Simulating Woodchip Bioreactor Performance Using a Mobile-Immobile Flow Model

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Introduction

Due to the strong bimodal pore distribution of the woodchips used in bioreactors, we hypothesized that nitrate transport through woodchip bioreactors would be best described by a dual porosity transport model where the bioreactor water is divided into a mobile domain between the woodchips where water is free to flow and solute movement is by advection and dispersion; and an immobile domain of water mostly within the woodchips that is stagnant and solute movement is by diffusion alone.

Methods

- A pilot-scale woodchip bioreactor was installed and used to treat water draining plots used to grow corn and soybean
- Nitrate concentrations entering and leaving a woodchip bioreactor were measured for 2 y, along with bioreactor temperature and flow rate
- Drainage through the bioreactor was determined by the natural drainage of the field plots
- A 1D mobile/immobile (MIM) model was used to describe nitrate transport through the bioreactor
- A KBr tracer was added during the 1st year to measure the Br breakthrough curve
- The HYDRUS model was used to fit the MIM model parameters θ_{im}, D_m, and α to the Br data
- The HYDRUS model was then used to fit the nitrate data for 2013 and 2014 using the parameters found from the Br data and fitting either 0-order (γ) or 1st order (μ) reaction rate and the Q_{10} temperature dependence.

Model

We used the MIM model to describe the transport and fate of nitrate moving through the dual porosity woodchip bioreactor. The MIM model can be expressed as:

$$\theta_m R \frac{\partial C_m}{\partial t} = \theta_m D_m \frac{\partial^2 C_m}{\partial x^2} - v_m \theta_m \frac{\partial C_m}{\partial x} - \alpha(\theta_m - \theta_{im}) - \theta_m \mu C_m - \theta_m \gamma$$

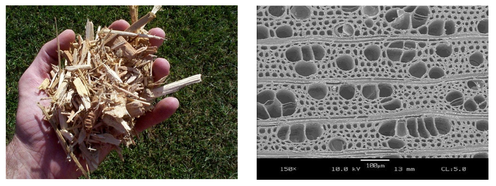
$$\theta_{im} R \frac{\partial C_{im}}{\partial t} = \alpha(C_m - C_{im}) - \theta_{im} \mu C_{im} - \theta_{im} \gamma$$

Where θ_m is the mobile and θ_{im} the immobile volumetric water content; and there sum being the total water content; C_m and C_{im} are the solute concentrations (mg L^{-1}) in the mobile and immobile domains; α (d^{-1}) is a first-order diffusion coefficient between the mobile and immobile liquid regions; t is time (d); R is the retardation ($R = 1 + \rho_b K_d \theta^{-1}$); ρ_b is the bulk density (g cm^{-3}); K_d is the equilibrium distribution constant (L kg^{-1}); x is distance (cm); D_m is the hydrodynamic dispersion in the mobile domain (cm^2 d^{-1}); v_m is pore water velocity (cm d^{-1}), D_m/v is the dispersivity (λ), and μ and γ are the 1st-order (d^{-1}) and 0-order (mg L^{-1} d^{-1}) water phase degradation rates.

Results

- The bioreactor removed 38% of the nitrate in 2013 and 49% of the nitrate in 2014
- Denitrification rates varied over the range of 0.04 – 13.2 g N m^{-3} during the 2 yr
- The MIM model fit the Br data well with $R^2 = 0.964$, NSSI = 0.94, and RMSE = 0.46 mg L^{-1}
- The MIM model fit the NO_3 data well with $R^2 > 0.7$, NSSI > 0.75, and RMSE < 2 mg L^{-1}.
- There was no consistent improvement in assuming either 0 - or 1st - order denitrification kinetics
- The Q_{10} was variable and often could not be fitted precisely , probably because of the limited temperature range observed
- The MIM concept is a promising approach for modeling nitrate fate and transport in woodchip bioreactors

Figure 1. Woodchips used in bioreactor and photo showing internal woodchip porosity (right), Br breakthrough curve and MIM model fit (below), and fitting results for Br data (below right).



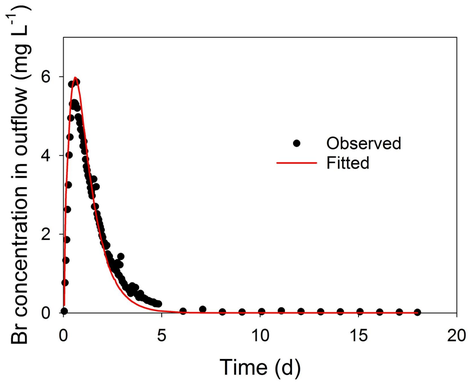


Table 1. MIM fitted parameters to Br data

Parameter	Fitted (95%cl)
λ (cm)	26.7 (18.32 – 35.2)
θ_{im} (-)	0.553 (0.521 – 0.585)
α (d^{-1})	5.29 (4.54 – 6.04)

Table 2. Fitted MIM model parameters, their 95% c.l., and fitting statistics for denitrification.

Year	γ (mg N L^{-1} d^{-1})	μ (d^{-1})	Q_{10}	R^2	RMSE	NSSI	Pbias
		0-order					
2013	8.7	-	1.7	0.80	1.58	0.77	-5%
	4.3-14.7		1.0-4.0				
2014	6.82		1.2	0.84	1.62	0.79	14%
	3.1-11.6	-	1.0-4.5				
		1st- order					
2013	-	0.99	8.0	0.88	1.49	0.88	-4%
		0.76-1.22	2.9-32				
2014	-	1.02	1.2	0.77	1.72	0.76	-8%
		0.85-1.18	1.0-5.3				

NSSI = Nash Sutcliffe sufficiency index

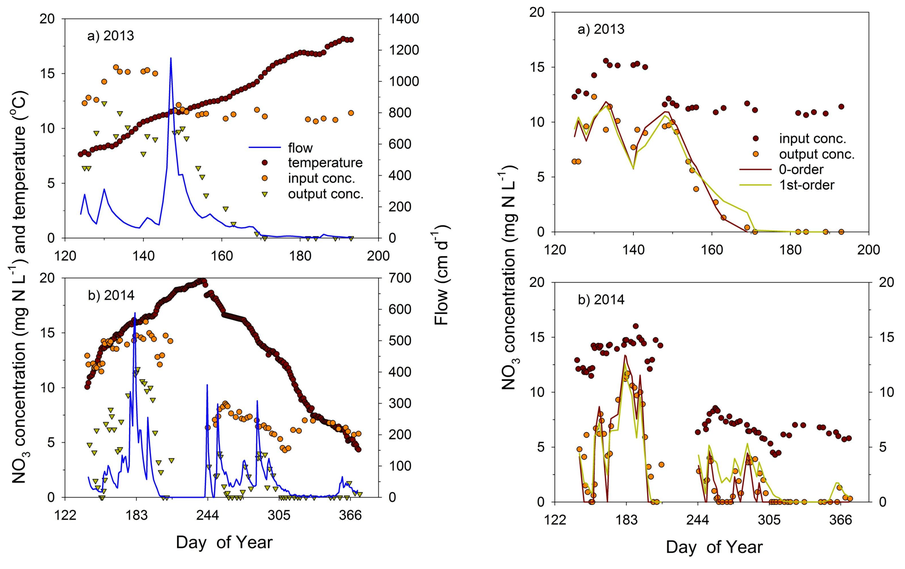


Figure 2. Measured NO_3 input and output concentration to bioreactor, flux and temperature (left) and best fit 0- and 1st-order nitrate removal kinetics in HYDRUS simulations (right).