S$ is a deadly gas, whose toxicity has been ranked along with that of hydrogen cyanide by the US Environmental Protection Agency (USEPA 1985), and is considered the primary cause of work-related deaths of sewer system workers (Forsgren & Brinck 2017).

Emission of $H_2S$ to the sewer atmosphere is known to be related to turbulence, pH, temperature and wastewater constituents (Yongsiri 2004). Several studies have addressed the production of sulfide under free surface flow in gravity sewers and the corresponding air–water mass transfer of $H_2S$ (e.g., ASCE 1989; Hvitved-Jacobsen *et al.* 2013).

doi: 10.2166/wst.2017.595

Additionally, a number of formulas have been proposed for predicting emission rates along sewer reaches (e.g., USEPA 1985; Yongsiri *et al.* 2003).

Even though scientific knowledge about sulfides and their consequences in sewer systems has been continuously increasing, fundamental aspects remain relatively unknown. This is the case, for example, of $H_2S$ emissions under highly turbulent and intermittent flow conditions, which is one of the cornerstones to understanding and predicting local odor and corrosion problems encountered at force main discharges, sewer drop structures, and other similar sections throughout sewer networks. Consequently, methods or expressions developed to evaluate the risk of $H_2S$-related problems under these circumstances are still missing in the specialized literature.

For engineering purposes it is especially useful to be able to predict and control sewer corrosion rates and odor impacts as well as to design effective measures aiming to reduce effects related to $H_2S$ formation and release. In order to do so, it is important to use modeling tools that should at least be capable of assessing variations in terms of dissolved oxygen (DO), $S_D$ and $H_2S$ gas concentration for several environmental scenarios.

In this paper the main effects related to sulfide formation and release, as well as their impacts in a sewer system under intermittent and highly turbulent flow conditions, are described. Then, the applicability of two different approaches for modeling this system in terms of quality parameters is analyzed:

- AEROSEPT – AERObiose e SEPTicidade em sistemas de águas residuais, translated as 'aerobic conditions and septicity in sewerage collection systems' (Matos 1992), an empirical formulation; and
- WATS – Wastewater Aerobic/anaerobic Transformations in Sewers (Hvitved-Jacobsen *et al.* 2013), a conceptual and more complex rational approach.

The main objective of this work is to present and discuss the results obtained by the application of these models and evaluate the effects of transitions between pressure mains and gravity sewers in the air–liquid mass transfer of $H_2S$ in the Ericeira sewer system in Portugal. The obtained results are compared with those from local measurements.

It is believed that this type of approach should be thoroughly applied as a support tool on existing and planned systems to define solutions that are more suitable to the local circumstances (Matias *et al.* 2014). An example of this is presented by Vollertsen *et al.* (2015) where the WATS model was calibrated to the complete San Francisco Bayside drainage area, consisting of more than 1,050 km of pipes. Following the calibration, the model has and is being used to assess the operation of the San Francisco network and to aid decision making for both operation and planning.

## METHODS

In order to evaluate the effects that transitions and turbulence in the flow rate have on the $H_2S$ air–liquid mass transfer, the wastewater quality of Ericeira's sewer system was previously characterized in several sections of the network known to have odor problems, especially during the summer season (Matias *et al.* 2017a).

Subsequently, the applicability of two different approaches, AEROSEPT and WATS, for modeling this system is evaluated.

WATS is probably the most complete and well known model for forecasting sulfide build-up in the bulk water and $H_2S$ in the sewer's atmosphere. In this model, both water and gas transport are included, considering not only wastewater and biofilms processes but also those processes taking place on the corroding surfaces. It has been developed at Aalborg University, Denmark, over the last three decades (Hvitved-Jacobsen *et al.* 2013) and is still continuously extended and improved as knowledge on in-sewer processes increases. It exists as a mathematical model able to simulate extended sewer networks (Vollertsen *et al.* 2008, 2011a, 2011b). However, to be fully reliable, its application needs appropriate data for calibration.

AEROSEPT includes the modeling of relevant processes that occur in sewer systems under aerobic and anaerobic conditions and was selected because it has also a long record of practical applications, typically for design purposes, in different parts of the world (Engidro *et al.* 2015). Regarding this type of empirical model, however, it should be stressed that they are important particularly when only scarce knowledge on the performance of the system exists or when the available data are limited (Hvitved-Jacobsen *et al.* 2013), which is, unfortunately, often the case.

In addition, previous findings were used to strengthen the AEROSEPT model, namely by including empirical expressions translating relationships between the mass transfer of DO and $H_2S$ with physical parameters of drop structures such as flow rate, drop height and tailwater depth (Matias 2016; Matias *et al.* 2017c, 2017b) – AEROSEPT.V02.

Furthermore, results from intensive field measurements in terms of hydraulic and wastewater quality parameters and $H_2S$ gas phase concentrations (Matias *et al.* 2017a) were used to verify the overall hydraulic behavior of the system using the Storm Water Management Model (SWMM) and, in some measure, calibrate both models.

## AEROSEPT model

The AEROSEPT model was initially developed by Matos (1992) and is based on the experimental and theoretical studies of Pomeroy (1959), Parkhurst & Pomeroy (1972); Pomeroy & Parkhurst (1972, 1977) and Matos & Sousa (1989, 1990). This model was calibrated and validated with several experimental data obtained in Portugal and in the USA.

For the aerobic phase, the expressions for reaeration and oxygen consumption in the liquid phase of ASCE (1989) were used and oxygen consumption in the biofilm was modeled according to Matos (1992). For the prediction of sulfide build-up along rising mains, the empirical equation proposed by Pomeroy (1959) was applied and, for partially filled sewer pipes, the Pomeroy & Parkhurst (1977) model was used. Regarding the $H_2S$ in the sewer's confined atmosphere, it assumes that it cannot escape from the system and that the air velocity may be estimated taking into account the liquid drag force according to the results of Pescod & Price (1982).

## WATS model

WATS is a concept for sewer process modeling developed over the last three decades (Hvitved-Jacobsen *et al.* 2013) that describes the transformation of organic matter, oxygen, oxidized nitrogen compounds and sulfurous compounds. Based on this concept a computer model capable of simulating complex catchments was developed (Vollertsen *et al.* 2008, 2011a, 2011b).

WATS consists of a number of non-linear differential equations describing a number of different wastewater transformations, including: aerobic, anoxic and anaerobic processes in the bulk water, biofilms and sediments as well as oxidation of sulfur compounds on moist sewer surfaces and consequent corrosion (Hvitved-Jacobsen *et al.* 2013).

## Description of the sewer system infrastructures

The Ericeira's wastewater intercepting sewer system includes 13 pumping stations (EE), more than 15 km of main gravity sewers, and a wastewater treatment plant (WWTP), Figure 1.

The formation of sulfide in this intercepting system is closely related to the existence of pumping stations in sequence discharging into gravity trunk sewers, some of which with significant slopes and turbulent conditions. Additionally, high temperatures, especially during summer, are known to worsen the sulfide problem.

## Field measurements

In order to assess the evolution of various quality parameters, both in the liquid and in the gas phase, field studies were carried out with *in situ* measurements of the following parameters:

- liquid phase: dissolved oxygen (DO), pH, temperature (T), redox potential (ORP), conductivity (Cond), $S_D$ (in the form of $HS^-$), wastewater flow rate (Q), velocity ($v_{liq}$) and depth (h);
- gas phase: $H_2S_g$, air-flow velocity ($v_{air}$), temperature ($T_{air}$) and relative humidity (RH).

The procedure has been previously described in detail by Matias *et al.* (2017a). In summary, the following equipment was used:

- YSI556 Multi-Probe System sensors for the continuous measurements of DO, pH, T, ORP and Cond;
- UV-VIS spectrometer to determine $HS^-$ concentration (spectro::lyser™, s::can);
- two gas detectors (models GFM130, 0–5,000 ppm, or GFM101, 0–200 ppm, GASDATA) depending on the expected $H_2S$ concentration in the confined atmosphere;
- a Testo 435 instrument to measure $v_{air}$, $T_{air}$ and RH; and
- four flow meters (one Hawk-eye, Flow Electronics, and three ADS 3600, ADS Environmental Services) depending on the local conditions regarding Q, $v_{liq}$ and h.

The field measurements were done on the 18th, 19th, 25th and 26th of July 2013 on two sections of the intercepting system, Figure 2(a), both consisting of plastic pipes and concrete manholes:

- section 1 – a gravity trunk sewer with low turbulence conditions and no drop structures, receiving intermittent discharges from a rising main with a maximum flow of 6 $L\,s^{-1}$: length of 1,000 m, 200 to 300 mm pipe diameters, and average slope and velocity of 1.4% and 0.9 $m\,s^{-1}$, respectively.
- section 2 – a gravity trunk sewer with high slopes and several drop structures, receiving intermittent discharges from a second rising main with a maximum flow of 54 $L\,s^{-1}$: length around 600 m, pipe diameters from 400

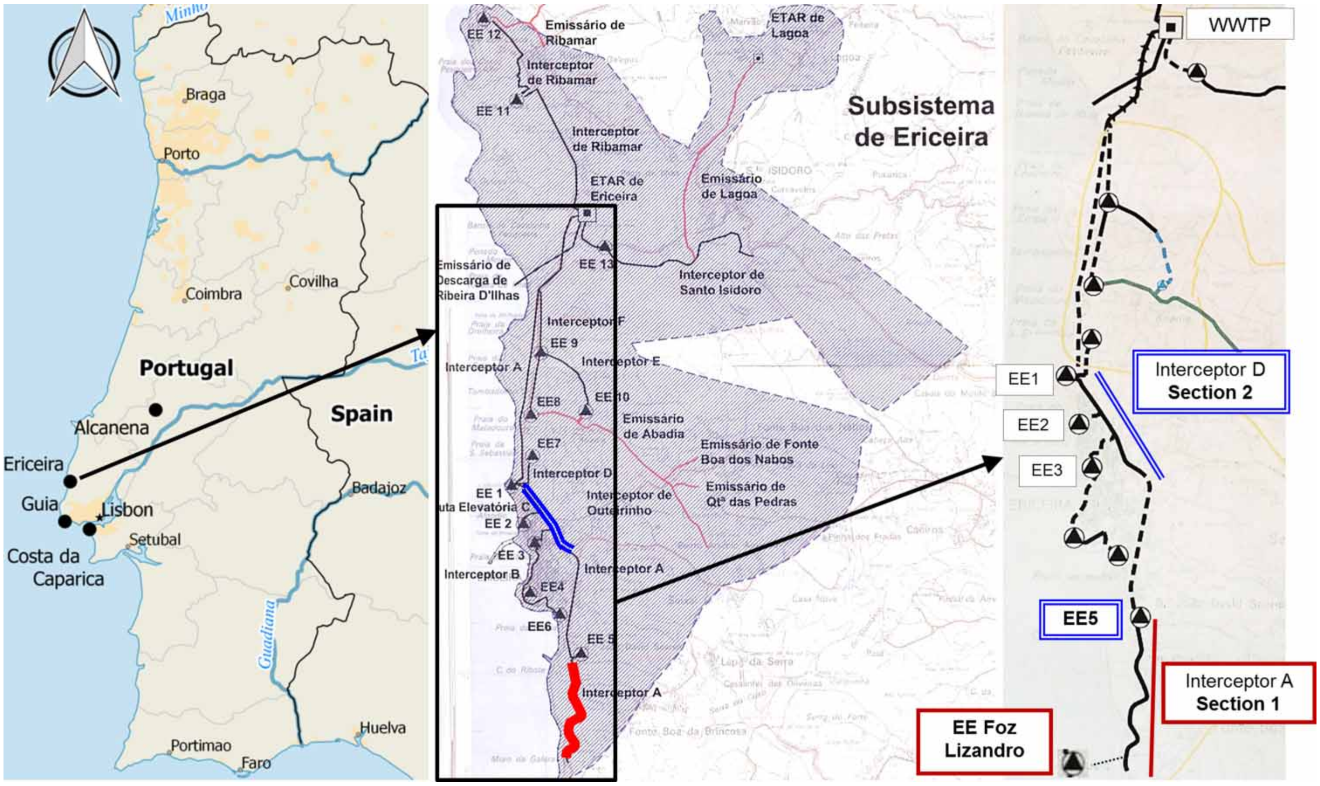

**Figure 1** | Location of Ericeira village, schematic representation of Ericeira's intercepting sewer system and relative position of the sections where field measurements were performed.

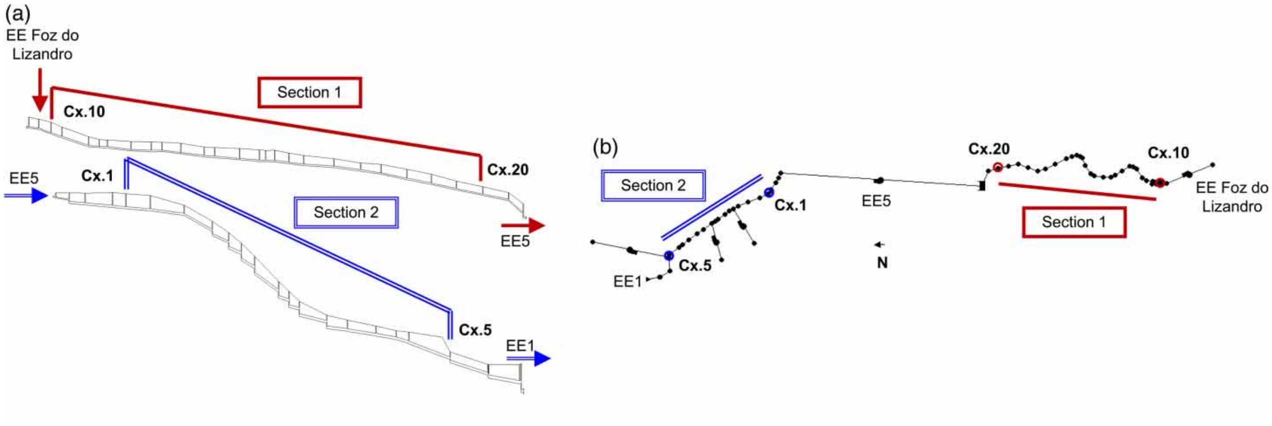

**Figure 2** | (a) Longitudinal profile of sections 1 and 2 including links to the pumping stations (EE) and (b) SWMM scheme of studied area.

to 600 mm and slopes between 0.8 and 7.3%, leading to velocities of up to 4 m $s^{-1}$.

Sampling of two consecutive pumping events were conducted on the 18th and 25th in section 2 and on the 19th and 26th in section 1. Continuous measurements of an additional pumping event in section 1 were also carried out each day. In this case, instead of wastewater sample collection, the YSI equipment was placed at the invert of both Cx.10 and Cx.20, Figure 2(a), and set to save measured data each 20 seconds during an entire pumping event, which lasted between 8 and 10 minutes.

For liquid phase measurements, samples were collected using buckets. This resulted in non-optimal conditions for gas phase measurements as the manhole covers were partially open. Therefore, a specific field study for the gas phase was undertaken in October 2013 and July 2014.

The complete obtained results are presented in Matias *et al.* (2017a) divided into: hydraulic parameters (Q, $v_{liq}$ and h); gas phase measurements ($H_2S_g$, $v_{air}$, $T_{air}$ and RH); and liquid phase measurements (DO, $S_D$, T, pH, ORP and Cond). In this paper, only the ones relevant in terms of the modeling are presented.

## Hydraulic simulation

To estimate hydraulic parameters such as water depth, velocity and flow rate at Ericeira's sewer system SWMM version 5.0, from the USEPA, was used.

The modeled network included only the infrastructures that were part of the field study between Foz do Lizandro and EE1 pumping stations (Figure 1), namely: Foz do Lizandro pumping station and respective rising main, interceptor A, EE5 pumping station and respective rising main, and interceptor D, with a last node, where the discharge from the modeled system was defined, corresponding to EE1, Figure 2(b).

In section 1, and based on the results from the flow meters installed and $H_2S$ gas measurements carried out previously (Matias *et al.* 2017a), the Foz do Lizandro pumping station was set to work hourly between 04:00 and 20:00 with a fixed flow rate of $6\ L\ s^{-1}$ during 10 minutes. Manning's coefficient of the pipes was set at $0.012\ s\ m^{-1/3}$ (typical value for plastic pipes) and the diameters varied according to the information provided by the utility company responsible for the system (SIMTEJO – Saneamento Integrado dos Municípios do Tejo e Trancão, S.A., now AdVT – Águas do Vale do Tejo).

Regarding section 2, EE5 pumping station was not set to work with a specific schedule, but controlled according to the level reached in the well and with a maximum flow rate discharge of $54\ L\ s^{-1}$ (information provided by the utility company). From the discharge of the EE5 rising main up to EE1, the 26 existing manholes were characterized, of which 16 include drop structures with heights ranging from 0.08 to 1.15 m. Since this part of Ericeira's sewer system is older, and based on the observed hydraulic data, Manning's coefficient of the conduits was overall defined as $0.015\ s\ m^{-1/3}$.

Then, existing important tributaries were added to each section and their value used to calibrate the model to the field measurement results.

Results from field measurements and simulations were compared considering a time step for the simulation report equal to the pacing of the flow meters installed in the respective manhole, i.e., 1 minute for Cx.10 and 5 minutes for Cx.20, Cx.1 and Cx.5. Flow rate, velocity and wastewater depth were then analyzed at the link upstream of the manhole or at the node itself.

## AEROSEPT and WATS model scenarios

Following field measurements and hydraulic characterization of sections 1 and 2, both AEROSEPT.V02 and WATS models were applied. Two scenarios were analyzed assuming steady state conditions and compared with the results obtained *in situ*:

- '*Qm*' – system modeled according to the real physical characteristics and so, in order to obtain approximately the same retention time, the flow rate was set to its mean value – in this case, reaeration along the pipes is expected not to be realistic compared to what really occurs after a pumping event;
- '*Qp*' – flow rate set in agreement to what was really being pumped in each event; consequently, turbulence effects at each drop structure and along the pipes are closer to the real conditions. In this scenario, to attain the same residence time as in *Qm*, fictitious pipes with nominal diameter DN = 2 m and the necessary slope to guarantee h/D = 0.5 (area similar to the pumping station well's cross-area), were introduced. Therefore, the effect of the residence time in the wells was considered.

# RESULTS AND DISCUSSION

To simulate Ericeira's sewer system in terms of quality parameters, both AEROSEPT.V02 and WATS models were applied. To do so under equivalent conditions, and as a way to verify the overall hydraulic behavior of the system, the SWMM model was used to estimate hydraulic parameters such as water depth, velocity and flow rate.

## SWMM model

In section 1, to obtain a total travel time and flow rate similar to the ones measured, an existing tributary, which conveys wastewater from a nearby residential neighborhood, was added to the model two manholes upstream of Cx.20 with $2.5\ L\ s^{-1}$.

The simulated hydraulic behavior resembled well those obtained by the flow meters. At Cx.10 a flow rate of $6\ L\,s^{-1}$ entailed liquid velocity and depth around $0.77\ m\,s^{-1}$ and 61 mm, respectively, Figure 3(a). The equivalent values obtained with the flow meter were $0.77\ m\,s^{-1}$ and 67 mm, Figure 3(b). However, both the frequency and duration of the simulated pumping events, Figure 3(a), were set to be higher than the shown measured ones, Figure 3(b). This is due to the fact that the modeled infrastructure, namely Foz do Lizandro pumping station, was set in the model to work for 10 minutes based on the average behavior observed during the field measurements (summer season), but the flow meter available data refer to October. Outside the summer season the wastewater production is significantly reduced, which necessarily leads to lower frequency and duration of the resulting pumping events.

The simulated travel time was 22 minutes which is quite close to the 23 minutes observed on average while conducting the *in situ* measurements (Matias *et al.* 2017a). This travel time corresponds at Cx.20 to a flow rate of about $6.25\ L\,s^{-1}$, liquid velocity of $1.05\ m\,s^{-1}$ and depth of 42 mm. For the same flow rate, the flow meter returned liquid velocity and depth of $1.04\ m\,s^{-1}$ and 41.8 mm, respectively (graph not shown).

Regarding section 2, the objective values, when choosing the most common value after an EE5 pumping event discharge, were:

- Cx.1 – $Q \approx 54\ L\,s^{-1}$, $v_{liq} \approx 0.94\ m\,s^{-1}$ and $h \approx 190$ mm (DN = 380), Figure 3(c);
- Cx.5 – $Q \approx 62\ L\,s^{-1}$, $v_{liq} \approx 2.00\ m\,s^{-1}$ and $h \approx 107$ mm (DN = 520).

In this case, and in order to obtain simulation results similar to the measured ones, close to Cx.1 a Manning's coefficient value of $0.022\ s\,m^{-1/3}$ was considered instead of the generally applied value for section 2, $0.015\ s\,m^{-1/3}$. This difference in roughness was probably due to biofilm on the pipe's walls and/or sediments.

Tributaries were added at the first node with $2\ L\,s^{-1}$, and, between Cx.1 and Cx.5, at 10 manholes with constant inflow values of $0.6\ L\,s^{-1}$. This was intended to simulate the highly densified urban area with quite a number of neighborhoods flowing directly into existing manholes. Under the assumptions presented above, the simulated results from SWMM were satisfactorily close to the average measured flows:

- Cx.1 – $Q \approx 53.04\ L\,s^{-1}$, $v_{liq} \approx 1.00\ m\,s^{-1}$ and $h \approx 180$ mm, Figure 3(d);
- Cx.5 – $Q \approx 61.54\ L\,s^{-1}$, $v_{liq} \approx 2.03\ m\,s^{-1}$ and $h \approx 104$ mm (graph not shown).

## Definition of parameters to model with AEROSEPT and WATS

Following field measurements and hydraulic characterization of sections 1 and 2, both AEROSEPT.V02 and WATS models were applied and scenarios *Qm* and *Qp*

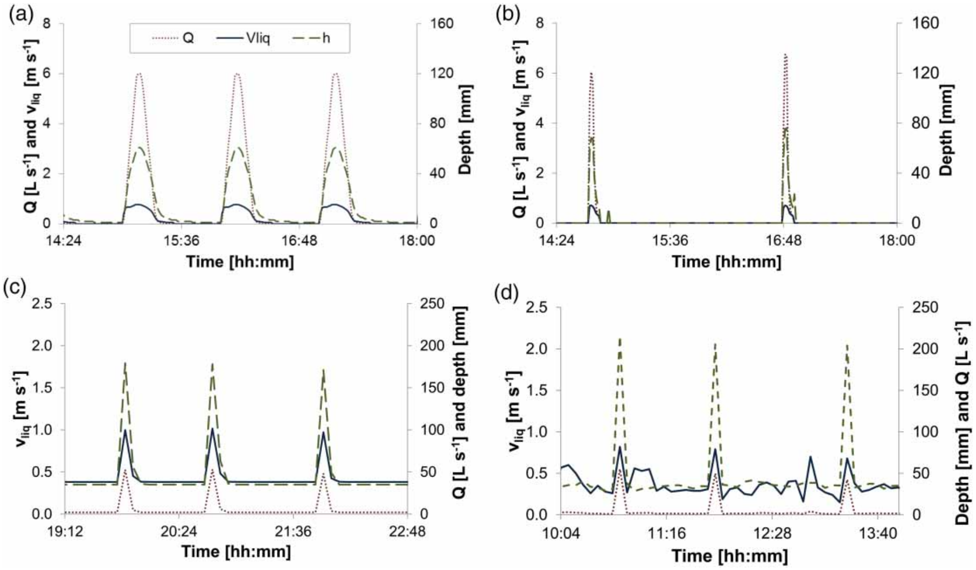

**Figure 3** | SWMM versus flow meter results: flow rate [Q], water depth and velocity [$v_{liq}$] for: (a) Cx.$10_{SWWM}$, (b) Cx.$10_{flow\_meter}$, (c) Cx.$1_{SWWM}$ and (d) Cx.$1_{flow\_meter}$.

analyzed assuming steady state conditions and compared with the *in situ* obtained results.

The mean flow rate was determined through the gas phase continuous measurements which allowed the average number of pumping events occurring in a typical summer week to be defined (Matias 2016; Matias *et al.* 2017a). The flow meter results were also used not only to validate this number of events but also to identify the average duration of each pumping event and the correspondent flow rate value. This resulted in mean flow rates of 0.42 and 2.52 L $s^{-1}$, respectively, for Foz do Lizandro and EE5 pumping stations.

The average measured values of T and pH, T = 24.3 °C and pH = 7.5, were used on both models. The default value for sulfate ($SO_4^{2-}$) is usually considered to be around 30 mg $SO_4^2$ $L^{-1}$. However, from preliminary simulations, this value was found to be too low and limiting the dissolved sulfide formation to values below what was systematically measured at Cx.10. Instead, a value of 45 mg $SO_4^{2-}$ $L^{-1}$ was applied.

In AEROSEPT.V02, the DO content set for the tributaries, as a way to define the travel time of the respective wastewater, was assumed to be 40% of the saturation level. This model was also calibrated admitting the empirical constant N of the Pomeroy & Parkhurst (1977) formulation, related to the formation rate in pipes flowing with free surface, equal to 0.64. These authors have proposed two values: N = 0.96 and N = 0.64. A relatively high value of N may be applied when focusing on corrosion, whereas odor problems may be best taken into account by a relatively lower value. For full flowing pipes or rising mains, and depending on the ratio between resting and pumping periods as suggested by Matos (1992), the M value of Pomeroy's (1959) expression assumes values from 0.0004 to 0.001 m $h^{-1}$. Values close to the lower limit should be chosen when the resting times are long and predominate relative to pumping periods. A conservative condition is often to apply values close to 0.001 m $h^{-1}$. In this case, the M value was set to 0.0004 m $h^{-1}$ for AEROSEPT_*Qm* and the more conservative value of 0.001 m $h^{-1}$ for AEROSEPT_*Qp*. Biochemical oxygen demand ($BOD_5$) is another required parameter. Following complementary laboratory results (Matias 2016), this parameter was defined as $BOD_5 =$ 300 mg $O_2$ $L^{-1}$.

The wastewater parameters in WATS were set to its default values for similar mainly domestic sewer systems (common average values). This model only allows slope values above 0.001%. Therefore, it was not possible to force a slope that would guarantee the h/D = 0.5 for the fictitious pipes introduced to include the effect of residence time in the pumping stations' wells. Consequently, a more conservative scenario was simulated, *Qp**, where these fictitious pipes were assumed as pressure pipes. Under this assumption, no reaeration occurs. Then, this model was calibrated taking into account the measured chemical oxygen demand (COD) value of 500 mg $O_2$ $L^{-1}$ (Matias 2016) and assuming a sulfide formation rate of 14 mg S $(m^2\,h)^{-0.5}$ for WATS_*Qm* and, a more conservative value, of 30 mg S $(m^2\,h)^{-0.5}$ for WATS_*Qp**.

## AEROSEPT.V02 model

In Figure 4(a) the results of $S_D$ and DO concentrations in the liquid phase obtained with AEROSEPT.V02 for the two scenarios is depicted. Figure 4(c) displays the concentration of $H_2S$ in the gas phase. In both Figure 4(a) and Figure 4(c), minimum, median and maximum measured values (Matias *et al.* 2017a) at Cx.10/Cx.20 (section 1) and Cx.1/Cx.5 (section 2) are shown.

As can be seen from Figure 4(a), scenario *Qm* shows results in terms of $S_D$ that can be considered very good when comparing between the simulation (full dark line) and the average measured values (square dots). From these results, it can be inferred that this model was able to simulate sulfide build-up along both rising mains and partially filled sewer pipes under intermittent flow conditions as it was able to predict the main observed results after a reduced set of parameters calibration. However, the same is not possible to state for DO as AEROSEPT.V02 does not allow $S_D$ and DO to coexist.

For scenario *Qp*, even adding a fictitious pipe to achieve the same residence time at the discharge of the two modeled rising mains, the amount of sulfide produced did not match scenario *Qm* nor the *in situ* measurements. In this case, it seems that, for simulation purposes with this model, it is better to have the correct travel time, and the corresponding sulfide formation in the rising mains, than to promote the correct reaeration and turbulence effects in the gravity pipes.

Regarding $H_2S$ in the gas phase, Figure 4(c), the range of measured values, especially at Cx.10, is very high (minimum, average and maximum values of 22, 74 and 260 ppm, respectively). Nonetheless, in scenario *Qm*, the average $H_2S_g$ concentration, and the overall system's behavior, are considered generally quite good. For example, the concentrations obtained with the model at Cx.10 and Cx.1 were 73 and 11 ppm, while the average measured values were 74 and 16 ppm, respectively, Figure 4(c).

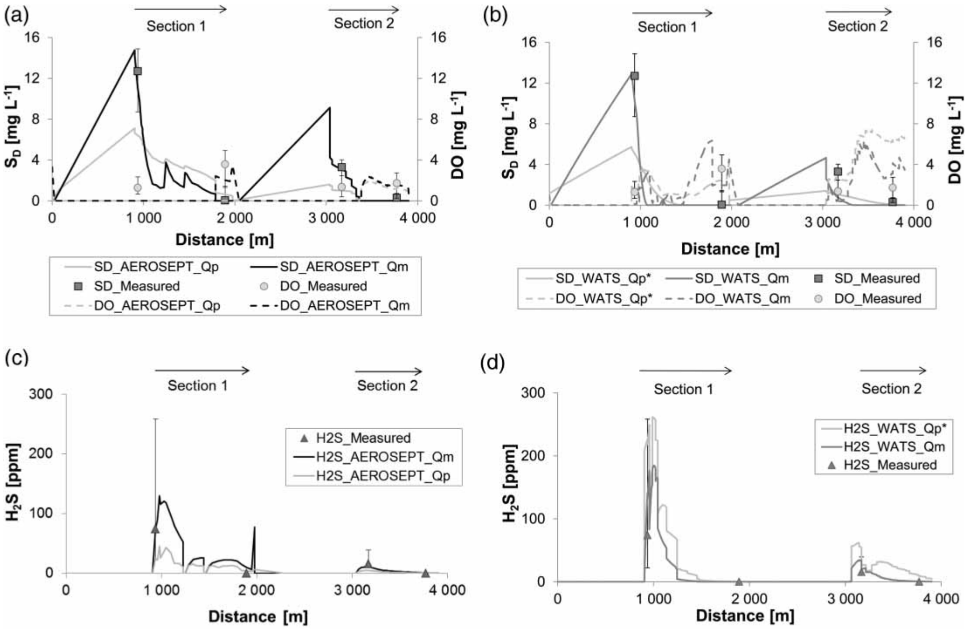

**Figure 4** | Results for DO and $S_D$ in the liquid phase: (a) AEROSEPT.V02 and (b) WATS; and $H_2S$ in the gas phase: (c) AEROSEPT.V02 and (d) WATS. Scenarios: *Qm* and *Qp/Qp**.

On the other hand, even with increased flow rates and associated turbulence, the $H_2S$ amount released to the gas phase in scenario *Qp* was considerably lower and far from the measured values. This is believed to be partially explained by the lower sulfide content in the liquid phase but also by some limitations of the model to properly simulate the influence of turbulence in the $H_2S$ releasing process.

The pH values obtained in the field measurements exhibited high variability (Matias 2016; Matias *et al.* 2017a). To demonstrate how this parameter can influence the simulation results of the gas phase, Figure 5 presents $H_2S_g$ for scenario *Qm* when changing the average measured value (pH = 7.5) to 7 or 8.

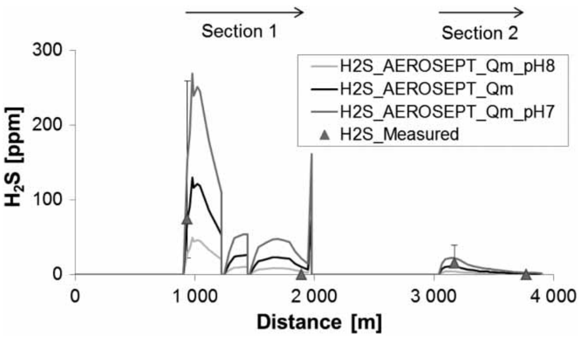

**Figure 5** | AEROSEPT.V02 results for $H_2S_g$ in the gas phase. Scenarios: *Qm* (pH = 7.5) and *Qm* with pH = 7 and 8.

From Figure 5 it can probably be assumed that part of the high range in the measured values at Cx.10 is due to pH variations in the liquid phase. These results are also in accordance with data obtained by Sharma *et al.* (2014), where the authors modeled the effect of pH in biofilm sulfidogenesis, having observed higher sulfate reduction rates at pH values close to neutral (6.5–7.5), and decreased rates when otherwise. Nevertheless, and despite the uncertainty of the unsteady flow rates, air velocities and turbulence, the obtained simulation results show that the model was able to adequately predict the average values occurring in the system.

The AEROSEPT.V02 version applied in these simulations include new equations for $H_2S$ release at drop structures (both free-fall and backdrop type of structures, Matias (2016)). The application of the original version would lead to $H_2S$ gas concentrations 10% lower. However, the obtained results, both from field measurements and simulations, still present some limitations to truly be able to represent real conditions in sewer systems at these specific transition locations.

## WATS model

Figure 4(b) depicts the results of $S_D$ and DO obtained by applying the WATS model to the two previously presented scenarios, and Figure 4(d) shows the ones regarding $H_2S$

in the gas phase. In both figures, the median measured values at Cx.10/Cx.20 (section 1) and Cx.1/Cx.5 (section 2) are also shown.

From Figure 4(b) it seems that, in terms of $S_D$, WATS for scenario *Qm* was also adequately calibrated by using the average measured values of T, pH, $SO_4^{2-}$, COD and sulfide formation rate (for example, at Cx.10, the sulfide content obtained with WATS was 12.73 mg $S^{2-}$ $L^{-1}$ and the average measured one was 12.70 mg $S^{2-}$ $L^{-1}$). In this case, however, DO was also more accurately predicted as it was measured and simulated coexisting with $S_D$. In contrast to what was obtained with AEROSEPT.V02 at Cx.10 (73 ppm for scenario *Qm* and 37 ppm for scenario *Qp*), WATS for scenario *Qp* resulted in an increased amount of $H_2S$ released to the gas phase, Figure 4(d), even with lower $S_D$ content predicted in the liquid phase (142 and 223 ppm, respectively, for scenario *Qm* and *Qp**).

## Comparison between model concepts

Results considering the mean diurnal flow rate in scenario *Qm* for both AEROSEPT.V02 and WATS are presented in Figure 6(a) for $S_D$ and DO in the liquid phase and, in Figure 6(b), for $H_2S$ in the gas phase.

Despite some similarities, differences arise from the fact that AEROSEPT.V02 assumes that DO and $S_D$ cannot coexist in the wastewater. Regarding the forecast of sulfides build-up, AEROSEPT.V02 seems more conservative both in rising mains and gravity sewers.

In terms of $H_2S$ in the gas phase, and despite WATS returning higher values in the upstream part of the system, with AEROSEPT.V02, more pipes are expected to have levels above 10–30 ppm. Nevertheless, WATS, even with lower $S_D$ content predicted in the liquid phase for scenario *Qp**, was able to more accurately take into account turbulence and predict the $H_2S$-gas concentrations that were measured in the gas phase.

Another comparison between the two modeling approaches and the field measurements can be the air velocity at Cx.10. Taking into account the time between the measured $H_2S$ gas concentration peaks, shown previously in Matias *et al.* (2017a) as taking 9 to 11 minutes to travel 33.3 m, the expected average air velocity would be around 0.05 to 0.06 m $s^{-1}$. In WATS_Qp* the gas phase velocity was 0.22 m $s^{-1}$ while for AEROSEPT_Qp the result was 0.19 m $s^{-1}$. The difference is probably due to the fact that the air velocity in both models is determined along the pipes, and the measurements were influenced by the air volume existing in the manholes, which inevitably influences the mean velocity.

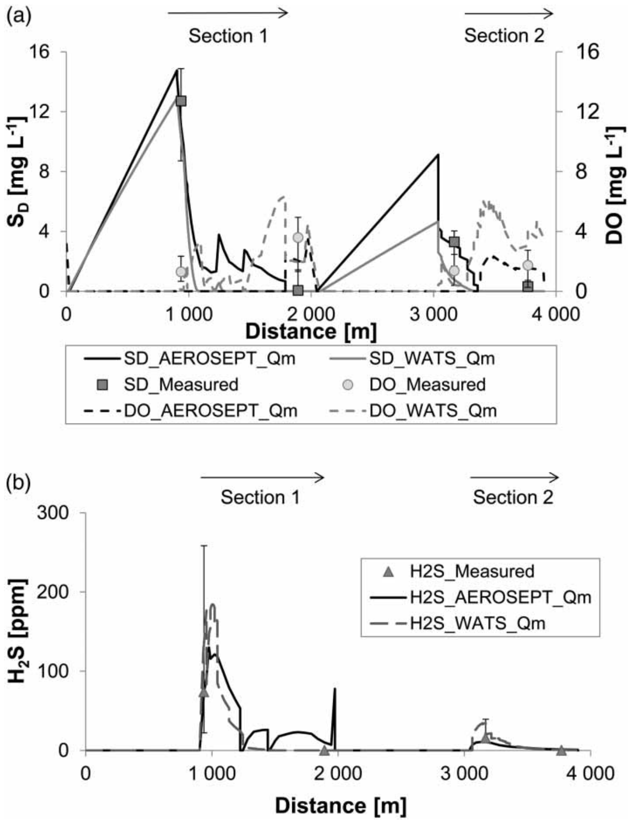

**Figure 6** | AEROSEPT.V02 and WATS results for (a) DO and $S_D$ in the liquid phase and (b) $H_2S$ in the gas phase. Scenario: *Qm*.

## CONCLUSIONS

The aim of this work was to present the results obtained by applying two different approaches for modeling wastewater quality in sewer systems under intermittent and highly turbulent flow conditions. One approach was based on an empirical formulation (AEROSEPT) and the other on a conceptual and more complex framework (WATS). The main sewer system of Ericeira, in Portugal, was chosen as a case study. To apply both models under equivalent conditions and to verify the overall hydraulic behavior of the system, SWMM was used to quantify all hydraulic variables. Additionally, the results from intensive field measurement campaigns were used for calibration.

Despite the unavoidable uncertainties due to the unsteady flow rate and the quantification of air velocity and turbulence, the simulation results obtained with both models have been shown to adequately predict concentrations of dissolved sulfide and oxygen as well as hydrogen sulfide gas levels in the confined atmosphere.

Overall, simulation results estimated by both models were similar. Despite this similarity, a significant difference stemmed from the fact that AEROSEPT assumes that oxygen and sulfide cannot coexist in the wastewater. Additional differences correspond to the build-up of sulfides, AEROSEPT being more conservative in both the rising mains and gravity trunk sewers. In terms of $H_2S$ gas concentration, and despite the fact that WATS tends to simulate higher values in upstream sections, according to AEROSEPT more pipes should be expected to have values above 10–30 ppm. WATS, even with a lower predicted dissolved sulfide content, was able to more accurately take into account turbulence and predict the $H_2S$-gas concentrations as they were measured in the gas phase.

The WATS model is considered more complete and useful; however, it requires more experimental data in order to calibrate its parameters and be fully reliable for supporting planning and operational decisions. Under those circumstances uncertainty is not large and average and maximum values of sulfides and $H_2S$ gas concentrations can be reasonably estimated. In cases of limited data AEROSEPT gives comparable results with less effort. It can be considered as fairly reliable in terms of predicting average values in a conservative way, being appropriate for design purposes.

For practical purposes, it is recommended to apply both models for a range of hydraulic and environmental scenarios, e.g., in terms of flows, temperatures, and influent COD and DO characteristics, in order to obtain, in different critical sections, ranges of possible values.

Case studies such as the one presented in this paper highlight the fact that processes occurring in sewer systems are complex and interlinked, and show that simple rule-of-thumb can easily fail when it comes to predicting sewer corrosion rates and odor impacts, leading to suboptimal or even incorrect sulfide management approaches. This may be especially relevant in the case of intermittent discharges that often translate into highly unsteady wastewater flows and variable ventilating conditions.

Wastewater quality in sewer systems depends on very complex processes whose outcomes are often difficult to generalize. We recommend that this type of approach becomes a standard as a support management tool on existing systems as it helps in defining solutions that are truly suitable to local conditions.

## ACKNOWLEDGEMENT

For the success of this field study, the support of AdVT (previously designated SIMTEJO) was essential. This work was supported by the Portuguese Foundation for Science and Technology (Fundação para a Ciência e a Tecnologia, FTC) under the scholarship SFRH/BD/60361/2009.

## REFERENCES

ASCE (American Society of Civil Engineers) 1989 *Sulfide in Wastewater Collection and Treatment Systems.* ASCE Manual 69, ASCE, New York, USA.

Engidro, HIDRA & Aquapor 2015 *Master Plan for Sanitation and Drainage of the Metropolitan Area of Maputo - Analysis of the Existing Situation. Volume 2 - Maputo and Marracuene - Final Report (Plano Director de Saneamento e Drenagem da Área Metropolitana de Maputo - Análise da Situação Existente. Volume 2-Maputo E Marracuene - Relatório Final).* Engidro, Lisbon, Portugal.

Forsgren, A. & Brinck, K. 2017 *Airborne Occupational Hazards in Sewer Systems.* Taylor & Francis, CRC Press, Boca Raton, FL, USA.

Hvitved-Jacobsen, T., Vollertsen, J. & Nielsen, A. H. 2013 *Sewer Processes: Microbial and Chemical Process Engineering of Sewer Networks.* 2nd edn. CRC Press, Boca Raton, FL, USA.

Jiang, G., Keller, J. & Bond, P. L. 2014 Determining the long-term effects of $H_2S$ concentration, relative humidity and air temperature on concrete sewer corrosion. *Water Research* **65**, 157–169.

Matias, N. M. 2016 *Release of Hydrogen Sulfide and Other Volatile Compounds in Sewer Systems under Turbulent Conditions.* PhD thesis, Instituto Superior Técnico, IST, Lisbon, Portugal.

Matias, N. M., Mutuvúie, R., Vollertsen, J., Nielsen, A. H., Ferreira, F. & Matos, J. S. 2014 Sulfide formation and its impacts on a sewer system of a developing country – a case study in Maputo, Mozambique. In: *13th IAHR/IWA International Conference on Urban Drainage, 13ICUD, 7–11 September 2014, Kuching, Malaysia.*

Matias, N. M., Matos, R., Ferreira, F., Vollertsen, J. & Matos, J. S. 2017a Release of hydrogen sulfide in a sewer system under intermittent flow conditions – the Ericeira case study, in Portugal. *Water Science & Technology* **75** (7), 1702–1711.

Matias, N. M., Nielsen, A. H., Vollertsen, J., Ferreira, F. & Matos, J. S. 2017b Liquid-gas mass transfer at drop structures. *Water Science & Technology* **76** (6), 1584–1594.

Matias, N. M., Nielsen, A. H., Vollertsen, J., Ferreira, F. & Matos, J. S. 2017c Liquid-gas mass transfer of volatile substances in an energy dissipating structure. *Water Environment Research* (accepted/in press).

Matos, J. S. 1992 *Aerobiose e Septicidade em Sistemas de Drenagem de Águas Residuais (Aerobic Conditions and Septicity in Sewerage Collection Systems).* PhD thesis, Instituto Superior Técnico, IST, Lisbon, Portugal.

Matos, J. S. & Sousa, E. R. 1989 *Modelação Sanitária do Escoamento de águas Residuais em Pressão em Condutas de Pequena Extensão (Modeling of Wastewater in Small Extent Rising Mains) (Vol. Projecto C&T, JNICT, 2° Relatório de Execução).* CEHIDRO, Lisbon, Portugal.

Matos, J. S. & Sousa, E. R. 1990 *Modelação de Oxigénio Dissolvido em Redes de Drenagem de águas Residuais Comunitárias*

*(Modeling of Dissolved Oxygen in Community Wastewater Collection Systems) (Vol. Projecto I&D, 1° Relatório (2° Ano de Execução))*. CEHIDRO, Lisboa.

Parkhurst, J. D. & Pomeroy, R. D. 1972 Oxygen absorption in streams. *Journal of the Sanitary Engineering Division* **98** (1), 101–124.

Pescod, M. B. & Price, A. C. 1982 Major factors in sewer ventilation. *Journal of the Water Pollution Control Federation* **54** (4), 385–397.

Pomeroy, R. D. 1959 Generation and control of sulfide in filled pipes. *Sewage & Industrial Wastes* **31** (9), 1082–1095.

Pomeroy, R. D. & Parkhurst, J. D. 1972 Self purification in sewers. In: *6th International Conference of the Water Pollution Research, Jerusalem*.

Pomeroy, R. D. & Parkhurst, J. D. 1977 The forecasting of sulfide buildup rates in sewers. *Progress in Water Technology* **9** (3), 621–628.

Sharma, K., Derlon, N., Hu, S. & Yuan, Z. 2014 Modeling the pH effect on sulfidogenesis in anaerobic sewer biofilm. *Water Research* **49**, 175–185.

Sun, X., Jiang, G., Bond, P. L. & Keller, J. 2015 Impact of fluctuations in gaseous $H_2S$ concentrations on sulfide uptake by sewer concrete: the effect of high $H_2S$ loads. *Water Research* **81**, 84–91.

Talaiekhozani, A., Bagheri, M., Goli, A. & Khoozani, M. R. T. 2016 An overview of principles of odor production, emission, and control methods in wastewater collection and treatment systems. *Journal of Environmental Management* **170**, 186–206.

USEPA (United States Environmental Protection Agency) 1985 *Odor and Corrosion Control in Sanitary Sewerage Systems and Treatment Plants*. USEPA 625/1-85/018, USEPA, Washington DC, USA.

Vollertsen, J., Nielsen, A. H., Jensen, H. S. & Hvitved-Jacobsen, T. 2008 Modeling the formation and fate of odorous substances in collection systems. *Water Environment Research* **80** (2), 118–126.

Vollertsen, J., Nielsen, A. H., Jensen, H. S., Rudelle, E. A. & Hvitved-Jacobsen, T. 2011a Modeling the corrosion of concrete sewers. In: *12th International Conference on Urban Drainage (ICUD 2011), 11–16 September 2011, Porto Alegre, Brazil*.

Vollertsen, J., Nielsen, L., Blicher, T. D., Hvitved-Jacobsen, T. & Nielsen, A. H. 2011b A sewer process model as planning and management tool – hydrogen sulfide simulation at catchment scale. *Water Science & Technology* **64** (2), 348–354.

Vollertsen, J., Revilla, N., Hvitved-Jacobsen, T. & Nielsen, A. H. 2015 Modeling sulfides, pH and hydrogen sulfide gas in the sewers of San Francisco. *Water Environment Research* **87** (11), 1980–1989.

Yongsiri, C. 2004 *Emission and Fate of Hydrogen Sulfide in Sewer Networks*. PhD thesis, Aalborg University, Aalborg, Denmark.

Yongsiri, C., Hvitved-Jacobsen, T., Vollertsen, J. & Tanaka, N. 2003 Introducing the emission process of hydrogen sulfide to a sewer process model (WATS). *Water Science & Technology* **47** (4), 85–92.

First received 1 August 2017; accepted in revised form 8 November 2017. Available online 23 November 2017