

Supplementary material on Liedl et al. (2011) model

Paper Title: Direct computation of critical plume quantities required for initial assessment of contaminated sites

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1 The conceptual model setup

The Liedl et al. (2011) model considers a 3D domain, which is infinite along the x and y directions and finite up to the aquifer depth (M [L]) along the z direction. The aquifer is homogeneous and isotropic with the uniform groundwater flow entering the domain from the left (Fig. 1). The origin $(0,0,0)$ of the domain is at the top of the aquifer.

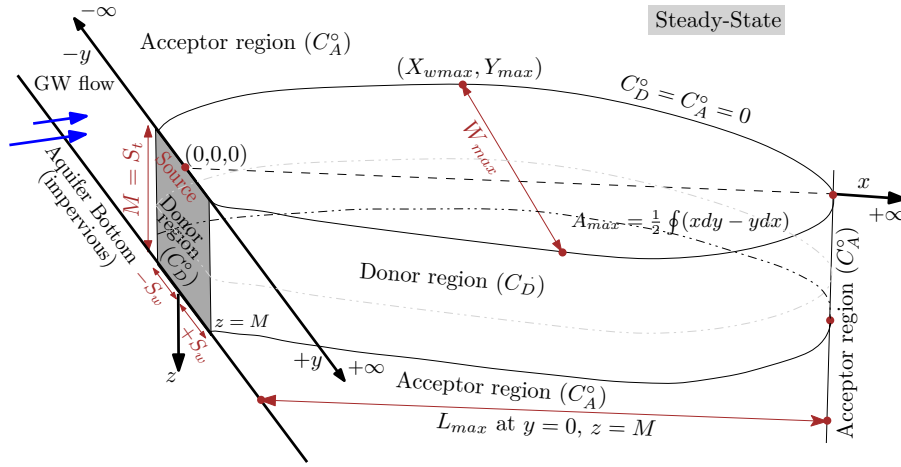


Figure 1: The Liedl et al. (2011) conceptual setup.

The continuous contaminant source called Electron Donor (or ED) with concentration C_D^0 [ML⁻³] appears as a rectangular patch extending from the origin to $\pm S_w$ [L] (called source width) along $\pm y$ directions and penetrating the entire thickness of the aquifer, i.e., $M = S_t$, where S_t [L] is referred as source thickness. The model considers bi-molecular reaction between ED and the partner reactant, called Electron Acceptor (or EA), C_A^0 [ML⁻³]. An instantaneous type reaction r [ML⁻³T⁻¹] between the reactants is considered in the model. Such extremely fast reactions are possible, for e.g., between strong acid and strong base or respiratory reactions, e.g. between fuel (e.g., CH₄) and oxygen (O₂). Wiedemeier et al. (1999) provide a detailed description on instantaneous reactions including that between fuel and oxygen. The assumption of instantaneous reaction leads to the two distinct reactant regions in the domain: the Donor region and the Acceptor region (Fig. 1). This further leads to both reactants only meeting at the edge of the plume, where they react and neutralize each other (i.e., at plume fringe $C_D^0 = C_A^0 = 0$). For the steady-state system, which is considered in Liedl et al. (2011), and since the contaminant source is continuous and penetrating the entire thickness of the aquifer, the maximum longitudinal (called L_{max}) and transverse (called W_{max}) travel of the contaminant/donor will appear at the bottom of the aquifer. The longitudinal location of W_{max} called X_{wmax} will, however, depend on the source shape (S_t and S_w) and other transport quantities such as dispersion (discussed below). For practical reasons, a critical concentration $C_D = C^* > 0$, which lies in the donor region of the domain, can be defined at which L_{max} and W_{max} is quantified. C^* can be for e.g., the maximum allowable water quality standard concentration.

2 The mathematical model setup

The consideration of a steady, homogeneous and isotropic aquifer with a uniform flow field allows (Liedl et al., 2011) to safely assume that transport and reaction quantities such as direction dependent dispersions, reaction rate (r) are also uniform in the domain. Additionally, assuming equal pore diffusion coefficients for both reactants leads to identical dispersivity for both reactants. Further, Liedl et al. (2011) ignore the effect of longitudinal dispersion. All of these assumptions are quite extensively detailed in Liedl et al. (2005), which considers the similar problem in a 2D domain. With all these assumptions, the transport equation (Advection-Dispersion-Reaction or ADR in short) for each reactant is (also numbered **Eq. 3 and Eq. 4 in the paper**):

$$\frac{\partial C_D}{\partial x} - \alpha_{Th} \frac{\partial^2 C_D}{\partial y^2} - \alpha_{Tv} \frac{\partial^2 C_D}{\partial z^2} = -\frac{r}{v} \quad (3)$$

$$\frac{\partial C_A}{\partial x} - \alpha_{Th} \frac{\partial^2 C_A}{\partial y^2} - \alpha_{Tv} \frac{\partial^2 C_A}{\partial z^2} = \frac{-\gamma r}{v} \quad (4)$$

in which α_{Th} [L] and α_{Tv} [L] are dispersivity along the transverse horizontal and vertical directions, respectively. v [LT^{-1}] is the uniform average groundwater flow velocity and $\gamma[-]$ is the stoichiometric coefficient, which represents the molecular ratio of reactants required for the instantaneous reaction to take place. The boundary conditions of the problem are defined as per the distinct donor and acceptor regions based on the conceptual setup (Fig. 1). Thus, the following boundary conditions are defined for the problem:

A. In the donor region:

1. $C_D(0, y, z) = C_D^\circ$ (source)
2. $\frac{\partial C_D}{\partial z}(x, y, M) = 0$ (no flux)
3. $C_A(x, y, z) = 0$

B. In the acceptor region:

1. $C_A(0, y, z) = C_A(x, \pm\infty, z) = C_A(x, y, 0) = C_A^\circ$
2. $\frac{\partial C_A}{\partial z}(x, y, M) = 0$ (no flux)
3. $C_D(x, y, z) = 0$

In addition, the boundary conditions at the plume fringe, which is unknown a priori, has to be specified. Since a single-step irreversible instantaneous reaction is considered, the following boundary condition is defined at the plume fringe:

$$C_D(x, y, z) = C_A(x, y, z) = 0$$

$$\gamma \alpha_{Th} v \frac{dC_D}{dy} - \alpha_{Th} v \frac{dC_A}{dy} = 0$$

$$\gamma \alpha_{Tv} v \frac{dC_D}{dz} - \alpha_{Tv} v \frac{dC_A}{dz} = 0$$

Here, the first condition indicates that donor and acceptor concentration vanish at the fringe due to their mutual neutralization. The second and third condition guarantee that the required proportions of donor and acceptor mass fluxes arrive at the fringe to maintain the instantaneous reaction. To simplify further, a variable $C(x, y, z) = \gamma C_D(x, y, z) - C_A(x, y, z)$ is introduced. C thus represents the deficit in acceptor concentration as compared to the acceptor concentration actually needed in the reaction to achieve a complete consumption of the donor. This deficit concentration appears in the paper (Eq. 2) as C^d , although the general symbol C is used for representing it in remaining of the text. Multiplying Eq. (3) by γ and subtracting it from Eq. (4), and then using the variable C results to the following single system equation (**Eq. 5 in the paper**) for the considered (Fig. 1) problem:

$$\frac{\partial C}{\partial x} - \alpha_{Th} \frac{\partial^2 C}{\partial y^2} - \alpha_{Tv} \frac{\partial^2 C}{\partial z^2} = 0 \quad (5)$$

with the boundary conditions: $C(0, y, z) = \gamma C_D^\circ$ if $|y| < S_w$, $C(0, y, z) = -C_A^\circ$ if $|y| > S_w$, $C(x, \pm\infty, z) = C(x, y, 0) = -C_A^\circ$ and $\partial C / \partial z(x, y, M) = 0$.

It is to be noted that above-mentioned boundary conditions at the plume fringe are no longer required due to introducing the new variable C . This step converts the consideration of plume fringe boundary conditions to the determination of the isoline $C = 0$. Two important features of Eq. (5) requires an attention. First, the reaction quantity r does not appear in the Eq. (5), i.e., a conservative equation has been developed for a reactive problem. Second, the groundwater velocity v is also not part of the Eq. (5). These two features largely simplify the problem.

Eq. (2) in the paper is a solution of Eq. (5), which is manipulated ($y = 0$, and $z = M$) to provide L_{max} using Eq. (6) in the paper.

3 Difference between BIOSCREEN-AT and Liedl et al. (2011) model

For completion, this section very briefly distinguishes between the BIOSCREEN-AT (Karanovic et al., 2007) and the Liedl et al. (2011) model. The respective papers should be followed for complete clarity. In contrast to Liedl et al. (2011) model, the BIOSCREEN-AT is a transient model that considers a first order degradation at the source $\gamma [T^{-1}]$ and in the plume Λ_{EEF} . Further, the model also considers linear sorption of the contaminant on the solid. Thus, BIOSCREEN-AT is a more realistic models compared to Liedl et al. (2011) model. However, simplistic model such as Liedl et al. (2011) model are often advantageous for example when site data are limited such as for the early investigation of sites.

References

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