

Fate of organic contamination during bank infiltration

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Introduction

The purpose of this report is to show the movement, via advection, of nutrients from a polluted river source through an aquifer. In addition to this it will demonstrate the chemical reactions which occur as the pollutant travels through the aquifer, differentiating the different compounds which are formed.

The model will make use of the derived differential equations used for stoichiometry and the reaction rates which were deemed appropriate given the constituent parts in the system.

Within the model different chemical processes are added to show their interconnection and dependence upon concentrations produced through reactions within the aquifer and the transport of compound concentrations from outside (the river). These processes are primarily, aeration, nitrification, denitrification and aerobic mineralisation. Aeration of the soil is Aerobic mineralisation affects the dissolved organic nitrogen, this process reduces the DON to a consumable form of the nitrogen in the form of Ammonia (Doussan et al., 1997). Nitrification is the reduction of ammonia to other nitrogen based product, in this case, Nitrate (Soetaert et al., 1996). Once the oxygen concentration within the aquifer has been lowered by the nitrification process, denitrification can take place (Spiteri et al., 2008). This process involves making use of the ammonia which has been produced in the nitrification process and finishes its reduction to nitrogen gas.

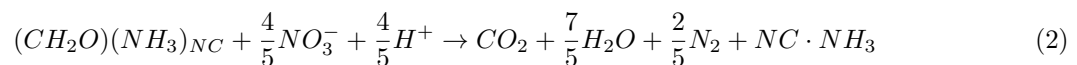
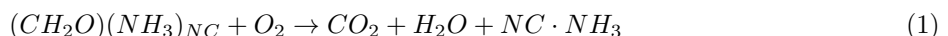
The overall process described by this model is bank filtration used for the cleaning of surface water to a grade suitable for human use. The use of bank filtration is of particular importance as for many counties it is used for the pre-treatment or treatment of water before human use (Hiscock & Grischek, 2002). Bank infiltration makes use of the naturally occurring processes present in the banks of rivers, namely; aeration, aerobic mineralization, nitrification and denitrification. These processes allow for the removal of DON. The layers of sand and silt at the bed of a river act as filter system through which nutrients and pathogens may be removed (Tufenkji et al., 2002). The system presented is a simplified version of the naturally occurring riverbanks where distance from the source and rate limiting elements, such as oxygen, play an important role not only in the chemical processes occurring but also where these chemical processes occur (Tufenkji et al., 2002).

The consequences of this distance related limitation on the processes will be demonstrated within the model. As this is a simplified model in a real scenario the ratio of nitrogen and phosphorus in the system would be greater than the redfield ratio of 16:1. These affects are the result of anthropogenic discharges via farming and industry.

Methods

Model concept

In this model, the processes involved in organic matter mineralization are simplified to a subset of three main reactions. While the full nitrogen cycle is more involved, including processes such as anammox, these are beyond the scope of the current project.



Equation 1 describes the reaction of the process of aerobic mineralization, with NC standing for the nitrogen to carbon ratio in organic matter, also known as the Redfield ratio (16/106). As this is the energetically most favorable reaction, microbes will use oxygen as an electron acceptor first for the organic matter degradation. The process, therefore, is limited by the amount of available oxygen (Tesoriero & Puckett, 2011). Equation 2 is the reaction for denitrification. For this process, nitrate availability is the limiting component. Only when the conditions become anoxic, or nearly anoxic, nitrate is used as an electron acceptor; therefore, oxygen concentration is an inhibiting component of this reaction. Both aerobic mineralization and denitrification are considered to be first-order processes with respect to the DOM concentration. Nitrogen is fixed in both of these reactions and released in the form of ammonia. Through the process of nitrification (equation 3), this can be converted back into nitrate, although only under oxic conditions. This is mediated by nitrifying bacteria. Through the process of aeration, atmospheric oxygen dissolves into the aquifer water up to the

saturation concentration of oxygen, dependent on the salinity, temperature, and the partial pressure of oxygen in the atmosphere.

$$R_{aerobic\ mineralization} = r_{aerobic\ mineralization} \cdot \frac{[O_2]}{[O_2] + k_{O_2}} \cdot [DOM] \quad (4)$$

$$R_{denitrification} = r_{denitrification} \cdot \frac{[NO_3^-]}{[NO_3^-] + k_{NO_3^-}} \cdot \frac{k_{O_2}}{[O_2] + k_{O_2}} \cdot [DOM] \quad (5)$$

$$R_{nitrification} = r_{nitrification} \cdot [O_2] \cdot [NH_3] \quad (6)$$

$$R_{aeration} = r_{aeration} \cdot (O_{2,solubility} - [O_2]) \quad (7)$$

Equation 4 and 5 give the reaction rates (R) of aerobic mineralization and denitrification respectively [$mol\ DOM\ m^{-3}h^{-1}$]. Equation 6 gives the reaction rate of nitrification [$mol\ NH_3\ m^{-3}h^{-1}$]. Equation 7 gives the rate of aeration in the aquifer [$mol\ O_2\ m^{-3}h^{-1}$]. In these rate equations, r stand for the rate constants [h^{-1}] of the respective reactions. The k stands for the Michaelis-Menten rate limitation term of the respective reactant. The term $O_{2,solubility}$ is the solubility of oxygen in the aquifer water.

The model developed in this study takes into account five state variables; DOM, O_2 , NO_3^- , NH_3 and N_2 , given in $mol\ m^{-3}$ of their respective molecules. Other molecule concentrations involved in the reactions are not considered in this model implementation, therefore, C and H^+ . Albeit aerobic mineralization, denitrification and nitrification being mediated by microbes, any change of biomass due to these processes is deemed to be negligible compared to the concentrations in the aquifer water. This all leads to a conceptual model figure 1.

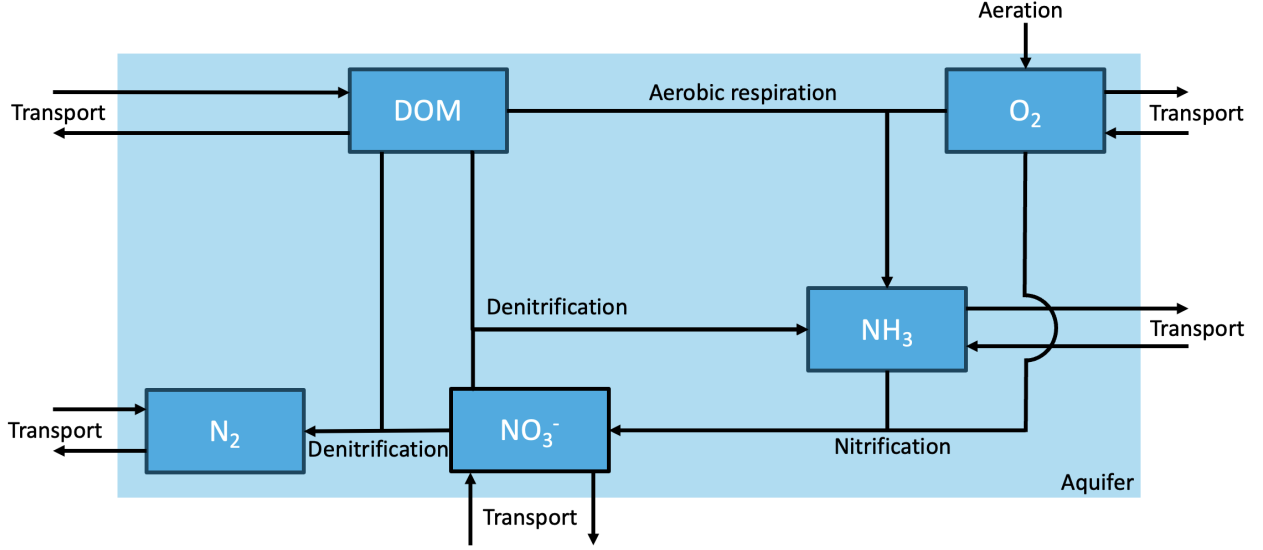


Figure 1: Conceptual diagram of the bank infiltration model.

For the transport processes, 1-dimensional flow from the river through the aquifer is assumed. Considering the time and spatial scales involved, diffusion processes can be ignored compared to advection and dispersion processes. The porosity is taken as constant over the length of the aquifer. The upper boundary condition (at the river-subsurface interface), is taken as the respective river concentrations of the state variables, so a constant concentration boundary condition. The lower boundary condition (at the end of the modeled aquifer length), is a zero concentration gradient.

$$\frac{\partial[DOM]}{\partial t} = Transport(DOM) - R_{aerobic\ mineralization} - R_{denitrification} \quad (8)$$

$$\frac{\partial[O_2]}{\partial t} = Transport(O_2) + R_{aeration} - R_{aerobic\ mineralization} - 2 \cdot R_{nitrification} \quad (9)$$

$$\frac{\partial[NO_3^-]}{\partial t} = Transport(NO_3^-) - \frac{4}{5} \cdot R_{denitrification} + R_{nitrification} \quad (10)$$

$$\frac{\partial[NH_3]}{\partial t} = Transport(NH_3) + \frac{16}{106} \cdot (R_{aerobic\ mineralization} + R_{denitrification}) - R_{nitrification} \quad (11)$$

$$\frac{\partial[N_2]}{\partial t} = Transport(N_2) + \frac{2}{5} \cdot R_{denitrification} \quad (12)$$

Equations 8, 9, 10, 11 and 12 give the mass balances of DOM, oxygen, nitrate, ammonia and molecular nitrogen. Each in $mol\ m^{-3}\ h^{-1}$ of the respective state variable. The mass balance equations are used to calculate the change in concentration of the state variables over the length of the aquifer.

Model implementation

The model is implemented in R (Team, 2021) as follows.

The model grid is setup using the ReacTran package (Soetaert & Meysman, 2012). The aquifer has a length of 500 m and is divided into 500 cells, each of one meter.

```
# units: time=hours, space=meters, amount=moles, concentration=mol/m3

# Spatial domain of aquifer
Length    <- 500    # Length of model grid (i.e. aquifer length [m])
N         <- 500    # number of grid cells

# grid with equally sized boxes
Grid      <- setup.grid.1D(L = Length, N = N)
```

The parameters not varying in space are defined. The solubility of oxygen in water is calculated using the marelac package (Soetaert, 2023).

```
temp      <- 10      # Temperature in degrees
salinity  <- 0        # Salinity
O2_sol    <- gas_solubility(S = salinity, t = temp, species = "O2") / 1000 * 0.21 # Oxygen solubility

f         <- 1/1000   # Factor to convert from µM to mol/m3

def.pars <- c(
  r_aeromin = 0.002, # [/h] Aerobic mineralization rate constant
  r_denitr  = 0.002, # [/h] Denitrification rate constant
  r_nitri   = 0.36,  # [/(mol/m3) /h] Nitrification rate constant
  r_aera    = 0.0003, # [/h] Aeration rate constant
  Length    = 500,   # [m] Modelled length of aquifer
  v_adv     = 10 / 100, # [m/h] Transport velocity
```

```

a          = 1.5,      # [m]                Dispersivity
kO2        = 20 * f,   # [mol/m3]           The affinity constant in the Michaelis-Menten rate limitati
kNO3       = 35 * f,   # [mol/m3]           The affinity constant in the Michaelis-Menten rate limitati
riverDOM    = 6/12e-3*f, # [mol/m3]        River dissolved organic matter
riverO2     = 210 * f,  # [mol/m3]        River oxygen concentration
riverNO3    = 100 * f,  # [mol/m3]        River Nitrate concentration
riverNH3    = 0 * f,    # [mol/m3]        River oxygen concentration
O2_sol     = O2_sol,   # [mol/m3]        Solubility of oxygen
por         = 0.4      # [-]            Porosity
)

```

State variables are defined, the initial conditions for each concentration in the aquifer is 0.

```

# Create a vector for each state variable of length N which contains the initial condition
DOM      <- rep(0, times = N)
Oxygen   <- rep(0, times = N)
Nitrate  <- rep(0, times = N)
Ammonia  <- rep(0, times = N)
Nitrogen <- rep(0, times = N)

# Save the state variables as one long vector and make a vector with their respective names
state.ini <- c(DOM, Oxygen, Nitrate, Ammonia, Nitrogen)
SVnames   <- c("DOM", "Oxygen", "Nitrate", "Ammonia", "Nitrogen")
nspec     <- length(SVnames)

```

A model is defined that calculates transport, reaction rate and concentration change for a time step.

```

AquModel <- function(t, state, parms)
{
  with(as.list(parms),{

    # Unpacking state variables
    DOM      <- state[ (0*N+1) : (1*N) ]    # Next N elements: DOM
    O2       <- state[ (1*N+1) : (2*N) ]    # Next N elements: O2
    NO3      <- state[ (2*N+1) : (3*N) ]    # Next N elements: NO3
    NH3      <- state[ (3*N+1) : (4*N) ]    # Next N elements: NH3
    N2       <- state[ (4*N+1) : (5*N) ]    # Last N elements: N2

    # === transport rates ===
    # Transport by dispersion and advection
    # Lower boundaries are zero gradient by default

    tran.DOM <- tran.1D(C = DOM, C.up = riverDOM, # upper boundary: fixed concentration
                        dx = Grid, VF = por,       # grid and volume fraction (por)
                        D = a * v_adv, v = v_adv)  # dispersion (dispersivity * flow velocity) and advection

    tran.O2 <- tran.1D(C = O2, C.up = riverO2,
                       dx = Grid, VF = por,
                       D = a * v_adv, v = v_adv)

    tran.NO3 <- tran.1D(C = NO3, C.up = riverNO3,
                        dx = Grid, VF = por,
                        D = a * v_adv, v = v_adv)
  })
}

```

```

tran.NH3 <- tran.1D(C = NH3, C.up = riverNH3,
  dx = Grid, VF = por,
  D = a * v_adv, v = v_adv)

tran.N2 <- tran.1D(C = N2, C.up = 0,
  dx = Grid, VF = por,
  D = a * v_adv, v = v_adv)

# === reaction rates ===

# DOM mineralisation, first order relation with DOM concentration, limited by oxygen concentration
aeroMin <- r_aeromin * (O2 / (O2 + kO2)) * DOM

# Denitrification, first order relation with DOM concentration, limited by nitrate concentration, i
denitri <- r_denitr * (NO3 / (NO3 + kNO3)) * (kO2 / (O2 + kO2)) * DOM

# Nitrification, first order relation with oxygen and ammonia
nitri <- r_nitri * O2 * NH3

# Aeration rate, calculated as the difference between the maximum solubility of oxygen and oxygen c
aeration <- r_aera * (O2_sol - O2)

# === mass balances : dC/dt = transport + reactions ===

dDOM.dt <- ( tran.DOM$dC - # transport
  aeroMin - denitri) # reactions, [mol DOM /m3]

dO2.dt <- ( tran.O2$dC + aeration # transport
  - aeroMin - 2 * nitri) # reactions, [mol O2 /m3]

dNO3.dt <- ( tran.NO3$dC - # transport
  4/5 * denitri + nitri) # reactions, [mol NO3 /m3]

dNH3.dt <- ( tran.NH3$dC + # transport
  (aeroMin + denitri) * 16/106 - nitri) # reactions, [mol NH3 /m3]

dN2.dt <- ( tran.N2$dC + # transport
  + 2/5 * denitri) # reactions, [mol N2 /m3]

# Reaction rates integrated over aquifer length
TotalAeroDeg = sum(aeroMin * Grid$dx * por) # [mol DOM /m2 /h]
TotalDenitri = sum(denitri * Grid$dx * por) # [mol DOM /m2 /h]
TotalNitri = sum(nitri * Grid$dx * por) # [mol NH3 /m2 /h]
TotalAeration = sum(aeration * Grid$dx * por) # [mol O2 /m2 /h]

return(list(c(dDOM.dt, dO2.dt, dNO3.dt, dNH3.dt, dN2.dt), # The time-derivatives, as a long vector

  # Reaction rates
  Aerobic_mineralisation = aeroMin, # Aerobic mineralisation rate [mol DOM /m3 /h]
  Denitrification = denitri, # Denitrification rate [mol DOM /m3 /h]
  Nitrification = nitri, # Nitrification rate [mol NH3 /m3 /h]
  Aeration = aeration, # Aeration rate [mol O2 / m3 / h]

```

```

# Aquifer integrated reaction rates for budget
TotalAeroDeg      = TotalAeroDeg,          # [mol DOM /m2 /h]
TotalDenitri      = TotalDenitri,          # [mol DOM /m2 /h]
TotalNitri        = TotalNitri,            # [mol NH3 /m2 /h]
TotalAeration     = TotalAeration,         # [mol O2 /m2 /h]

# Transport fluxes at system boundaries for budget
DOM.up.Flux       = tran.DOM$flux.up,      # [mol DOM /m2 /h]
DOM.down.Flux     = tran.DOM$flux.down,    # [mol DOM /m2 /h]
O2.up.Flux        = tran.O2$flux.up,      # [mol O2 /m2 /h]
O2.down.Flux      = tran.O2$flux.down,    # [mol O2 /m2 /h]
NO3.up.Flux       = tran.NO3$flux.up,     # [mol NO3 /m2 /h]
NO3.down.Flux     = tran.NO3$flux.down,   # [mol NO3 /m2 /h]
NH3.up.Flux       = tran.NH3$flux.up,     # [mol NH3 /m2 /h]
NH3.down.Flux     = tran.NH3$flux.down,   # [mol NH3 /m2 /h]
N2.up.Flux        = tran.N2$flux.up,      # [mol N2 /m2 /h]
N2.down.Flux      = tran.N2$flux.down))   # [mol N2 /m2 /h]
})
}

```

To find the steady state solution, the function `steady.1D` from the `rootSolve` package is used Soetaert (2009).

```

def.std <- steady.1D (y = state.ini, func = AquModel, parms = def.parms,
                     nspec = nspec, dims = N, names = SVnames,
                     positive = TRUE, atol = 1e-10, rtol = 1e-10)

```

The system budget is evaluated by getting fluxes from the steady state solution

```

# Select which output form the steady state solution to include in the budget
toselect <- c("TotalAeroDeg", "TotalDenitri", "TotalNitri", "TotalAeration", "DOM.up.Flux", "DOM.down.Flux")
BUDGET   <- def.std[toselect]
unlist(BUDGET) # display BUDGET as a vector with named elements rather than a list

```

For parameter calibration, load in the field data, to be plotted against the default parameters. The R package `shiny` was used for this purpose (Chang et al., 2024). The `shiny` package allows the user to generate an environment where the parameters can be changed interactively by the use of sliders. By visual examination, the parameters were changed to correspond with the field data. For the code used in the shiny application, see the appendix.

```

# Load in the data file with field data, to be used to calibrate the parameters. Set working directory
aquifer_fielddata <- read.csv("./aquifer_fielddata.txt")

```

For the sensitivity analysis, code was written that gets the value of the NH_3 concentration at a distance of 200m from the river, for different parameter values. These graphs give information about the effect of fluctuations on the water quality in the aquifer.

```

# make a function with as input a parameter value and the name of that parameter
sens <- function(parameter, par_name){
  # save the parameters in a new vector
  pars.sens <- def.pars
  # change the value of the parameter

```

```

pars.sens[par_name] <- parameter

# calculate the steady state solution with the changed parameter
sens <- steady.1D (y=state.ini, func=AquiModel, parms=pars.sens,
                  nspec=nspec, dimens=N, names=SVnames,
                  positive = TRUE, atol = 1e-10, rtol = 1e-10)
# return the concentration distribution of the ammonia state variable
return((sens$y[, "Ammonia"]))
}

# make a vector with the range in which to vary the parameter
DOM_vect <- seq(from = 0, to = 0.7, length.out = 50)
# initialize the output array
NH3_DOM_vect <- NULL

# loop over every parameter value
for (riverDOM in DOM_vect){
  # run the sens function with the parameter value as input, which gives the concentration of ammonia o
  model_output <- sens(riverDOM, "riverDOM")
  # determine the value at 200m by taking the average between 199.5m and 200.5m
  conc_200 <- (model_output[200] + model_output[201]) / 2
  #store this value in the output array
  NH3_DOM_vect <- c(NH3_DOM_vect, conc_200)
}

# repeat this process for three other parameter values to chance
NO3_vect <- seq(from = 0, to = 0.3, length.out = 50)
NH3_NO3_vect <- NULL

for (riverNO3 in NO3_vect){
  model_output <- sens(riverNO3, "riverNO3")
  conc_200 <- (model_output[200] + model_output[201]) / 2

  NH3_NO3_vect <- c(NH3_NO3_vect, conc_200)
}

NH3_vect <- seq(from = 0, to = 0.1, length.out = 50)
NH3_NH3_vect <- NULL

for (riverNH3 in NH3_vect){
  model_output <- sens(riverNH3, "riverNH3")
  conc_200 <- (model_output[200] + model_output[201]) / 2

  NH3_NH3_vect <- c(NH3_NH3_vect, conc_200)
}

aera_vect <- seq(from = 0, to = 0.0006, length.out = 50)
NH3_aera_vect <- NULL

for (r_aera in aera_vect){
  model_output <- sens(r_aera, "r_aera")
  conc_200 <- (model_output[200] + model_output[201]) / 2

```



```
NH3_aera_vect <- c(NH3_aera_vect, conc_200)
}
```

For the method section as an .Rmd file (and all the other sections of the report), see *GitHub*, where it is publicly accessible.

Results

Zonation and shape

The steady state condition of the system shows the spatial distribution of concentrations and process rates after the system has set into equilibrium (figure ??). This gives insight into the different processes occurring along the length of the aquifer and how they interact.

Aerobic mineralization rate is high in the beginning of the aquifer, however, over a distance of 50m, it quickly drops off. This is due to the process consuming oxygen, thereby limiting its own reaction rate. Moving further from the river, after its initial convex decrease, it flats out and very slowly decreases over the remaining length of the aquifer, as the organic matter is almost depleted.

The denitrification rate rises from the river to 50m into the aquifer, where it peaks and subsequently decreases in a convex manner. As denitrification is oxygen inhibited, the initially high oxygen concentration slows the process until most of the oxygen is exhausted by aerobic mineralization. The rate of denitrification peters off due to the nitrate and organic matter depleting.

The nitrification rate is dependent on the oxygen and ammonia concentrations present in the aquifer. An increase in the beginning of the aquifer is followed by a sharp drop off due to the decrease in oxygen concentration. This is then followed by a slight comeback due to the increasing ammonia concentrations caused by aerobic mineralisation and denitrification. Afterwards, the nitrification rate settles and nears zero as the ammonia is depleted.

The aeration rate is dependent on the difference between oxygen concentration and oxygen saturation level. As oxygen is depleted by aerobic mineralisation, the aeration rate increases to a maximum while the oxygen concentration remains near zero. Once the oxygen consuming processes slow down due to low concentrations of organic matter and ammonia, the aeration rate decreases for the rest of the aquifer. As oxygen concentration is inversely related to the aeration rate, the shape of the aeration rate in the aquifer is the shape of the oxygen concentration flipped.

The DON is introduced into the aquifer through the river, giving an initially high concentration before dropping off as it continues through the aquifer. This is due to it being consumed via denitrification. This gives the depth profile its convex shape.

The Oxygen profile demonstrates a convex shape with the oxygen concentration dropping as a result of the oxygen being required for the nitrification and aerobic mineralisation processes. As these processes end the concentration of oxygen is able to recover to its normal level.

The nitrate profile initially shows a concave profile before becoming a convex profile. This is due to the already existing concentration of nitrate in the system being added to from the river, however this drops off due to the denitrification process taking place in the system.

The ammonia concentration rises from a concentration value of zero from the processes of aerobic mineralisation and denitrification. This abundance of ammonia is the used in the nitrification process forming nitrate, giving the curve its concave shape.

The Nitrogen concentration profile forms a concave curve due to its continual increase due to the denitrification coming from the dissolved organic nitrogen pool and the nitrate pool. This increase continues until both pools are exhausted.

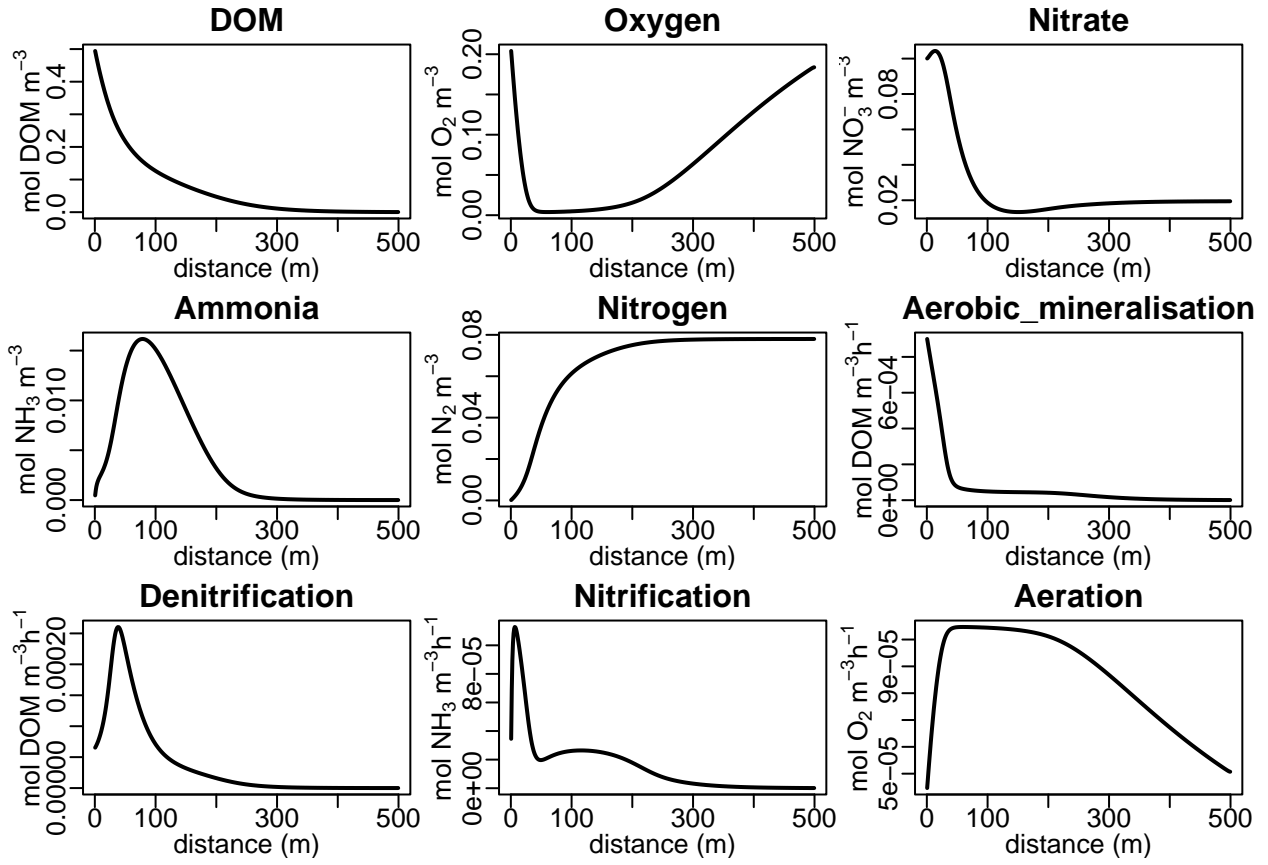


Figure 2: Concentration and rate profiles over the aquifer length.

Budgets

A budget of the system is set up to evaluate the fate of the state variables in the system ???. These fluxes can be further visualized in the conceptual diagram of the system ???

Table 1: Budget for the bank infiltration model. Unit of fluxes are in $\text{mol m}^{-3} \text{h}^{-1}$ of their respective state variable.

	flux
TotalAeroDeg	0.0128
TotalDenitri	0.0079
TotalNitri	0.0031
TotalAeration	0.0172
DOM.up.Flux	0.0207
DOM.down.Flux	0.0000
O ₂ .up.Flux	0.0091
O ₂ .down.Flux	0.0074
NO ₃ .up.Flux	0.0040
NH ₃ .up.Flux	-0.0001
NH ₃ .down.Flux	0.0000
N ₂ .up.Flux	0.0000
N ₂ .down.Flux	0.0031

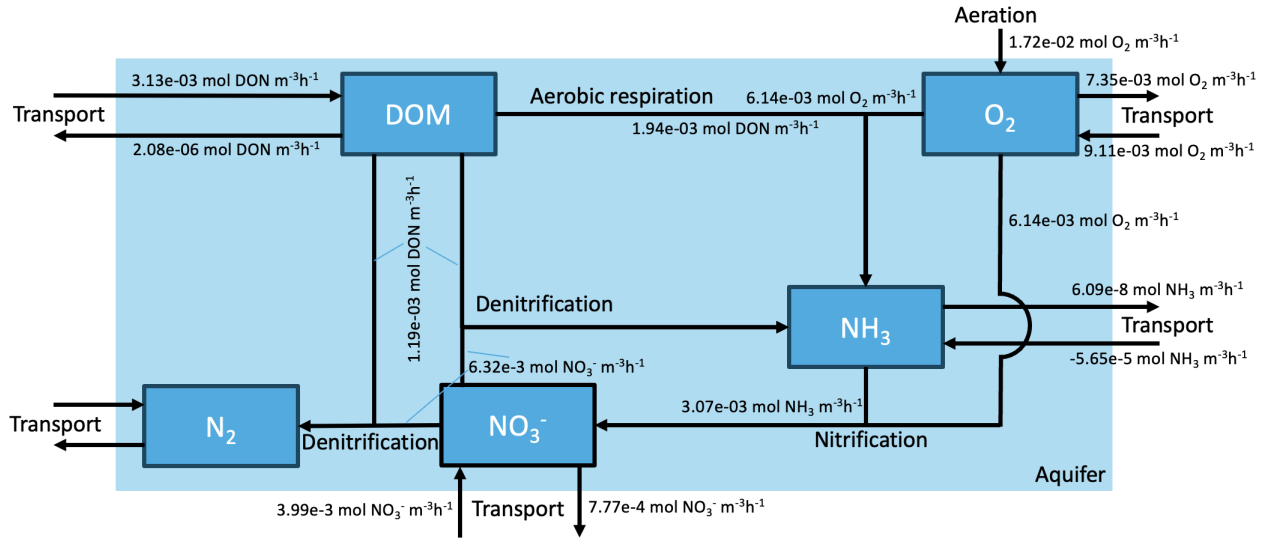


Figure 3: Conceptual diagram of the bank infiltration model with process fluxes

The amount of oxygen coming in from the river and the oxygen supplied by aeration give the total amount of oxygen supplied to the system. Aerobic mineralization and nitrification both consume oxygen, the latter of which at two molecules per reaction. Therefore, the amount of oxygen used for aerobic matter mineralization is 49% of the total oxygen supplied, 28% is used for nitrification and the rest is transported out of the aquifer.

The amount of organic material making its way into the aquifer is $0.021 \text{ mol m}^{-3} \text{h}^{-1}$, using the Redfield ratio, this is $3.13\text{e-}03 \text{ mol DON m}^{-3} \text{h}^{-1}$. Of this, 62% is consumed by means of aerobic mineralization, and 38% by denitrification.

Nitrate enters the system by supply from the river and by the process of nitrification. About $3.99\text{e-}3 \text{ mol}$

$\text{NO}_3^- \text{ m}^{-3} \text{ h}^{-1}$ is supplied by the river, while $3.07\text{e-}3 \text{ mol NO}_3^- \text{ m}^{-3} \text{ h}^{-1}$ is formed in the aquifer by nitrification. 89% of this is transformed back into ammonia by denitrification, the remaining 11% is transported away.

Nitrogen!!!!

Fitting to field data

The model output with the default parameters differs substantially from field data (??). The field data show slightly lower DON levels across the aquifer and the oxygen concentration in the further reaches of the aquifer increases slower. Lastly, the ammonia concentration peaks further into the aquifer in the field and is more spread out than with the default model parameters.

The aeration and nitrification rate constant and the river DON concentration were adapted to fit the model with the default parameters to the field data [table reference]. Reducing the river DON concentration decreases the river boundary concentration of DON and consequently, the concentration across the first half of the aquifer. This increases oxygen concentration across the whole aquifer, since less oxygen is consumed by aerobic mineralisation. Furthermore, less ammonia is produced by aerobic mineralisation and denitrification, reducing its concentration. By reducing the aeration rate constant, less oxygen is replenished over the aquifer length. In turn, this causes less ammonia to be converted to nitrate by nitrification, increasing the ammonia concentration. Lastly, decreasing the nitrification rate constant further increases the ammonia concentration in the aquifer. These changes in parameter fitted the field data the best (table ??).

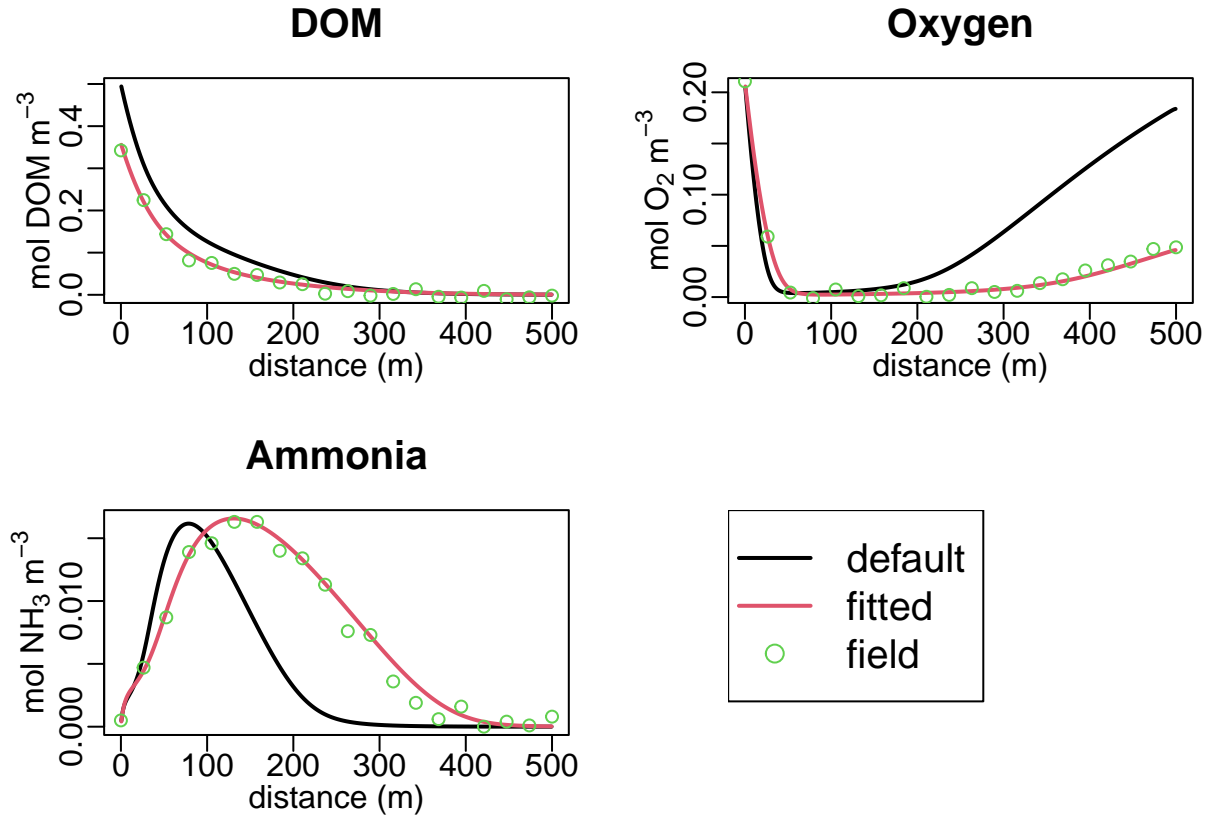


Figure 4: Concentrations for three state variables , showing the steady state conditions for both default parameters and fitted parameters.

Table 2: Default and fitted parameter values for the bank infiltration model.

parameter	default	fitted
riverDOM [mol DOM m ⁻³]	0.5000	0.36000
aeration rate [h ⁻¹]	0.0003	0.00009
nitrification rate [/(mol/m ³) h ⁻¹]	0.3600	0.19000

Safety concentrations

While the nitrate concentration in the aquifer stays well below the safety concentration, elevated concentrations of organic matter and ammonia make the water unsafe for human consumption in the first 200m of the aquifer [figure ??]. The first 50m of the aquifer have too high of organic matter concentrations, due to the river concentration. Aerobic mineralisation and denitrification break down the organic matter, but produce ammonia, which is subsequently elevated to concentrations above the safety criteria for drinking water. Only once enough ammonia has been converted to nitrate by nitrification becomes the water safe enough to drink. Therefore, any well used to extract drinking water from this aquifer should be located at least 200 m from the river.

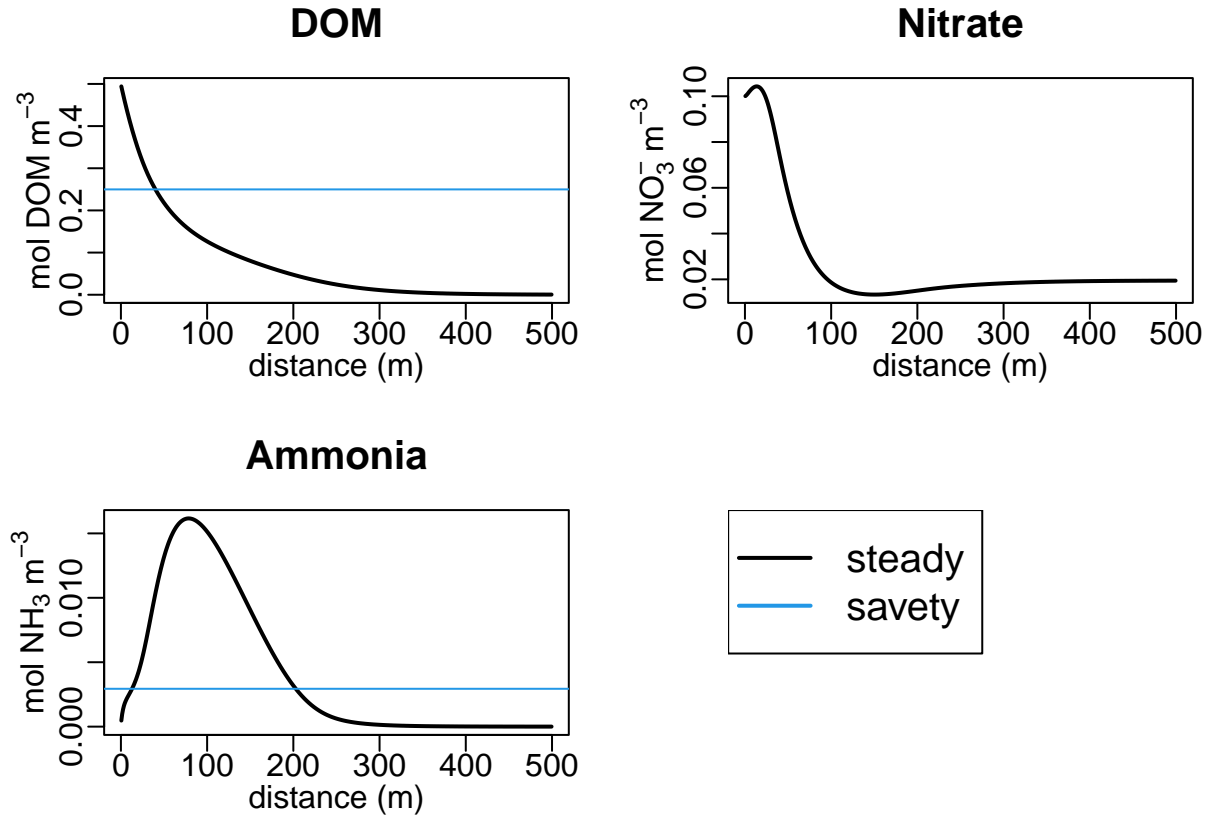


Figure 5: Concentration profiles of three state variables and their respective drinking water safety concentrations. The safety concentration for nitrate (0.4 mol NO₃⁻ m⁻³) falls off the graph.

Sensitivity analysis

When no denitrification is present in the water the dissolved organic Nitrogen increases. Oxygen concentration in the water becomes less, Nitrate concentration increases, Ammonia decreases in the short path of the water but over a longer path the concentration is higher than the default concentration. Nitrogen stays zero, aerobic mineralization increases, the nitrification increases but over time decreases.

With the aerobic mineralization being 0, then there will be an increase in Dissolved organic nitrogen and oxygen. The nitrate will decrease with a uniform pattern. Nitrogen concentration will be less than the default concentration for nitrogen. Denitrification and nitrification will decrease in productivity and decline towards 0.

The nitrification rate can have a value of 0, if that's the case then the oxygen and ammonia concentration will become higher relative to the default concentration where the nitrification rate is 0.36. DON, nitrate and nitrogen become less than the default concentrations. Aerobic mineralization increases relative to the default rate of when the nitrification rate is 0. Nitrification becomes 0 and denitrification in the first 120 meters is still above 0 and after stays 0 along the distance from the aquifer.

For the Aeration rate with a value of 0 the concentrations increase for DON and Ammonia, for the oxygen, nitrate and nitrogen the concentrations become 0. The reactions for aerobic mineralization and nitrification decline towards a value of 0, for denitrification the first 70 meters the process occurs more often than the default rate of the denitrification.

For DOM concentrations in rivers with values below 0.5 [mol/m³] the water is suitable for human consumption. When the values go above 0.5 [mol/m³] the river will have too much Ammonia in the water, thus the water will not be suitable for human consumption. Range DOM \leq 0.5 [mol/m³] When changing the NO₃ concentration in the river, it shows that for values above 0.1 [mol/m³] the water will stay suitable for human consumption. Range concentrations NO₃ \geq 0.1 [mol/m³] For NH₃ concentrations in the river, every amount added to the water concentration will make the water unsuitable for human consumption, because the ammonia concentration will be too high.

The rate constant of aeration (r Aeration) should stay at 0.003 [/h] or above, if it reaches values below 0.003 [/h] the Ammonia concentration will exceed the limit and the water will become unsuitable for drinking water.

These value ranges were all taken when the other values remained the same values as before. However the NH₃ concentrations can become higher than 0 when the DOM concentration has a value of 0, for NO₃ concentrations they can range to values beyond 0.1 [mol/m³]. The Ammonia concentration remains constant in these cases and stays at 0.0 [mol/m³] (figure ??).

[1] "DOM"

Discussion

The results shown above show the concentrations produced as a result of the processes occurring in the aquifer as the water travels down through the soil. While these processes may come across as being separate entities, they are in fact interlinked with one another. The model produced makes use of the dependences of these rates and the corresponding concentrations produced as a result. The coupling of the processes allows for an added level of complexity as well as a greater understanding of the processes themselves. It demonstrates how each of the processes are dependent upon the others as they will have an impact on the concentrations of the pollutants as well as the distribution of the concentrations and processes in the aquifer.

The well is located at a distance of 200 meters from the riverbank. This distance is shown to be a good position for the pumping well as the water quality is safe and when the well is situated closer to the river the water quality is not high enough for safe human consumption. This is due to the fact that as the distance is

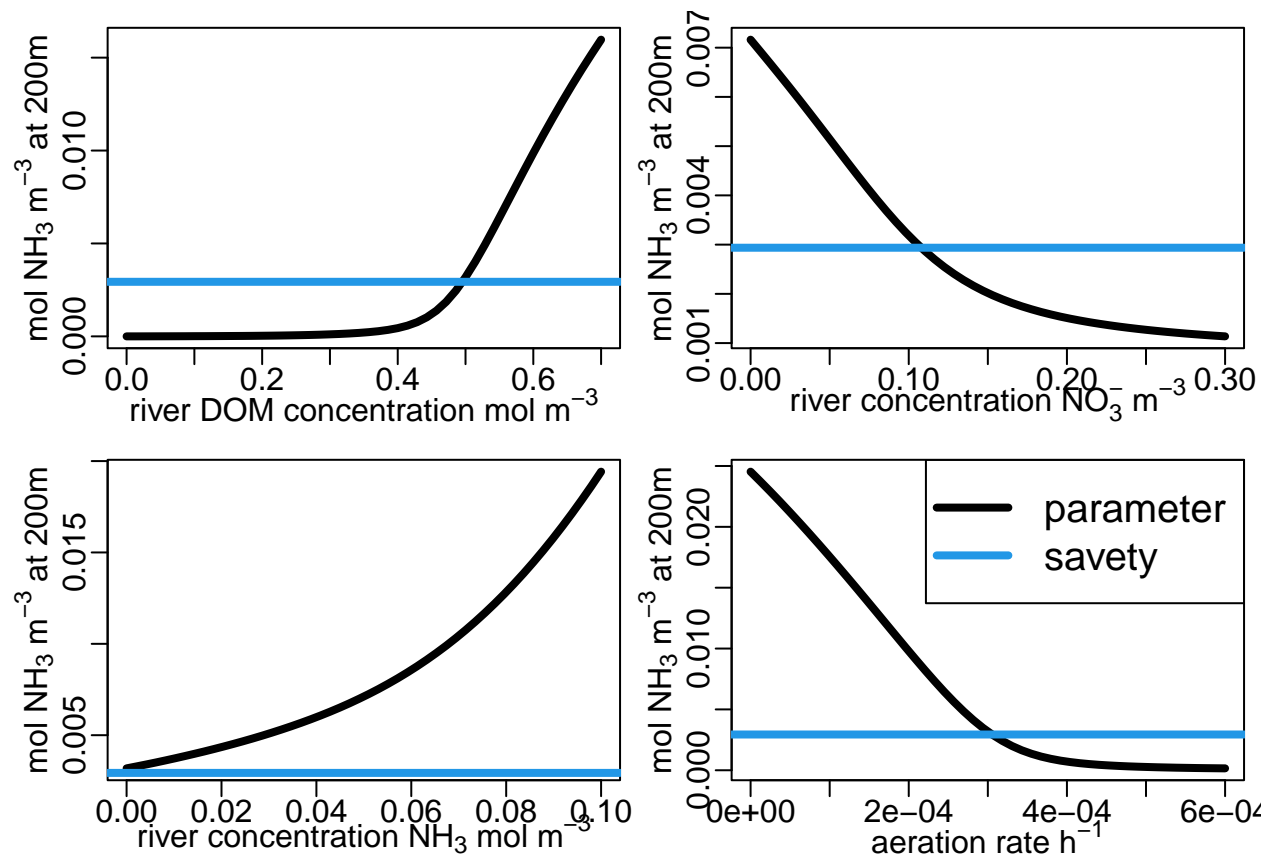


Figure 6: Sensitivity analysis of four parameters for the NH_3 concentration in the aquifer.

less than what is required to remove enough of the Ammonia from the water. The Ammonia concentration is the main cause of concern regarding water quality, as the concentrations remain high between 20 and 200 meters. Following this the concentration of Dissolved Organic Nitrogen is particularly high until it reaches a distance of 40 meters from the edge of the river. The Nitrate and Oxygen concentrations do not go over the threshold of a dangerous concentration. The aerobic mineralisation of the dissolved Organic Nitrogen is what contributes to the increase in the Ammonia concentration. Due to this high concentration, it takes the process of nitrification much longer, which therefore requires a much longer distance, to reduce the ammonia into a reduced form, in this case, nitrate. The increased distance required for the ammonia concentration to drop to a safe concentration will cause the location of the well to be further away from the aquifer in order to produce water with a good quality.

In order for the Dissolved organic Nitrogen to be broken down into a consumable element for the bacteria the dissolved organic nitrogen needs to go through the process of aerobic mineralisation. During this process the dissolved organic nitrogen will be broken down into ammonia. While the amount of ammonia produced in this step is of concern given how far it forces the extraction well to move from the edge of the river there are also benefits. Were the aerobic mineralisation rate to be increased there would be an increase in the amount of ammonia produced, it would however reduce the concentration of the dissolved organic nitrogen much quicker. However, this would in turn cause a greater strain upon the nitrification process as the ammonia would need a much farther distance to travel before it could be considered safe to drink.

As ammonia is shown to have the highest concentration of all the pollutants moving through the aquifer it is of more concern than the others. The easiest way to help remove as much of the ammonia in as short a space of time is to increase the nitrification rate. However, this comes with its own number of setbacks. Nitrification is an aerobic process within the nitrogen cycle and in order to increase the rate of nitrification there would be an increased demand on the amount of oxygen present in the ground. This creates the problem of a reduction in oxygen concentration in the soil. Should the oxygen concentration in the soil be increased however this would require a continued addition of oxygen as it is consumed through the process of nitrification. Steps such as these while they would reduce the concentration of ammonia and the distance the well is required to be located out may prove to be too costly.

The levels of nitrate present in the aquifer are not of major concern as even at their highest level they exist below what is considered a safe threshold. It is however important to ensure that these levels do not rise and as much of the nitrate from the pollutants is removed. The process removing the nitrate is denitrification, which is the anaerobic process involved in the nitrogen cycle. At this point oxygen is no longer available and this final step involved the nitrate reducing further to Nitrogen gas. As the increase in denitrification would require the concentration of nitrate to be higher it would also need the oxygen concentration to be reduced faster. This would have a negative effect upon the breakdown of ammonia to nitrate increasing the distance required to ensure that the water is at a safe quality.

Conclusion

This study showed a simplified model for bank infiltration from a river. It is shown that bank infiltration can substantially improve the water quality, given sufficient length of aquifer for the process to take place. The coupling between processes has been discussed. Increase in nitrification or aeration rates cause the aquifer water to remove ammonia faster and thus increase the water quality overall. The processes are a relatively effective and cheap way for cleaning up of river water and making it safe for human consumption.

Contributions

Conceptual model: Jorrit Bakker

Initial model setup: Jorrit Bakker and Denis Power

Further model coding and result generation: Jorrit Bakker

Report:

- Introduction: Denis Power
- Methods: Jorrit Bakker
- Results: Denis Power, Jorrit Bakker and Willem Poelman
- Discussion: Willem Poelman, Denis Power
- Conclusion: Willem Poelman and Jorrit Bakker
- RMarkdown: Jorrit Bakker

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Appendix

Shiny application

The code used to perform the fitting of the parameters, using the R shiny package.

```
## Loading required package: shiny
```

```

# Define UI (user interface)
UI.Aquifer <- shinyUI(pageWithSidebar(

  # Application title
  headerPanel("OM degradation in aquifer model"),

  # Make a panel in the sidebar which contains sliders for the various parameters
  sidebarPanel(
    sliderInput(inputId="r_aeromin",
      label = "r_aeromin: rate constant of aerobic mineralization [/h]",
      min = 0, max = 0.02, step = 0.0002, value = def.pars["r_aeromin"]),
    sliderInput(inputId="r_denitr",
      label = "r_denitr: rate constant of denitrification [/h]",
      min = 0, max = 0.02, step = 0.0002, value = def.pars["r_denitr"]),
    sliderInput(inputId="r_nitri",
      label = "r_nitri: rate constant of nitrification [/(mol/m3)/h]",
      min = 0, max = 1, step = 0.01, value = def.pars["r_nitri"]),
    sliderInput(inputId="r_aera",
      label = "r_aera: rate constant of aeration [/h]",
      min = 0, max = 0.003, step = 0.00003, value = def.pars["r_aera"]),
    sliderInput(inputId="kO2",
      label = "kO2: Affinity constant in Michaelis-Mentan rate limitation/inhibition term for O2 [mol/m3]",
      min = 0, max = 100/1000, step = 1/1000, value = def.pars["kO2"]),
    sliderInput(inputId="kNO3",
      label = "kNO3: Affinity constant in Michaelis-Mentan rate limitation term for NO3 [mol/m3]",
      min = 0, max = 100/1000, step = 1/1000, value = def.pars["kNO3"]),
    sliderInput(inputId="riverDOM",
      label = "riverDOM: Dissolved organic matter concentration in river [mol/m3]",
      min = 0, max = 1000/1000, step = 10/1000, value = def.pars["riverDOM"]),
    sliderInput(inputId="riverO2",
      label = "riverO2: O2 concentration in river [mol/m3]",
      min = 0, max = 1000/1000, step = 10/1000, value = def.pars["riverO2"]),
    sliderInput(inputId="riverNO3",
      label = "riverNO3: NO3 concentration river [mol/m3]",
      min = 0, max = 500/1000, step = 5/1000, value = def.pars["riverNO3"]),
    sliderInput(inputId="riverNH3",
      label = "riverNH3: NH3 concentration river [mol/m3]",
      min = 0, max = 100/1000, step = 1/1000, value = def.pars["riverNH3"]),

    # Make an action button, which triggers an effect once pressed (defined in server)
    actionButton (inputId="resetButton",
      label="Reset Parameters"),

    # Make an check box, which toggles an effect on or off
    checkboxInput(inputId="defaultRun",
      label=strong("Add default run"), value = TRUE),

    checkboxInput(inputId="fieldData",
      label=strong("Add calibration field data"), value = TRUE),

    checkboxInput(inputId="safetyLimit",
      label=strong("Add water concentration safety limit"), value = TRUE),
  )
)

```

```

checkboxInput(inputId="wellLocation",
           label=strong("Add well location at 200m"), value = TRUE),

br()    # HTML break
),

# Define contents of the main panel
mainPanel(
  plotOutput("PlotAquifer", height = "700")
))

# Define server (back-end)
Server.Aquifer <- shinyServer(function(input, output, session) {

  # Define the action of clicking on clicking the action button
  observeEvent(input$resetButton, {

    # Convert the default parameters to a list
    def.pars.list <- as.list(def.pars)

    # Change the current parameter values to the default ones
    updateNumericInput(session, "r_aeromin", value = def.pars.list$r_aeromin)
    updateNumericInput(session, "r_denitr", value = def.pars.list$r_denitr)
    updateNumericInput(session, "r_nitri", value = def.pars.list$r_nitri)
    updateNumericInput(session, "r_aera", value = def.pars.list$r_aera)
    updateNumericInput(session, "kO2", value = def.pars.list$kO2)
    updateNumericInput(session, "kNO3", value = def.pars.list$kNO3)
    updateNumericInput(session, "riverDOM", value = def.pars.list$riverDOM)
    updateNumericInput(session, "riverO2", value = def.pars.list$riverO2)
    updateNumericInput(session, "riverNO3", value = def.pars.list$riverNO3)
    updateNumericInput(session, "riverNH3", value = def.pars.list$riverNH3)
  })

  # Get the model parameters set by the sliders as defined in the UI
  getpars <- reactive( {

    # Get the default parameters as a list
    pars <- as.list(def.pars)

    # Set the adaptable model parameters to the ones given by the sliders
    pars$r_aeromin <- input$r_aeromin
    pars$r_denitr <- input$r_denitr
    pars$r_nitri <- input$r_nitri
    pars$r_aera <- input$r_aera
    pars$kO2 <- input$kO2
    pars$kNO3 <- input$kNO3
    pars$riverDOM <- input$riverDOM
    pars$riverO2 <- input$riverO2
    pars$riverNO3 <- input$riverNO3
    pars$riverNH3 <- input$riverNH3

    # Return pars and convert to a vector
    return(unlist(pars))
  })

```

```

})

# Get and plot the output, which is visible in the main panel
output$PlotAquifer <- renderPlot({

  # Get the adapted model parameters, as defined above
  pars <- getpars()

  # Calculate the steady state solution with these new parameters
  out <- steady.1D(y = state.ini, parms = pars, func = AquModel,
                  names = SVnames, nspec = nspec, dims = N,
                  positive = TRUE, atol = 1e-10, rtol = 1e-10)

  # Make vectors for the variables to be plotted, the y-axis names and the safety concentrations of s
  plt_variables <- c("DOM", "Oxygen", "Nitrate", "Ammonia", "Nitrogen", "Aerobic_mineralisation", "Denitr
  plt_title <- c("DOM", "Oxygen", "Nitrate", "Ammonia", "Nitrogen", "Aerobic_mineralisation", "Denitr
  plt_ylabel <- c(expression(paste("mol DOM m"-3")), expression(paste("mol O"2", " m"-3")), exp

  plt_savelimit <- c(2.498e-1, 0, 4.032e-1, 2.937e-3, 0, 0, 0, 0)

  # Make the plots as a 3x3 matrix
  par(mfrow = c(3, 3),
      mgp=c(2,0.5,0))

  # Loop over each variable to be plotted
  for (i in 1:length(plt_variables)) {
    # If the defaultRun checkbox is toggled, plot both the default values and dynamix output
    if (input$defaultRun) {
      plot(def.std, out, grid=Grid$x.mid, lty=1, lwd=2, col = 1:2,
          which = plt_variables[i], mfrow=NULL,
          main = plt_title[i],
          ylab = plt_ylabel[i],
          xlab = "distance (m)",
          cex.main = 2, cex.axis = 1.5, cex.lab = 1.5)
      # Otherwise, only plot the dynamix output
    } else {
      plot(out, grid=Grid$x.mid, lty=1, lwd=2, col = 2,
          which = plt_variables[i], mfrow=NULL,
          main = plt_title[i],
          ylab = plt_ylabel[i],
          xlab = "distance (m)",
          cex.main = 2, cex.axis = 1.5, cex.lab = 1.5)
    }

    # For specific variables, plot the field data if the check box fieldData is toggled
    if (plt_variables[i] == "DOM" & input$fieldData) {
      points(aquifer_fielddata$distance_m, aquifer_fielddata[[plt_variables[i]]] / (16/106), col = :
    }

    if (plt_variables[i] %in% c("Oxygen", "Ammonia") & input$fieldData) {
      points(aquifer_fielddata$distance_m, aquifer_fielddata[[plt_variables[i]]], col = 3)
    }
  }

```

```

# For specific variables, plot the water savety concentration if the check box savetyLimit is tog
if (plt_variables[i] %in% c("DOM", "Nitrate", "Ammonia") & input$savetyLimit) {
  abline(h = plt_savelimit[i], col = 4)
}

if (plt_variables[i] %in% c("DOM", "Nitrate", "Ammonia") & input$wellLocation) {
  abline(v = 200, col = 6)
}
}

# Plot the legend in the remaining panel of the matrix
plot.new()

legend("topright", legend = c("default", "output", "field", "savety", "well"),
      lty = c(1, 1, -1, 1, 1), lwd = c(2, 2, 1, 2, 2), pch = c(-1, -1, 1, -1, -1), col = c(1,2,3,4
      cex = 2)

}) # end output$plot

}) # end of the definition of shinyServer

```

To run the shiny application, run the following chunk

```
shinyApp(ui = UI.Aquifer, server = Server.Aquifer)
```