EXPERIMENTAL STUDY AND NUMERICAL SIMULATION OF
DENITRIFICATION IN SATURATED POROUS MEDIA

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Abstract. The effect of denitrification on the behavior of nitrate in saturated sandy soil was studied in the laboratory and the results were compared with the temporal and spatial concentration of nitrate in nonreactive (without denitrification) and reactive (with denitrification) cases. A laboratory model was fabricated to study steady one-dimensional flow and to transport nitrate with or without denitrification. Denitrification at various rates has been simulated with varied C:N ratios and detention time. Retardation constant, dispersivity, and degradation constants have been computed using existing analytical models supporting adsorption and zero and/or first order production or decay. It was found that such analytical models can be used to fit the concentration of nitrate in saturated porous media for a C:N ratio between 2 and 5.

1. Introduction

The leaching of nitrate from agricultural land has been a major focus of investigation throughout the decade [1-12]. Major field investigation on the occurrence and rate of denitrification has been reported by Hendry et al. [13] and Trudell et al. [14]. Nitrate concentration in groundwater in many regions of the world has been exceeding the World Health Organization and European Economic Community recommended standard limit of 11.3 mg NO$_3$-N L$^{-1}$ (50 mg NO$_3$ L$^{-1}$).

It has been recognized for about 30 yr that excessive quantities of nitrate in the drinking water can cause methaemoglobinemia in infants and ruminants by depleting O$_2$ in their bloodstream [15]. Nitrates may also have possible carcinogenic effect on the human body, being converted to nitrites or nitrosamines [16]. Recent reports link nitrate intake to gastric cancer [17, 18]. The UK Government has set up a study group to investigate the problems posed by high nitrate levels in UK water supplies. Wolfe and Wasserman [19] have discussed the health hazards due to ingestion of water and food items high in nitrate and the US Public Health Service [20] has set a mandatory limit of 45 mg L$^{-1}$ nitrate (NO$_3^-$) for domestic water supplies.

Besides denitrification, several methods are available for the removal of nitrate...
from drinking water. These include: chemical reduction; ion exchange; reverse osmosis; electrodialysis; etc. A combination of ion-exchange and denitrification has also been suggested. In fact, much research has been directed towards the removal of N from drinking water as well as groundwater. However research on the effects of chemical reactions on transport and dispersion of contaminants like NO$_3^-$, in connection with quantification of flow, are relatively few.

The objective of this paper is to study on the effects of denitrification, a biochemical reaction that has had a salutary effect on NO$_3^-$ pollution, and its effect on the behavior of nitrate in saturated porous media.

2. Theoretical Background

Various Researchers have attempted to quantify contaminant transport by solving the advection dispersion equation. However a satisfactory level of understanding of all relevant processes is not complete yet, and consequently there is a lack of theories which adequately describe or predict subsurface contaminant transport.

Parker and van Genuchten [21] suggest the following equation for the transport of a single reactive solute species subject to first-order decay, zero-order production, and adsorption during steady flow in a one-dimensional homogenous system:

$$\frac{\rho}{\theta} \frac{\partial S}{\partial t} + \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - \nu \frac{\partial C}{\partial x} - \mu_w C - \frac{\mu_s \rho}{\theta} S + \gamma_w + \frac{\gamma_s \rho}{\theta}$$

(1)

where $C$ is the volume averaged resident concentration of the solute in the liquid phase; $S$ is the adsorbed concentration per unit mass of the solid phase; $\theta$ is the volumetric water content; $D$ is the dispersion coefficient; $\nu$ is the seepage or average pore water velocity in the $x$ direction; $\mu_w$ and $\mu_s$ are rate constants for first-order decay in the liquid and solid phase of the soil respectively; and $\gamma_w$ and $\gamma_s$ are the corresponding zero-order production coefficients. Considering the case where adsorption is defined by a linear or linearized isotherm of the form

$$S = kC$$

(2)

where $k$ is an empirical distribution constant. Substituting (2) into (1) we get

$$D \frac{\partial^2 C}{\partial x^2} - \nu \frac{\partial C}{\partial x} - \mu C + \gamma = \frac{R \frac{\partial C}{\partial t}}{\theta}$$

(3)

where the dimensionless retardation factor $R$ is defined as

$$R = 1 + \rho k / \theta$$

(4)

and the new rate constants $\mu$ and $\gamma$ are given by

$$\mu = \mu_w + \mu_s \rho k / \theta$$

(5)

$$\gamma = \gamma_w + \gamma_s \rho k / \theta.$$