Modelling spatial oscillations in soil borehole bacteria

M.J. McGuinness [a,*], L.B. Cribbin [b], H.F. Winstanley [b], A.C. Fowler [b,c]

[a] School of Mathematics, Statistics and Operations Research, Victoria University of Wellington, New Zealand
[b] MACSI, University of Limerick, Limerick, Ireland
[c] OCIAM, University of Oxford, Oxford, UK

HIGHLIGHTS

- A simple mathematical model.
- Spatial oscillations in groundwater contaminants.
- Microbial competition between fermenters and respiring heterotrophs plays the key role.
- Self-sustained temporal oscillations plus spatial diffusion can give travelling waves.

ARTICLE INFO

ABSTRACT

Spatial oscillations in groundwater contaminant concentrations can be successfully explained by consideration of a competitive microbial community in conditions of poor nutrient supply, in which the effects of spatial diffusion of the nutrient sources are included. In previous work we showed that the microbial competition itself allowed oscillations to occur, and, in common with other reaction–diffusion systems, the addition of spatial diffusion transforms these temporal oscillations into travelling waves, sometimes chaotic. We therefore suggest that irregular chemical profiles sometimes found in contaminant plume borehole profiles may be a consequence of this competition.

© 2014 Elsevier Ltd. All rights reserved.

1. Introduction

Groundwater contaminant concentration profiles have been observed to oscillate spatially (Broholm et al., 1998; Jones et al., 1999; Smits et al., 2009). In recent work, Fowler et al. (2014) suggested that one mechanism whereby such oscillatory profiles could occur was through a competitive interaction between respiring heterotrophic and fermentative bacteria. In conditions of limited nutrient supply, self-sustained oscillations in both microbe species and nutrient carbon source can occur in a Continuous Stirred Tank Reactor (CSTR) model, and Fowler et al. (2014) suggest that when this model is studied in a spatially inhomogeneous medium, the effects of diffusion may cause oscillatory waves to occur, corresponding to the spatial oscillations which are actually seen. The purpose of the present paper is to demonstrate that this is true.

An extensively studied site of groundwater contamination is the Rexco site in Mansfield, UK, where the ammoniacal waste liquor from a coal carbonisation plant, which operated from the early 1930s to 1970s (Smits et al., 2009), has penetrated some 18 m into unsaturated sandstone, forming a contaminant plume of about 25 m depth. In the course of a large field investigation (Broholm et al., 1998; Jones et al., 1999), groundwater and soil samples were taken from a series of boreholes and the minerals in the aquifer were characterised. The results from borehole BH102 (data collected May 2003) are shown in Fig. 1. Data for each contaminant was recorded along 25 cm intervals beginning 18 m underground at the top of the saturated zone, so that we can see a vertical section through the contaminant plume. The interpretation of data such as these follows standard explanations of redox zonation by sequential depletion of terminal electron acceptors (TEAs) (e.g. Chapelle, 2001). The most striking feature of the data is the nitrate spike at 19 m depth, suggestive of coupled nitrification–denitrification, presumably at the lower margin of the oxic zone, though oxygen data are not available. The steady decrease of nitrate from 19 m to 22.5 m indicates denitrification in the absence of oxygen, with a depletion at 22.75 m in a sharp front. The dominant TEA process in this region is not evident from the data, but dissimilatory iron reduction or sulphate reduction are plausible candidates. Our interest is in the zone below this front (from 23 m depth), where concentrations of the electron donors' organic carbon and ammonium

* Corresponding author: School of Mathematics, Statistics and Operations Research, Victoria University of Wellington, New Zealand. Tel.: +64 4 463 5059.
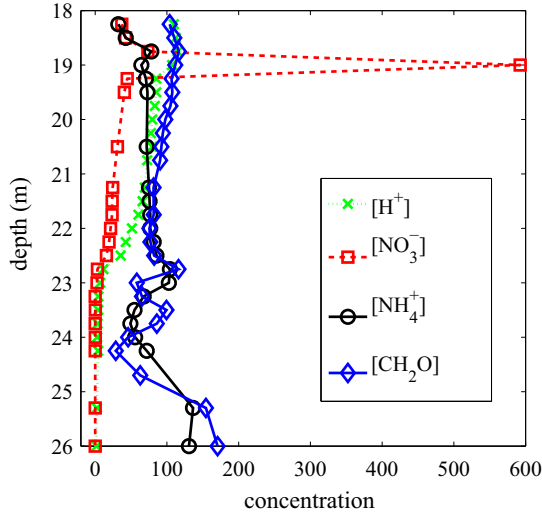E-mail address: Mark.McGuinness@vuw.ac.nz (M.J. McGuinness).

Fig. 1. The data from the Rexco site, borehole 102, May 2003, showing concentrations of NH_4^+ (mg l^{-1}), NO_3^- (mg l^{-1}), H^+ (nmol l^{-1}) and CH_2O (10^{-5} mol l^{-1}). Note that the zero concentration is offset from the left hand axis, and both H^+ and NO_3^- go to zero at a reaction front at depth 22.75 m. Oscillations in concentration profiles are observed from 22.5 m. The data was kindly provided by David Lerner and Arne Hüttmann at the Groundwater Protection and Restoration Group, University of Sheffield.

appear to show out-of-phase spatial oscillations. While only a single period of these oscillations is visible, the important feature is the coherence of the data points within this period; the signal does not appear noisy. Other borehole profiles from the same site also show similar coherent oscillations (Smits et al., 2009). Although oscillations in chemical reactions can occur, for example in the Belousov–Zhabotinskii reaction (e.g., Murray, 2002), we have sought vainly in models of nitrification for processes which might oscillate. Instead, we suggested (Fowler et al., 2014) that the cause of spatial oscillations might lie in competition between microbial populations. While microbial competition is commonly thought of as providing for competitive exclusion (Smith and Waltman, 1995), we showed (Fowler et al., 2014) that in a simple model of microbial competition oscillations could occur.

We wish to emphasise that while our interest in spatial oscillations is motivated by Fig. 1, our concern is not to explain that particular data set, but simply to ask the question whether realistic mathematical models of microbial growth are consistent with such oscillations. The model described in the following section should be divorced from any direct connection with Fig. 1.

The model system which we studied earlier represented a fairly general system in which two competing microbial populations used two different carbon sources, provided typically by hydrolysis from an organic carbon feed. A population of heterotrophs could utilise either source, but preferred the simpler, broken down carbon, which itself was provided by the action of fermenters on the complex source. The resulting activator–inhibitor system led to pronounced oscillations in conditions of relative starvation.

In this short note, we show that the same model kinetics, when incorporated in a spatial domain with the effects of spatial diffusion added, allow spatial oscillations to occur, with a wavelength comparable to that which is seen in Fig. 1, although we emphasise again that a direct application is not intended.

2. Activation-inhibition system

2.1. The model

The interactions between respiring heterotrophic bacteria (H) and fermentative bacteria (F), consuming complex (C_n) and simple

(C_1) organic carbon are given by the model (Fowler et al., 2014)

$$\frac{\partial H}{\partial t} = \frac{r_n C_n H}{C_n + K_n} + \frac{r_1 C_1 H}{C_1 + K_1} - d_H H,$$

$$\frac{\partial F}{\partial t} = \frac{r_F C_n F}{C_n + K_F} - d_F F,$$

$$\frac{\partial C_n}{\partial t} = -\frac{r_F C_n F}{Y_{Fn}(C_n + K_F)} - \frac{r_n C_n H}{Y_n(C_n + K_n)} + S + D\frac{\partial^2 C_n}{\partial z^2},$$

$$\frac{\partial C_1}{\partial t} = \frac{r_F C_n F}{Y_{F1}(C_n + K_F)} - \frac{r_1 C_1 H}{Y_1(C_1 + K_1)} + D\frac{\partial^2 C_1}{\partial z^2}, \tag{2.1}$$

which differs from our earlier model by the inclusion of diffusion terms for the soil carbon concentrations in a one-dimensional spatial domain $-\infty < z < \infty$.

Diffusive transport is assumed here because we are concerned with the vertical structure of the profile. In fact, transport in groundwater plumes is essentially by horizontal advection, and is measured by the size of the (reduced) Péclet number, which has a typical value somewhat larger than one.[1] However, such advection simply causes the vertical diffusive term to be relative to a uniformly advected horizontal spatial coordinate, with respect to which (2.1) provides the appropriate model.

Units for H, F, C_n, and C_1 are mg$_{COD}$ l^{-1}. Fermenters activate respiring heterotrophs as they break down complex carbon and produce simple organic carbon. The respiring heterotrophic bacteria that consume the complex organic carbon inhibit the fermenters. S denotes the constant source of complex organic carbon and r_i denotes reaction uptake rates. We have used simple Monod uptake terms with maximal uptake rates r_i, half-saturation constants K_i, yield coefficients Y_i, and linear death rates with coefficients d_i, for the bacteria. We have ignored an additional source term for complex carbon released upon death by organic material, involving a conversion ratio ζ, which is noted in Fowler et al. (2014) can lead to chaotic oscillations if $\zeta \neq 0$.

Typically, organic carbon would be supplied through advection from upstream, diffusion from the plume centre, or by hydrolysis. The latter would provide a source term in the equation, and following Fowler et al. (2014), we take this source S to be constant.

2.2. Non-dimensionalisation

We non-dimensionalise the equations in the same way as Fowler et al. (2014), additionally choosing an appropriate length scale:

$$H = \frac{S}{d_H}h, \quad F = \frac{S}{d_F}f, \quad C_1 = \frac{K_1 d_H}{r_1}c, \quad C_n = \frac{K_F d_F}{r_F}s,$$

$$t \sim t_0 = \sqrt{\frac{K_n}{r_F S}}, \quad z \sim l = \sqrt{D t_0}. \tag{2.2}$$

Parameter values are listed in Table 1; these are as given by Fowler et al. (2014), with the additional choice of a diffusion coefficient D of $\sim 10^{-9}$ m^2 s^{-1}. Most of the parameter values are taken from Langergraber et al. (2009).

The resulting dimensionless model is given by

$$\varepsilon \lambda h_t = \frac{\delta h s}{1 + \gamma s} + \frac{hc}{1 + \alpha c} - h,$$

$$\varepsilon f_t = \frac{sf}{1 + \beta s} - f,$$

$$s_t = \varepsilon\left[\sigma - \frac{sf}{Y_{Fn}(1 + \beta s)} - \frac{\delta h s}{Y_n(1 + \gamma s)}\right] + s_{zz},$$

---

[1] A typical example is for a horizontal flow of $U = 10$ m year^{-1}, over a horizontal distance $L \sim 1$ km and vertical extent $h \sim 10$ m; if the transverse dispersion coefficient is $D \sim 10^{-9}$ m^2 s^{-1}, then the reduced Péclet number is $Pe = Uh^2/LD \sim 30$.