

Implementation of the bacterial transformation and biodegradation processes model CWM1 into the COMSOL Multiphysics simulation software environment

Roger Samsó^a, Esther Llorens^b, Joan Garcia^a.

^a Hydraulics, Maritime and Environmental Engineering Department, Technical University of Catalonia, 08034 Barcelona, Spain (roger.samsó-campa@upc.edu).

^b Catalan Institute for Water Research, H2O building, Scientific and Technological Park of the University of Girona, c/ Emili Grahit 101, E-17003 Girona, Spain.

ABSTRACT

The aim of this work is to provide a new and flexible tool based on the equations described in CWM1 and built on top of the Comsol Multiphysics simulation software environment, to model the biochemical transformation and degradation processes of organic matter, nitrogen and sulphur in subsurface flow constructed wetlands. The model has been developed to overcome some of the limitations of the pre-existing implementation CWM1-RETRASO, with which the model presented in this paper was benchmarked. To this end, both models have been applied on an existing subsurface flow constructed wetland located in Catalonia and the results obtained with each platform have been compared. The results obtained with the two models show a good match. Therefore, the model presented is capable of simulating the internal functioning of constructed wetlands and represents a good starting point for further development and increased complexity.

INTRODUCTION

Constructed wetlands have long been used to improve water quality. During this time, several researchers have focused their attention on trying to comprehend the processes that lead to the removal of pollutants within them. However, there are still some areas of its internal functioning that are not yet well understood. To help understand the internal behaviour of these systems, several numerical models of diverse complexity have been developed (Langergraber 2008). However, the models developed so far are not yet capable of simulating all the processes involved in the water treatment nor have they caught the attention of the constructed wetlands' designers.

At present, the best implementation of the well accepted Constructed Wetlands Model Number 1 (Langergraber et al. 2009) is CWM1-RETRASO (Llorens et al. 2009). This is the only mechanistic model that has successfully simulated the processes described in CWM1 on a real subsurface flow constructed wetland (Les Franqueses del Vallès, Catalonia) (Llorens et al. 2010). Despite its good performance, this model and specifically the platform on which it was developed (RetrasoCodeBright) (Saaltink et al. 2004; Llorens et al. 2009) has certain limitations that have hindered its wider adoption among the industry and that do not allow adding further complexity. The steep learning curve due to the lack of a user interface is bound to be one of the causes of the little adoption of the model. Among the most significant limitations of the model itself are the fact that the bacteria responsible for the

water quality improvement travel at the flow velocity and that the development of clogging cannot be simulated.

These limitations have encouraged the development of a new model, which takes on the work by Langergraber 2009, Llorens et al., 2009 and Llorens et al. 2010 and aims at providing a more flexible and comprehensive simulation platform to further extend the knowledge of these complex systems.

METHODS

Comsol Multiphysics is a complete simulation software environment which uses an underlying finite elements platform to solve the model differential equations.

The model presented, which is built on the Comsol Multiphysics platform, is subdivided in two separate models running one on top the other; the base model describes the hydraulics of the simulated wetland, while the one running on top describes the reactive transport processes taking place within the granular media. The hydraulic model uses the Darcy equations to simulate a stationary water flow through the bed. It was calibrated using real data obtained from a wetland in Les Franqueses del Vallès (Barcelona, Catalonia) with a tracer test carried out by Garcia et al. 2004. The main features of this wetland are shown in Table 1. On the other hand, the solute transport is modelled using 16 equations (one for each component of CWM1) that consider advection, dispersion and diffusion. In each of these equations there is a term for chemical reactions, in which the equations describing bacterial reaction rates in CWM1 (Langergraber et al. 2009) were added. All the modifications introduced by Llorens et al. 2010 to the stoichiometric and kinetic parameters of CWM1 were implemented in the present model as well.

Table 1. Main features of the simulated wetland.

Bed geometry	Length (m)	10,3
	Width (m)	5,3
Granular media	Porosity	0,41
	Cu	1,6
	D ₆₀ (mm)	10
	Hydraulic conductivity	14,76
Hydraulic properties	HLR (mm/d)	36
	HRT (h)	132
	Water depth (m)	0,5-

This model has been benchmarked with CWM1-RETRASO taking into account different scenarios of inflow concentrations. These different scenarios are described in Llorens et al. 2010.

RESULTS AND DISCUSSION

Despite being in the initial stages of the implementation of CWM1 on the Comsol Multiphysics platform, so far the results obtained with the two platforms show a promising good match. However, there are still some minor issues that need to be addressed before the full power of the model can be extracted. Among these problems, the most significant one concerns the hydraulic model, in which more work needs to be put. Also, the differences in the results obtained after several simulations with the two models, can be partly attributed to the fact that in our implementation of CWM1, as opposed to that of CWM1-RETRASO, the biofilm is attached to the granular media. In this regard, we expect to have more results by the date of the congress.

CONCLUSIONS

The new implementation of CWM1 in the Comsol Multiphysics platform shows great potential and represents a good starting point for further development. The friendly user interface and the ease of use of Comsol Multiphysics adds to the value of the model which, when tested extensively, will be applicable with design purposes.

REFERENCES

- García, J., Chiva, J., Aguirre, P., Alvarez, E., Sierra, J., and Mujeriego, R. (2004). Hydraulic behaviour of horizontal subsurface flow constructed wetlands with different aspect ratio and granular medium size. *Ecological Engineering* 23, no. 3 (November): 177–187. doi:10.1016/j.ecoleng.2004.09.002.
- Langergraber, G., Rousseau, D., García, J., and Mena, J. (2009). CWM1: a general model to describe biokinetic processes in subsurface flow constructed wetlands. *Water science and technology : a journal of the International Association on Water Pollution Research* 59, no. 9 (January): 1687–97. doi:10.2166/wst.2009.131.
- Langergraber, G. (2008). Modeling of Processes in Subsurface Flow Constructed Wetlands: A Review. *Vadose Zone Journal* 7, no. 2: 830. doi:10.2136/vzj2007.0054.
- Llorens, E., Saaltink, M., Poch, M., and García, J. (2010). Bacterial transformation and biodegradation processes simulation in horizontal subsurface flow constructed wetlands using CWM1-RETRASO. *Bioresource technology* (September): 1–9. doi:10.1016/j.biortech.2010.09.038.
- Llorens, E., Saaltink, M., García, J., (2009). CMW1-RETRASO: a dynamic numerical model of subsurface horizontal flow constructed wetlands. In: Bayona, J.M., García, J. (Eds.), *Proceedings of the 3rd Wetland Pollutant Dynamics and Control Symposium. WETPOL 2009, Barcelona*, pp. 75–76.
- Saaltink, M., Batlle, F., Ayora, C., Carrera, J., and Olivella, S. (2004). RETRASO, a code for modeling reactive transport in saturated and unsaturated porous media. *Geol. Acta* 2, no. 3: 235–251.