Reactive transport modeling of subsurface flow CWs using the HYDRUS wetland module

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Introduction

The HYDRUS software

- Software Package for simulating the two- and three-dimensional movement of water, heat, and multiple solutes in variably-saturated media
- HYDRUS numerically solves the Richards equation for saturated/unsaturated water flow and the convection-dispersion equation for heat and solute transport.
- Graphical User Interface
- Version 2 released in May 2011
- HYDRUS Wetland module (Langergraber and Šimůnek, 2006, 2011)

Content

Introduction
- Treatment wetlands
- Models for wetlands

The Wetland Module of HYDRUS

Simulation results

1. Vertical flow constructed wetlands
2. Batch-fed CWs (Master thesis Tamás Pálfy, BOKU)
3. HF beds with peak loads (Poster Rizzo and Langergraber)
4. HF beds for tertiary treatment (Poster Sanchez-Ramos and Langergraber)
5. Nitrate dynamics in a rural headwater catchment: measurements and modelling (Poster Smethurst and Langergraber)

Summary and conclusion
Introduction
Types of wetlands (Fonder and Headley, 2010)

- **Natural wetlands** are those wetland areas that exist in the landscape due to natural processes rather than having been created either directly or indirectly as a result of anthropogenic influences.
- **Constructed wetlands** are man-made systems that are designed to mimic many of the conditions and/or processes that occur in natural wetlands.

Purpose of constructed wetlands:
- **Restored wetlands**: Areas which were formerly natural wetlands
- **Created wetlands**: Non-wetland areas which have been converted
- **Treatment wetlands**: Artificially created wetland systems designed to provide a specific water treatment function

3 characteristics can be identified which are typical of all TWs:
- The presence of *macrophytic vegetation* that typically grows within natural wetlands;
- The existence of *water-logged* or *saturated substrate* conditions for at least part of the time; and
- The inflow of *contaminated waters* with constituents that have to be removed.
Introduction

Models for wetlands

- In wetlands a large number of physical, chemical, and biological processes are active in parallel and mutually influence each other.
- Therefore wetlands are complex systems and for a long time have been often considered as "black boxes".
- Also models for wetlands for a long time have been using "black box" approaches only, i.e. the processes in wetlands have not been considered in detail.
- Still today most "models" for wetlands are using a "black box" approach
- The number of models describing processes in wetlands in detail is limited.

"Simple" models ("black-box" approach)
- correlations between influent and effluent concentrations
- first-order rate equations (used for design of TWs)
- artificial neural network models
- etc.

- Data from experiments needed to derive model equations

Trang et al. (2009)
Introduction
Models for wetlands

Process-based models

- Mathematical model equations based on processes in wetlands (with various degree of complexity) - includes balance equations for energy, mass, charge, ...

\[ \frac{dm}{dt} = dC \cdot V \]

Typical mass balance equation

- Data are used for calibration and validation of model

- Better prediction is possible using these models

\[ \rightarrow \] should be better applicable for design

Models describing wetland processes
Processes in wetlands

For a WETLAND MODEL a number of different processes have to be considered:

- The flow model (describing water flow)
- The transport model (describing transport of constituents as well as adsorption and desorption processes)
- The biokinetic model (describing biochemical transformation and degradation processes)
- The influence of plants (growth, decay, decomposition, nutrient uptake, root oxygen release, etc.)
- The description of clogging processes
- Physical re-aeration


HYDRUS wetland module
Processes available

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- The transport model (describing transport of constituents as well as adsorption and desorption processes)
- The biokinetic model (describing biochemical transformation and degradation processes)
- The influence of plants (nutrient uptake, root oxygen release)
- Physical re-aeration

- The influence of plants (growth, decay, decomposition)
- The description of clogging processes \[ \rightarrow \] not available in HYDRUS

HYDRUS wetland module
General description

HYDRUS wetland module

- developed for SSF TWs
- includes two biokinetic model formulations:
  1. CW2D (Langergraber and Šimůnek, 2005)
  2. CWM1 (Constructed Wetland Model #1) (Langergraber et al., 2009).

<table>
<thead>
<tr>
<th>Model</th>
<th>CW2D</th>
<th>CWM1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Processes</td>
<td>Aerobic and anoxic (9)</td>
<td>Aerobic, anoxic and anaerobic (17)</td>
</tr>
<tr>
<td>Constituents</td>
<td>Oxygen, organic matter, nitrogen and phosphorus (12)</td>
<td>Oxygen, organic matter, nitrogen and sulphur (16)</td>
</tr>
</tbody>
</table>
Simulation Results 1
Pilot-scale subsurface VF CW for wastewater treatment

Flow simulations

Microbial biomass

Tietz et al., 2007, Sci Total Environ 380(1-3), 163-172
Langergraber et al., 2007, Water Sci Technol 56(3), 233-240
Simulation Results 1
Outdoor CW (Ernsthofen, NÖ) for treatment of wastewater

3 parallel beds
surface area 20 m² each
organic loading of 20, 27, 40 g COD/(m².d)
⇒ resp. 4, 3, 2 m³/PE


Simulation Results 2
Master thesis Tamás Pálfy

- Goal: to verify the implementation of CWM1 in the HYDRUS Wetland Module
- Uses column experiment data made by a research group at Montana State University as reference outcome
- Compare with simulation results published by Mburu et al. (2012, Ecol Eng 42, 304-315) … CWM1 implemented in Aquasim
Simulation Results 2
Master thesis Tamás Pálfy

Experiments at MSU
- D=20cm, h=50 cm batch-operated columns filled with pea gravel
- Synthetic domestic wastewater
  - 490 ± 4.3 mg/L COD
  - 14 ± 0.5 mg/L SO₄⁻-S
  - 40 ± 1.2 mg/L TN
  - 8 ± 0.3 mg/L PO₄⁻-P
- Operated at 12, 16, 20 and 24°C
- 20 days incubation
- Sedge, bulrush and cattail plus unplanted column for each run

Simulation Results 3
Poster: A. Rizzo* and Langergraber

Simulation of peak loads for horizontal flow CWs - A first step towards modeling stochastic behavior of HF CW

Objective
- Compare simulation results for a HF CW subjected to sudden peak loads (Galvão and Matos, 2012, Ecol Eng 49, 123-129)
- Data from laboratory experiment using synthetic wastewater
- COD load was applied
  - Lines A 11.4 g/m²/day for 3.5 months, then +22% load for 2 week
  - Lines B 5.3 g/m²/day for 3.5 months, then +7% load for 2 week

Main assumptions
- parameters CWM1 biokinetic model (Langergraber, G., Šimůnek, J., 2012)
  - rate constant of lysis of fermenting bacteria (Xₕ) → 0.5
  - Fraction of inert particulate (Xᵢ) generated in biomass lysis → 0.01
- no O₂ inflow, no plants
- maximum time step → 0.001 d (ca. 1.5 min)
- new time step check to limit numerical disturbance (code correction was implemented in the new HYDRUS version)
- CODᵢ fractionation for synthetic wastewater
  - Sₕ=62% CODᵢ, Sₐ=10% CODᵢ, Sᵢ=3% CODᵢ, Xᵢ=20% CODᵢ, Xᵢ=5% CODᵢ
Simulation Results 3
Poster A. Rizzo* and Langergraber

Results 1
- COD outflows
  → adequately simulated

<table>
<thead>
<tr>
<th></th>
<th>AE&lt;sub&gt;COD,out&lt;/sub&gt; (%)</th>
<th>Rem&lt;sub&gt;COD,meas&lt;/sub&gt; (%)</th>
<th>Rem&lt;sub&gt;COD,sim&lt;/sub&gt; (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>20</td>
<td>69</td>
<td>68</td>
</tr>
<tr>
<td>B</td>
<td>16.7</td>
<td>66</td>
<td>70</td>
</tr>
</tbody>
</table>

Simulation Results 4
Poster: D. Sanchez-Ramos* and Langergraber

Modelling horizontal flow constructed wetlands treating effluents of wastewater treatment plants

Objective
- Tablas de Daimiel National Park (Spain):
- Floodplain wetland (1928 ha) connected with an important aquifer (5500 km²)
- Intensive pumping → disconnection → drying
- Treated Sewage Effluents from several WWTPs in the surroundings as possible solution for maintenance of TDNP until aquifer recovery
- Direct use of TSE unsafe → CW systems to polish WWTP effluents

* School of Civil Engineering, University of Castilla-La Mancha, Ciudad Real, Spain

Simulation Results 3
Poster A. Rizzo* and Langergraber

Results 1
- NH₄⁺ outflows
  → not adequately simulated

<table>
<thead>
<tr>
<th></th>
<th>AE&lt;sub&gt;COD,out&lt;/sub&gt; (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>83</td>
</tr>
<tr>
<td>B</td>
<td>60</td>
</tr>
</tbody>
</table>
Simulation Results 4
Poster: D. Sanchez-Ramos* and Langergraber

Influent concentrations:
- 125 mg O2 L⁻¹ COD (mainly as slowly biodegradable particulate COD, XS)
- and 15 mg N L⁻¹ ammonium (SNH)

CWM1 parameters changed

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CWM1 original value</th>
<th>Simulation value</th>
<th>Variation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu_n ) (d⁻¹)</td>
<td>6</td>
<td>2.5</td>
<td>-58.33</td>
</tr>
<tr>
<td>( b_n ) (d⁻¹)</td>
<td>0.4</td>
<td>0.4</td>
<td>0</td>
</tr>
<tr>
<td>( K_{SN} ) (mg O₂/l)</td>
<td>0.2</td>
<td>0.4</td>
<td>100</td>
</tr>
<tr>
<td>( K_n ) (d⁻¹)</td>
<td>3</td>
<td>2</td>
<td>-33.33</td>
</tr>
<tr>
<td>( f_{MXL} ) (g CODₘX/g CODₘ)</td>
<td>0.1</td>
<td>0.02</td>
<td>-80</td>
</tr>
</tbody>
</table>

Simulation results
- Better treatment efficiency than expected in the design:
  - 66% COD removal
  - 39% NH₄ removal
- High HRT (19 cm d⁻¹) → important O₂ and COD supply in the inlet
- The high development of \( X_H \) has been the main difficulty on the simulation

Simulation Results 5
Poster: P. Smethurst* and Langergraber

Nitrate dynamics in a rural headwater catchment: measurements and modelling


* CSIRO Ecosystem Sciences, Hobart, Tasmania
SMZ plantation at 4 years of age

Simulation Results 5
Poster: P. Smethurst* and Langergraber

HYDRUS Wetland Modelling:
simulation of riparian buffer N dynamics

Important Capabilities:
• Denitrification
• Other organic C, N and P pools
• Rooting depth
• N uptake
• Rainfall, runoff, groundwater, and seepage
• Spatial and temporal flexibility

Main novel steps:
1. External spreadsheet: quick-flow/slow-flow analysis
2. HYDRUS: route slow-flow through HYDRUS as infiltration
3. External spreadsheet: recombine seepage as base-flow with quick-flow to estimate stream flow

Water and Nitrate:
hillslope modelling success at hourly and annual scales
Summary

Different applications of the biokinetic models CW2D and CWM1

| Biokinetic model | CW2D (Langergraber and Šimůnek, 2005) | CWM1 (Langergraber et al., 2009) |

Conclusions

The following conclusions can be drawn:

- Version 2 of the HYDRUS wetland module is the only publicly available implementation of the Constructed Wetland Model N°1 (CWM1).
- It is essential for modelling SSF CWs that fixed bacteria can be simulated.
- Since CWM1 is able to describe anaerobic processes, it is more suitable for modelling HF CWs.
- The influence of wetland plants on various biochemical transformation and degradation processes due to release of oxygen by plant roots in a HF bed is significant and therefore has to be considered.
- More experience still has to be gained in using the CWM1 biokinetic model.

Needs for improvement 1

(view of the Wetland module users)

- New time step adjustment linked with solute concentrations calculated in the wetland module
- Adjust default parameters for biokinetic models based on recent experiences
- Make limited outflow function again
- Particle transport and influence on hydraulic properties
- It is not possible to use physical non-equilibrium and chemical non-equilibrium at the same time (presentation Ania)
- Preferential flow is not possible while using the wetland module
- Implementation of flexible biokinetic model, i.e. addition of substances and processes to the wetland module should be possible by users

Needs for improvement 2

(view of the Wetland module users)

- Overland flow needs to be simulated by pre- and post-HYDRUS processing (hillslope application).
- For hillslope applications of HYDRUS, with or without the wetland module, it would be very useful to include outputs of pools and fluxes of both water and nitrate on a per area basis.
- Only one root type can be specified, wherever they are placed in the simulation domain (hillslope application).
- Preferential flow is not possible while using the wetland module.
- Implementation of flexible biokinetic model, i.e. addition of substances and processes to the wetland module should be possible by users.
Contact

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