DESCRIPTIVE ASSESSMENT AND AMENDMENT OF THE SIMPLETREAT MODEL

Modelling of Organic Chemicals in Sludge for Soil Application

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Abstract
This study presents a stepwise methodology to predict the fate of organic compounds (OCs) in both wastewater treatment plants (WWTPs) and soils by applying the easy accessible SimpleTreat model. The proposed methodology involves plant description, chemical data collection, calibration, validation and continuation step to investigate the effect of soil processes. Furthermore, the original SimpleTreat model was modified and proved to be applicable for predicting the fate of OCs with regard to a number of factors: i) model structure, ii) model parameters and iii) data quality. Hence, a total of 84 chemicals were modelled in the modified SimpleTreat model using four plant configurations. The selected WWTPs attested a good representation of the overall pollution removal rates via the effluent and sludge when compared with typical concentrations ranges of the IVL-database (Swedish Environmental Research Institute). The order of magnitude of the SimpleTreat model predictions proved to have 92% accuracy while in sludge it had 56%. Additional analysis of the chemicals in soil must be carried out to evaluate the overall risk of the sludge when applied as soil amendment.

Introduction

Large quantities and numbers of OCs from industries and domestic sources enter WWTPs everyday, which is an ever-increasing issue in modern society. In WWTPs, the organic pollutants are either degraded or emitted to the air, effluent or sludge. Even though the sludge may contain toxic contaminants and heavy metals, there is an incentive of recycling sewage sludge as a fertiliser to preserve the phosphorus that is a limiting resource. The quality of the sludge can be ensured with the certification system, REVAQ, which oblige the WWTP to set up an *upstream action* plan that requires continuous work of improving the sludge. However, the overall environmental risk of OCs, i.e. from entering the WWTP to exposing the sludge containing OCs to soil processes, has so far not been taken into consideration in the upstream actions.

The main objective of the project was to develop a methodology to predict the fate of OCs in sludge after being exposed to soil processes by applying and amending the easy accessible modelling tool SimpleTreat 3.1. Further investigation of how the soil processes will affect the removal of the OCs will not be assessed in this work. The SimpleTreat will as well be adapted to existing known parameters of generic Swedish WWTPs that have not been included in the original model. In addition, the applicability of the modified model for four generic Swedish WWTP configurations was validated by comparing the predicted results of effluent and sludge with measurements from the IVL-database. Finally, by simulating the measured OCs in the influent, a general view of expected concentration ranges in Swedish effluent and sludge was obtained, especially important since many of the emerging chemicals' presence, frequency of occurrence or source may be unknown.

This master's thesis was carried out at SWECO AB for the Swedish Water & Wastewater Association, in cooperation with four Swedish WWTPs: Ellinge, Käppala, Ryaverket and Sjölunda. Since two input parameters from Ellinge were missing, Ellinge was consequently left out in the investigation. The old and new sections of Käppala have different plant configurations and are therefore treated as two separate plants.

Organic Chemicals

Typical OCs that end up in WWTPs are predominantly hydrophobic, i.e. have a tendency to be sorbed into sludge. Hydrophobicity of a chemical can be described with the octanol-water partition coefficient (distribution or sorption coefficient), K_{OW}.

Moreover, the evaporation of a chemical can be described with the air-water partition coefficient K_{AW} that is also referred to as the dimensionless Henry's law constant, K_H, while Henry's constant with a unit is denoted as H.

SimpleTreat 3.1

SimpleTreat is a spreadsheet based (Excel®), steady-state box model, which predicts the fate of an OC in a WWTP. The modelled WWTP consists of a primary settler, an aeration tank and secondary clarifier. The primary settler and secondary clarifier are designed to settle suspended contaminants of the influent. In the aeration tank, the wastewater undergoes biological treatment to remove and separate OCs with the help of microorganisms. The elimination of organic contaminants in a WWTP can in general be divided into the following essential removal processes described with their characteristic parameters:

- Sorption (K_{OW});
- Volatilisation, air stripping (K_H, H);
- Biodegradation (aerobic degradation rate constant, k_{deg}).

Methodology

The methodology consists of five steps although the last step is not a part of this work.

STEP 1: Select a WWTP and thereafter collect plant characteristics which are necessary for the use of the prediction model in *STEP 3*.

STEP 2: Select an OC that has been measured in sludge used for soil application; either by searching in databases, e.g. the IVL-database, or performing field measurements of the chemical in the influent, effluent and sludge. For every chemical of interest, relevant physico-chemical properties need to be specified, e.g. using the estimation software, EPI Suite™ when experimentally measured values are not available.

STEP 3: Select a WWTP model that predicts the fate of a chemical in a WWTP, e.g. SimpleTreat, depending on the selected WWTP and chemical. The WWTP model is simulated by inserting three essential input data sets: i) the plant configuration, ii) the physico-chemical parameters and the iii) influent concentration. Model outputs are the expected concentrations in air, effluent and sludge.

STEP 4: The modelled effluent is compared with the measured effluent. If these concentrations do not match well, the current model can either be modified or reselected. Another possible option is to run additional measurements of the chemical concentration in influent, effluent and sludge.

STEP 5: Select a soil model that describes the soil processes using the predicted (persistence, bioaccumulation, toxicity, potential for long-range transportation etc) sludge concentration from the WWTP model to simulate the fate of OC in soil. When the results of OC's predicted concentration after being processed in soil is analysed to be insignificant, then no further action is taken. In other cases, the chemical ought to be monitored in the WWTP and included in the work of upstream actions as a part of the REVAQ certification.

Modifications of SimpleTreat

The SimpleTreat was modified to adapt to generic Swedish WWTPs and existing known parameter inputs of anaerobic and anoxic tanks were added: HRT, height and volume (see Figure 1). An additional sheet was included to simplify the modelling and simulation of multiple chemicals simultaneously.

The modified SimpleTreat proved to be applicable for predicting the fate of organic pollutants with regard to a number of factors: 1) the model structure, 2) the model parameters and 3) the data quality. Firstly, the structure of the modified SimpleTreat is limited to a primary settler, an activated sludge system (anaerobic, anoxic and aerobic zones) and a secondary clarifier. Secondly, although the physico-chemical parameters are preferably experimentally measured, they were in many cases estimated using the EPI Suite™. Thirdly, influent, effluent and sludge data have to be measured at the right location within a reasonable time frame and employing the same sampling and analysis method.

Outlook

To test the proposed methodology, Käppala (old and new), Ryaverket and Sjölunda were used as case studies. In the second step, a total of 84 different OCs were selected from the IVL-database. In the third step, the modified SimpleTreat was selected. In the fourth step, evaluation of the predicted minimum, average and maximum values in effluent and sludge were determined by comparing if they were within the order of magnitude and range of the measured concentrations.

For such a simple steady-state model, the modified SimpleTreat still generated 92% accuracy in predicting the order of magnitudes of a chemical's fate in the effluent and 56% in the sludge.

Conclusions

The thesis presents a practical methodology to predict the distribution of OCs to sludge in a WWTP, which comprises of a plant description, chemical data collection, calibration, validation and continuation step to investigate the effect of soil processes.

To improve the results for a specific compound, it is suggested to measure the specific partition coefficient K_p in raw sewage, primary settler, aeration tank and secondary clarifier to gain a more precise prediction of the partitioning in the specified WWTP.

For the modified SimpleTreat, the selected WWTPs represent fairly well the overall pollution removal rates via the effluent and sludge when compared with the concentrations ranges of the IVL-database. In the outlook, prediction of the concentrations' order of magnitude in Swedish effluent using the modified SimpleTreat proved to have a higher accuracy than in Swedish sludge.

The methodology provides information about the potential threat that OCs might pose to the environment and human health. Nevertheless, additional analysis of the OCs must be carried out to evaluate the overall risk of sludge when applied as soil amendment.

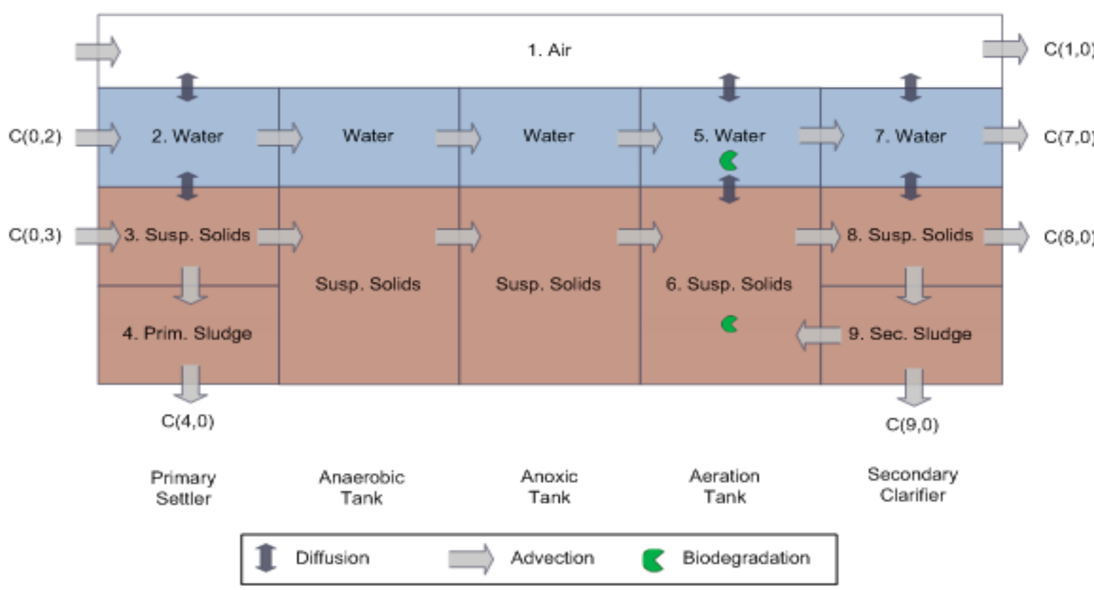

Figure 1. Process scheme of the modified SimpleTreat model.