Comprehensive process-based modelling of sand filters and subsurface flow constructed wetlands

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INTRODUCTION

Improved engineering design and optimization of sand filters and constructed wetlands require a process-based understanding of the numerous pollutant removal mechanisms, their interactions and feedbacks. Although in the recent years several mechanistic models have been developed and successfully applied to different type of systems, both fundamental research aimed at better understanding system functioning and development of more sophisticated biological and geochemical models is necessary (e.g., Langergraber et al., 2009). Investigation of the fate and removal efficiency of novel/non-traditional contaminants (e.g., pharmaceuticals, personal-care products, heavy metals) is needed as they pose a risk for receiving water bodies even at low concentrations (Imfeld et al., 2009). In this respect, reliable process-based modelling tools are necessary to corroborate and integrate experimental results, and to test hypotheses regarding contaminant transformation or detoxification. To this end, we have further developed and improved the capabilities of an existing numerical simulator. The numerical model was subsequently tested against experimental data, and used to conduct a sensitivity analysis in order to identify the conditions for which some of the processes can be safely neglected.

SUMMARY OF MODEL CAPABILITIES

The work we present extends the capabilities of the simulator discussed by Brovelli et al. (2006) and Langergraber et al. (2009). The model has a modular structure, and was originally designed for horizontal, subsurface flow constructed wetlands with saturated flow conditions only. The core of the simulator is based on a coupled variable-density flow and reactive transport code named PHWAT (Mao et al., 2006), which in turn was developed by coupling USGS codes for groundwater flow, solute transport and biogeochemical reactions using a split-operator algorithm. Several additional modules have now been developed, and the model capabilities have been extended to include:

1) *Unsaturated flow modelling*. This extends the model's applicability, for example, to vertical flow constructed wetlands by solving Richard's equation for unsaturated flow in porous media. This module is based on the VSF package for Modflow-2000 (Thoms et al., 2006). The soil characteristic function is described using the van Genuchten – Mualem parameterisation. Boundary conditions to simulate evaporation from the bed surface, ponding and the root-zone have been implemented.
2) *Complex biogeochemical reaction networks*. These include microbial transformations in anoxic conditions as well as multiple electron acceptors (nitrates, iron, sulphur). A schematic representation of the biological transformation included in the module is depicted in Figure 1. Production of gases is explicitly included, namely N_2, N_2O, CO_2, CH_4 and H_2S, and a separate gas phase can form when the partial pressure of the dissolved gases is larger than the local hydrostatic pressure in the wetland. Consequently, the model can also be used, for example, to estimate the amount of greenhouse gases produced, and to identify the operational conditions to treat the highest possible loading rate while minimizing the production of CH_4 and N_2O. In parallel to the complex, comprehensive reaction network outlined above, we also implemented a simplified set of biological aerobic and anaerobic transformations, based on the proposed CWM1 model (Langergraber et al., 2009).
3) *Wetland clogging*. A major problem in the maintenance of constructed wetlands and sand filters is the progressive decrease of the hydraulic conductivity of the substrate during the lifetime of the system, or clogging. Clogging is the result of several parallel processes, but it is

primarily due to filtration and precipitation of suspended solid particles (e.g., particulate organic matter, macromolecules, colloids, etc.) and to biomass growth. It is normally more pronounced near the inlet, and can lead to a significant decrease in the wetland performance. To study the clogging process, and identify some design criteria to minimize its adverse effects, we have also developed a module to simulate the feedback of biological reactions on porosity and hydraulic conductivity. This module is discussed in a separate contribution, together with simulation results illustrating some of its capabilities.

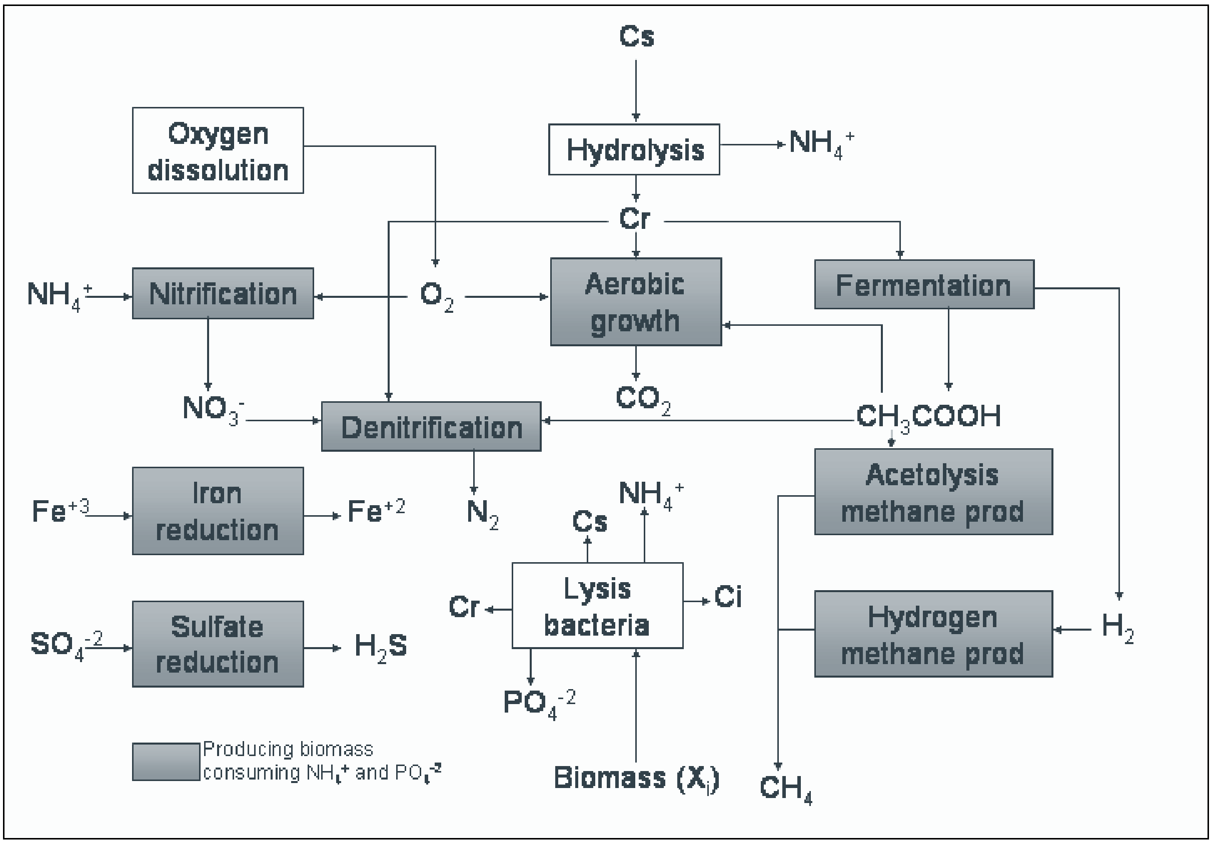

Fig. 1. Schematic representation of the complex geochemical reaction network implemented in the model. Cs, Cr and Ci represent soluble, recalcitrant and inert carbon sources, respectively. Iron and sulphate reduction are driven by hydrogen from the fermentation reaction, i.e. $H_2 \leftrightarrow 2H^+ + 2e^-$

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