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Calibration and validation of an integrated nitrate transport model within a well capture zone

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ABSTRACT

Groundwater contamination by nitrate was investigated in an agricultural area in southern Quebec, Canada, where a municipal well is the local source of drinking water. A network of 38 piezometers was installed within the capture zone of the municipal well to monitor water table levels and nitrate concentrations in the aquifer. Nitrate concentrations were also measured in the municipal well. A *Water flow and Nitrate transport Global Model* (*WNGM*) was developed to simulate the impact of agricultural activities on nitrate concentrations in both the aquifer and municipal well. The *WNGM* first uses the *Agriflux* model to simulate vertical water and nitrate fluxes below the root zone for each of the seventy agricultural fields located within the capture zone of the municipal well. The *WNGM* then uses the *HydroGeoSphere* model to simulate three-dimensional variably-saturated groundwater flow and nitrate transport in the aquifer using water and nitrate fluxes computed with the *Agriflux* model as the top boundary conditions. The *WNGM* model was calibrated by reproducing water levels measured from 2005 to 2007 in the network of piezometers and nitrate concentrations measured in the municipal well from 1997 to 2007. The nitrate concentrations measured in the network of piezometers, however, showed greater variability than in the municipal well and could not be reproduced by the calibrated model. After calibration, the model was validated by successfully reproducing the decrease of nitrate concentrations observed in the municipal well in 2006 and 2007. Although it cannot predict nitrate concentrations in individual piezometers, the calibrated and validated *WNGM* can be used to assess the impact of changes in agricultural practices on global nitrate concentrations in the aquifer and in the municipal well.

1. Introduction

In rural areas, groundwater contamination is frequently associated with agricultural activities, with nitrate being one of the most common contaminants. Previous assessments of groundwater quality in areas with intensive agriculture have shown significant nitrate contamination in unconfined aquifers, with concentrations varying from 35 to 85 mg NO_3^-/L (Chae et al., 2004; Kaown et al., 2007; Kim et al., 2009; Krapac et al., 2002; Lasserre et al., 1999; Molenat and Gascuel-Odoux, 2002). Consumption of water containing nitrate at levels higher than 49 mg NO_3^-/L could lead to methaemoglobinemia in infants (WHO, 2007) and, in the long term, could be potentially carcinogenic to humans (INSPQ, 2003). The US EPA (1991) suggests a threshold for nitrate in drinking water between 50 and 90 mg NO_3^-/L and points out that no risk for human health has been observed

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for infants consuming water containing less than 45 mg NO_3^-/L.

The protection of sources of groundwater in regions with intensive agriculture often creates conflicts. On one hand, farmers grow crops and produce food to satisfy consumer demand and, on the other hand, municipal and government authorities must protect public health by ensuring adequate drinking water quality. Therefore, most groundwater regulations require the delineation of a well capture zone, which corresponds to the portion of land contributing water to a well, along with wellhead protection areas. These wellhead protection areas are defined according to distance or travel time. Strategies for source water protection serve to define protection areas, identify potential sources of contamination within these areas and manage contamination sources. Regulations for groundwater source protection typically prohibit or restrict specific activities within protection areas, impose monitoring requirements and promote public education (US EPA, 2000). Prohibition or restriction of specific activities can create conflict, for example, with farmers as mentioned above.

Proper land use and groundwater protection within a well capture zone and protection areas require a scientific understanding of the impacts of agricultural activities on groundwater quality. These impacts are typically assessed with groundwater and solute transport models. Almasri (2007) reviewed state-of-the-art modeling of the fate of nitrate in aquifers and explained that accurately simulating nitrate concentrations may be difficult because of complex nitrogen transformation and transport processes occurring in soils as well as temporal and spatial variations of nitrate concentrations in groundwater. Soil nitrogen models are useful to estimate nitrate leaching from ground surface to groundwater. A number of mechanistic models were developed to simulate the dynamics of nitrogen transformation and nitrate transport in the root zone, such as *NLEAP* (Shaffer et al., 1991), *Leachm* (Huston and Waganet, 1992), *Agriflux* (Banton and Larocque, 1997), and *Coupmodel* (Jansson and Karlberg, 2004). An overview of these models is provided by Ma and Shaffer (2001). They are based mainly on the one-dimensional Richards equation (Todd and Mays, 2005) to simulate vertical flow in the unsaturated (or root) zone. They generally account for the main processes affecting water balance near ground surface, such as precipitation, surface runoff, drainage, infiltration, crop water uptake, evaporation, and snowmelt (Zhang et al., 2002). Soil nitrogen models also simulate the nitrogen cycle, including nitrogen input, mineralization, nitrification, denitrification, nitrogen uptake by crops, and nitrate leaching (Almasri and Kaluarachchi, 2007). However, these soil nitrogen models have limited capabilities to simulate the fate of nitrate in aquifers and they must be linked to models that simulate variably-saturated groundwater flow and solute transport in porous media.

The simulation of nitrate migration in groundwater can be grouped into two categories according to the main processes simulated: denitrification or nitrogen plant uptake. Kinzelbach and Schäfer (1991), Schäfer and Therrien (1995), MacQuarrie et al. (2001), and Molenat and Gascuel-Odoux (2002) present nitrate transport simulations that account for denitrification within an aquifer but do not consider nitrogen plant uptake. Contrary to these studies, the work presented here focuses on simulating nitrate transport in an oxygenated aquifer where denitrification can be neglected but where nitrogen uptake by plants must be considered. Table 1 presents a list of studies relevant to our work and where a soil nitrogen model was coupled to a groundwater flow and a solute transport model to investigate groundwater contamination by nitrate in agricultural areas. These studies considered nitrate contamination at scales ranging from 518 to 95 560 km^2 (Almasri and Kaluarachchi, 2007; Krause et al., 2008; Ledoux et al., 2007; Refsgaard et al., 1999; Savard and Somers, 2007), which is much larger than the scale considered here. The only study at a scale similar to the one considered here is presented in Lasserre et al. (1999) for an area of 20 km^2. These studies generally aim at simulating nitrate contamination in a catchment, and there are no reported studies where numerical models simulate nitrate transport for municipal well management at a local scale.

Model calibration is essential to ensure adequate representation of groundwater flow and nitrate transport in the aquifer. Calibration is generally divided into three steps (ASTM, 1994; ASTM, 1996). The first step is a sensitivity analysis to identify the parameters with the greatest impact on outputs. The second step is history matching, where values of the most sensitive parameters are modified to minimize the difference between observed and simulated outputs. The third step is validation of the model to test its predictive capabilities. In general, any model should be validated before its application. A set of wells or piezometers may be moni-

Table 1
Groundwater and nitrate transport studies in agricultural areas.

Author	Area (km^2)	Nitrogen transformation	Root zone and unsaturated zone model	Saturated zone model
Savard and Somers (2007)	5660	CANB (Yang et al., 2007)	HELP (Schroeder et al., 1994)	FEFLOW (Diersch, 2004)
Almasri and Kaluarachchi (2007)	973	NLEAP (Shaffer et al., 1991)	NLEAP (Shaffer et al., 1991)	MODFLOW (Harbaugh and McDonald, 1996); MT3D (Zheng and Wang, 1999)
Krause et al. (2008)	998	SWIM (Krysanova et al., 2000)	WASIM-ETH-I (Schulla, 1997)	MODFLOW (Harbaugh and McDonald, 1996); MT3D (Zheng and Wang, 1999)
Lasserre et al. (1999)	20	Agriflux (Banton and Larocque, 1997)	Agriflux (Banton and Larocque, 1997)	MODFLOW (Harbaugh and McDonald, 1996); MT3D (Zheng and Wang, 1999)
Refsgaard et al. (1999)	518/536	Daisy (Hansen et al., 1991)	Daisy/MIKE SHE (Hansen et al., 1991; Refsgaard and Storm, 1995)	MIKE SHE (Refsgaard and Storm, 1995)
Ledoux et al. (2007)	95 560	STICS (Brisson et al., 2003)	MODCOU/NEWSAM (Ledoux et al., 1989)	MODCOU/NEWSAM (Ledoux et al., 1989)