### 1 Introduction

### 1.1 Background

- 1.2 Objectives
- 1.2.1 To evaluate baseline model performance of forecasting  $NH_3N$  by developing models with traditional and deep learning algorithms.
- 1.2.2 To develop raw data cleaning methodologies for improved machine learning model performance of forecasting  $NH_3N$ .
- 1.2.3 To explore feature engineering with the use of domain knowledge in wastewater treatment to creating new variables for optimizing model performance of forecasting NH<sub>3</sub>N.
- 1.2.4 To construct an optimized procedure of training a machine learning model for NH<sub>3</sub>N forecasting.
- 1.3 Organization of the thesis

#### 2 Literature Review

- 2.1 Wastewater reclamation and reuse
- 2.1.1 Reclaimed water standard in wastewater treatment plant
- 2.1.2 Chlorination for reclaimed water disinfection
- 2.2 Control strategies for reclaimed water quality
- 2.2.1 Feed-forward control
- 2.2.2 Feed-back control
- 2.3 Water quality forecasting in wastewater treatment plant
- 2.3.1 Tools and technologies for parameter forecasting in wastewater treatment plant
- 2.3.2 Case study of machine learning models for water quality forecasting
- 2.4 Introduction to machine learning
- 2.4.1 Machine learning algorithms
- 2.4.2 Introduction to time-series data
- 2.4.3 Data pre-processing methodologies
- 2.4.3.1 Data cleaning
- 2.4.3.2 Outlier removal
- 2.4.3.3 Feature engineering

- 2.4.4 Model evaluation
- 2.4.4.1 Common metrics to evaluate model performance
- 2.4.4.2 Select baseline model performance

# 3 Materials and methods

- 3.1 Wastewater treatment plant description
- 3.1.1 Treatment processes in SHWEPP
- 3.1.2 Historical water quality data in SHWEPP
- 3.2 Raw data collection and preparation
- 3.2.1 NH<sub>3</sub>N data monitoring and collection
- 3.2.2 Data cleaning and pre-processing
- 3.2.2.1 Data smoothing with mathematical solutions
- 3.2.2.1.1 Exponentially Weighted Moving Average filter
- 3.2.2.1.2 Savitzky-Golay filter
- 3.2.2.2 Outlier detection and removal
- 3.2.2.2.1 Peak detection analysis
- 3.2.3 Feature Engineering
- 3.2.3.1 Positional encoding
- 3.2.4 Data transformation
- 3.2.4.1 Split train/test dataset fot model input

- 3.3 Architectures of the machine learning algorithms
- 3.3.1 Random Forest
- 3.3.2 Multilayer perceptron
- 3.3.3 Long Short-Term Memory
- 3.3.4 Transformer
- 3.4 Proposed time series forecasting workflow
- 4 Results and Discussion
- 4.1 Comparisons of forecasting accuracy with traditional and deep learning models
- 4.1.1 Selection of baseline model performance
- 4.2 The influence of data pre-processing on model performance
- 4.2.1 Data cleaning
- 4.2.2 Outlier removal
- 4.3 The influence of feature engineering on model performance
- 4.3.1 Positional encoding as new input features

# 5 Conclusions and recommendations

Title:

Forecasting the Ammonia Concentration in the Reclaimed Water using Machine Learning

Study 1: Algorithm Selections and Data Pre-processing Methodologies in Developing Machine Learning Models for NH<sub>3</sub>N Forecasting.

Study 2: To incoporate the use of domain knowledge in water/wastewater treatment and established methodology to construct a optimized model for NH<sub>3</sub>N forecasting.