Report by UWI doctoral researcher Abhinav Dixit (S2)

Project number: S2

First and last name of doctoral researcher: **Abhinav Dixit**

(Working) title of doctoral project: **Validation and application of a three phase simulation model for odour and corrosion control in sewer systems**

Name of supervisors: Prof. Dr.-Ing. **Reinhard Hinkelmann** (TUB), Prof. Dr.-Ing. **Matthias Barjenbruch** (TUB), Prof. Dr. rer. nat. **Dietmar Stephan** (TUB), Prof. Dr. rer. nat. **Gunnar Nützmann** (IGB)

2. Description of doctoral project and research results achieved to date:

State of the art

Biological corrosion of sewers and sewage treatment plants constitutes a serious problem and its effects result in the loss of billions of dollars every year (Tomala & Fiertaka 2016). Changing demography and more efficient use of water resources will lead to the reduction of the average volume of waste water and leads to higher residence times in the sewer canals. Due to climate change, i.e. warmer temperatures, the waste water in the canal will become more anaerobic. Therefore, sewer networks with a concrete construction are subjected to various mechanisms that subject it to rapid degradation. Due to the anaerobic conditions in sewage, sulfate present in the waste water can be reduced to sulfide by sulfate-reducing bacteria residing in the biofilms on the walls of the pipelines (Sharma et al. 2008). Hvitved-Jacobsen (2013) conclusively stated that this gas travels from the water phase to the air phase in the pipe system. Now in an aerobic environment this gas is oxidized to form sulphuric acid via microbial activities. These emissions not only increase the cost of maintenance but also pose a threat to human health of sewer workers. For more than 70 years, researchers have been committed not only to study the processes for odour and corrosion but also creating empirical and conceptual models for explanations (e.g. Gilchrist 1953). However, within the last 20 years a deeper understanding has been gained thanks to the efforts of research groups in Denmark and Australia (Rootsey & Yuan 2010, Rootsey et al. 2012, Hvitved-Jacobsen et al. 2013, Teuber et al. 2017). Nearly all current models are confined to a one-dimensional approach which is very suitable if only the water phase is considered. However, for processes which are affected by the concentration profiles (e.g. H_2S formation, mass transfer) and the air flow a three- dimensional approach should be preferred accounting for water and gas phase. In the 1st cohort, a model is being developed that can account for temperature and ph dependency on the mass transfer of H_2S.

Motivation and research idea

The processes and mechanisms that drive odour and corrosion in sewer systems are currently understood to an insufficient extent. Therefore, the motivation of this doctoral thesis is to improve the understanding through literature research and the experiments carried out by project S1 in the laboratory and pilot plant and to further develop the computational model of Teuber et. al. 2018 (1st cohort). This doctoral thesis is further practically motivated by the high costs which are required for the maintenance and repair and health risks imposed on sewer workers.

For this purpose, a high resolution three-dimensional model for water and air flow, multi-component reactive transport and mass transfer between the water and air phase must be developed. This will commence by furthering the research on the current OpenFOAM model developed by Teuber et al. 2018. For this a step by step approach will be intended starting from further validation of the established model using literature, laboratory experimentation and actual data collected from the pilot plant. Later research will include the study of natural degassing measures and multiphase reactive transport for dosage of reagents for H_2S stripping.

To study the causality of odour and corrosion a detailed research is required on all the processes leading to them (fig. 1). The production of hydrogen sulfide gas can be attributed to the various anaerobic microbial activities that persist in the water phase, however corrosion of the concrete wall occurs mainly due to four processes.

These are namely attack by acids (biogenic acids), carbonation, chloride corrosion and attack by sulfides (Tomala & Fiertaka 2016). At a later stage of the project, research will focus on the attack of sulfides (initial phase) and biogenic acids due to the biofilms (possibly in the later phase).

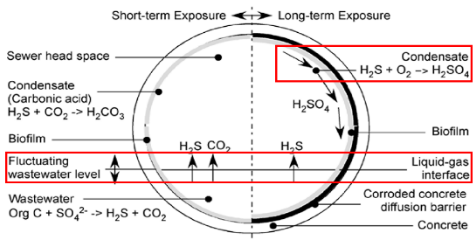


Figure 1: Short-term and long-term processes in the sewer network (Melchers et al. 2014)

Research demands
Following points will be the key focuses of this study:

1. Overall aim: Modelling multi-component reactive transport and mass-transfer of in-sewer processes.
2. Validation of the existing model and establishing the temperature and pH dependency of Henry's coefficient.
3. Using a turbulent H_2S reactor situated at BWB for understanding the odour and corrosion processes.
4. Modelling the structures for natural degassing and chemical stripping using dosage substances.
5. Optional targets: Study microbial processes and bionic corrosion; simplification and parameterization of the 3D model.

Objectives

Continuation and development of the model generated by Teuber et al. 2018 (Project T3) will be the focus of project S2- "Validation and application of a three phase simulation model for odour and corrosion control in sewer systems". Functionality and applicability of the model will be tested against data aggregated from literature, lab experiments and pilot plant.

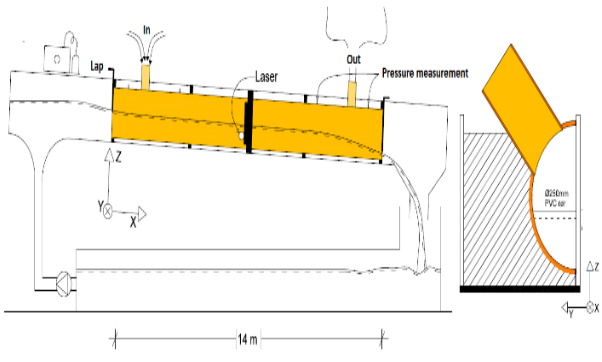
Work programme incl. proposed research methods

__WP 0__ ***'Literature review, familiarising with OpenFoam and collaboration'***

In this work package time will be utilized for understanding the basic chemical and biochemical processes happening in the sewer system. This includes the undergoing processes in the water phase, air phase and the corresponding reactions between the two phases. Certain amount of time will be devoted for revising the concepts of transport phenomena (mass and heat transport) and chemical kinetics of the two major reactions i.e. biochemical conversion of sulphates to sulfide via sulphate reducing bacteria (SRB) and conversion of sulfide to sulphuric acid at the wall. Key would be to establish a coherent relation between the chemical kinetics of ongoing reactions in a flowing network and corresponding solver in OpenFoam. Nevertheless, before establishing any correlations, OpenFoam software and CFD modelling will be studied in detail to ensure fluent process dynamics in the later parts of the research.
For this purpose, elective courses for Computational Fluid Dynamics and hydrodynamic modelling will be taken. Apart from electives, the core courses will be attended in order to get a broader prospect of urban water interfaces. This will help in future collaborations and in establishing a link between the ongoing researches.

__WP 1__ ***'Validation of the air phase and investigation of a semi-circular mesh'***

This work package will be strictly devoted to studying the current model developed by Katharina Teuber and furthering the validation using the experimental data. For having a better understanding of how the air in the sewage atmosphere moves, a refined semi-circular mesh will be generated developing on the works of collaboration partners from Aalborg University, Denmark (Fig. 2). By being able to model the air's motion in gravity lines, it is possible to assess mitigation measures for odour control (Kristensen 2015). Next step will include validation of the model by collecting the data from the pilot plant in BWB with the help of Kollegiate Danish Despot who has been responsible for the setup and testing. Due to previous experience in chemical analytics, if possible or needed, a certain amount of time will be allocated for design of experiments, lab tests etc. This step will give a better picture of the mass transfer processes (multi component reactive transport) and the temperature dependency of Henry's coefficient. The third part of this package will also contain a close collaboration with Kollegiate Danish Despot who will be working on H_2S gas reactor for investigating and validation of the air phase *(Fig. 3)*. H_2S emissions under turbulent conditions will be investigated and the concrete coupons placed in this reactor will be exposed to H_2S concentrations amounting a daily average of 100 ppm for 12 months (Sun et al. 2014).



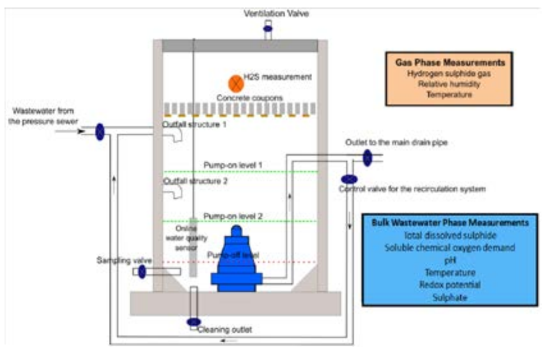


Figure 2: Experimental setup for the half mesh (Kristensen 2015) *Figure 3: Schematic of the H_2S gas reactor (Despot et al. 2014)*

There will be a close collaboration with project H2 for in-depth knowledge of the OpenFOAM tool and modelling concepts. The time line of this work package will conclude in summer semester 2019.

WP 2 ***'Natural degassing using mechanical structures (hydraulic jumps)'***

This work package will focus on considering structures, which enhance natural degassing, i.e. drop structures, steps etc. This will include the works of Arnau Bayón in the field of modelling hydraulic jumps (Bayón et al. 2016). The dynamics of physical structures such as drop structures associated with deep sanitary trunks can also lead to significant pressurization of headspaces of downstream sewer conduits and cause air to move (Edwini-Bonsu et al 2006). It would be interesting to understand how the design of such structures impacts the natural degassing of H_2S and the impact of energy dissipation in these hydraulic jumps. Another important point while designing these structure will be to avoid that the deposition of transported material is enhanced. Modelling and understanding these phenomena will be the main focus of this work package and will commence during the second year of the programme.

WP 3 ***'Finalization of the model and dissertation'***

The third step will include research on the dosage mitigation techniques against odour and corrosion. There can be multiple solutions for injection of dosage substances regarding different locations and temporal distribution of $NaNO_2$, $CaNO_3$ or $FeNO_3$ which reduce H_2S production in water and are toxic for biofilms. Major focus will be on modelling the injection of dosage substances while understanding and building up on the works of José González in the field of predictive control of ferrous chloride dosing to minimise corrosion and odour (González et al. 2015). There have been positive demonstrations of the predictive and localized dosage of substances to have an effective control on the H_2S production. Chemical interactions of these dosage substances with the H_2S will also be emphasized when modelling the multi-component reactive transport.

WP 4 ***'Optional: microbial processes and model simplification'***

Work package 4 could commence by the mid of the 3rd doctoral year, with the finalization of the model using the integral solver for the ongoing processes in a closed conduit sewer network. One option includes include establishing a fundamental model/theoretical approach for biochemical reactions at the biofilm-solid interface. The other option addresses simplifications, upscaling and parameterization of 3D effects in 1D models as the computational demand of the river is large. This package will also try to link to the 3rd cohort of UWI by opening the topic of reactive transport modelling to sediment transport in sewer networks.

Collaboration

Project T3 and H2 (Simulation models/OpenFOAM): Integral modelling approach for flow and reactive transport-Katharina Teuber (T3) and Vahid Sobhi Gollo (H2).

Project T2 and S1 (data exchange/experimentation): Thematic work related to in-sewer processes at the pilot plant in BWB and H_2S gas reactor for investigating biogenic concrete corrosion - Daneish Despot (Kollegiate), Maria Sielaff (T2) and Micaela Pacheco Fernandez (S1).

Further Collaborations: **F2** and **F3** for water quality modelling and **W1** for first flush pollution modelling concerning reactive transport.

References

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3. Comments on the qualification programme and supervision strategy:

Participation in the following Research Training Group events:

1. Core courses
   - Urban interface processes – fluxes, transport, interactions (3 ECTS)
   - Urban freshwater ecology (3 ECTS)
   - Modelling and measuring concepts of interface processes (3 ECTS)
2. Elective courses
   - Computational Fluid Dynamics course (6 ECTS),
   - Modelling Hydro- and Environmental Systems (6 ECTS)
   - Kolloquium Wasserwesen (3 ECTS)
3. UWI lectures and Colloquium Hydroscience
4. Other UWI Events
   - Summer School and Expose talk (19. – 20.09.2018)

Research stays or internships at other research institutions both at home and abroad:
Not planned yet.