Calibration and Reliability in Groundwater Modelling (Proceedings of the ModelCARE 99 Conference held at Zürich, Switzerland, September 1999). IAHS Publ. no. 265, 2000.

Validity and sensitivity analysis of a new comprehensive clogging model

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Abstract Evidence of the importance of clogging at many artificial recharge sites has led to the numerical implementation of an integrated mathematical model. The code, termed CLOG, pays attention to the most relevant clogging processes by considering three dimensional multiphase flow and reactive transport of suspended particles and solutes, and the associated porosity variations. A number of synthetic and real examples are currently being studied in order to determine the performance of CLOG. This paper presents the results obtained after validation of the model against laboratory and field data. The sensitivity of the simulations to the model parameters was also investigated in order to identify the more influential factors. This analysis confirmed that the kinetic rates and the apparent density of the clogging layer are critical. Furthermore, the issue of prediction is succinctly discussed, given the interest for design purposes. It is expected that existing generic tight guidelines could be relaxed and adapted to the prevailing site conditions.

INTRODUCTION

Clogging denotes the reduction in the efficiency of artificial recharge systems due to physical, biological and chemical processes. These processes affect the porosity of the medium, thus implying a lower filtration rate or an additional head build-up. Evidence of the clogging processes and their effects can be found elsewhere (Pérez-Paricio & Carrera, 1999a).

There are two approaches to quantifying the extent of clogging: *empirical* and *theoretical* modelling. The former approach uses a few meaningful parameters (concentration of suspended solids, organic carbon load) to achieve a satisfactory reproduction of the experimental results. In general, empirical models cannot be extrapolated to other plants, but are site-dependent.

The second approach employs physical balances to propose a mathematical framework to analyse the spatial and temporal evolution of a system. It is critical to correctly identify the basic processes, and to establish adequate relationships (usually kinetic) among the key variables. It is evident that this type of models require a lot of data and, more important, a sufficiently good previous identification of the controlling reactions. Theoretical models provide a better description of the system under study, although there are significant uncertainties involved in their application to real cases. Among these, the role of physical (heterogeneity) and process-related variability is crucial. Uncertainty as to the magnitude and distribution of the kinetic parameters can not be disregarded either. Prediction is difficult when these considerations are taken into account.

In recent years there has been a trend to produce more and more sophisticated codes. This is a consequence of the recognition of numerical modelling as an essential contribution to most scientific and technical projects. An integrated three-dimensional (3-D) finite element code, CLOG, has been developed recently (Pérez-Paricio *et al.*, 1998; Pérez-Paricio & Carrera, 1999b). CLOG features the following:

- multiphase flow of liquid and gas,
- transport of heat, solutes and suspended particles,
- compaction of the solid matrix,
- generic minerals: true minerals, attached bacteria and attached particles,
- reduction of porosity by physical, biological and chemical reactions (generic minerals),
- final change of intrinsic permeability caused by porosity modifications by means of the Kozeny-Carman equation.

In this paper we focus on two examples: physical clogging in a recharge well at Langerak, The Netherlands (Timmer *et al.*, 1999; Pérez-Paricio & Carrera, 1999c), and bacterial clogging in a sand column (Albrechtsen *et al.*, 1999; Pérez-Paricio & Carrera, 1999d). The main objective is to study the sensitivity of CLOG to the model parameters, gaining insight into the predictive capability of the code.

MATHEMATICAL MODEL

CLOG performs mass balances within the groundwater system. Given that most of the equations are well known in groundwater science, we only focus on the more specialized relationships. The calculations include:

- mass balance of water (liquid, gaseous and solid phases); liquid pressure is the state variable,
- mass balance of air (liquid and gaseous phases); gas pressure is the state variable,
- balance of momentum of the solid matrix; solid displacement velocity is the state variable,
- energy balance, where temperature is the state variable,
- mass balance of dissolved species or solutes, subject to the thermodynamic laws for solubility and partitioning (precipitation and dissolution of minerals, kinetically or in equilibrium, is particularly important),
- mass balance of suspended particles, which are linked to the concentration of attached particles (to the solid matrix) by means of a kinetic expression,
- mass balance of fixed bacteria, which grow and die-off as a function of the availability of nutrients and electron donors/acceptors.

Porosity is directly affected by the concentration of generic minerals. Equations (1) and (2) represent the mass balance of flowing species and generic minerals, respectively (Pérez-Paricio & Carrera, 1999b):

$$\rho_l S_l \phi \frac{D w_l^p}{D t} = \nabla \left[\rho_l D_l^p \nabla w_l^p\right] - \rho_l q_l \nabla w_l^p + f^w \left[w_{l/o}^p - w_l^p\right] + r^p (w_l^p) \qquad (1)$$

where w_l^p [L^0] is the mass fraction of species *i* in the liquid *l*, ρ_l [M L^{-3}] is the liquid density, ϕ [L^0] is porosity, S_l [L^0] is the saturation degree, *t* [T] is time, *D* [L^{-2} T^{-1}] is the dispersion coefficient (strictly a tensor), q_l [L T^{-1}] is Darcy's velocity, f^w [M L^{-3} T^{-1}] denotes the external sink/source term, and r^i is the reactive sink/source term [M L^{-3} T^{-1}]. Superscript i denotes the particular species under consideration, subscript l refers to the liquid phase and i/o the concentration of species i moving into/out of the system associated with the f^w term.

$$\frac{\partial a}{\partial t} = K_a(w_l^p) - K_d a \tag{2}$$

where a [L^0] is the mass fraction of retained particles and K_a [T^{-1}] and K_d [T^{-1}] are the attachment and detachment rate terms, respectively. Table 1 presents the exact form of the attachment and detachment parameters, which will be referred to later when analysing the sensitivity of the model.

Table 1 Explicit form of the attachment and detachment parameters for particles and bacteria (Pérez-Paricio & Carrera, 1999b). The corresponding term for precipitation of true minerals is not shown.

	Attachment rate term (K_a)	Detachment term (K_d)
Attached particles	$\frac{K_{att}}{d_g}\left\{\left[\frac{d_p}{d_g}\right]^{m_{int}} + \alpha_{por}\left[\frac{d_g - d_{g0}}{d_{g0}}\right]^{m_{por}}\right\}$	$K_{det}\delta_{\phi\phi_{crit}}$
Fixed bacteria	$\mu_{max}\frac{[De]}{[De]+g_{De}}\frac{[Ae]_0}{[Ae]_0+g_{Ae}^0}\prod_{k=1}^{N_{SEC}}\frac{g_{Ae}^k}{[Ae]_k+g_{Ae}^k}$	μ_{dec}

K_{att} [L T^{-1}] is the attachment coefficient; d_{g0} [L] is the mean diameter of the aquifer grains at the initial time; d_g [L] is the current grain diameter; m_{int} [L^0] is a real number ranging between 1.0 and 2.0 (interception exponent); α_{por} [L^0] and m_{por} [L^0] are two adjustable parameters (coefficient and exponent of cake filtration) controlling the magnitude and dynamics of this contribution; d_p [L] is the mean particle diameter (suspended solids); K_{det} [T^{-1}] is the detachment coefficient.

μ_{max} [T^{-1}] is the maximum growth rate; $[De]$ [L^0] is the concentration of electron donor; g_{De} [L^0] is the half-saturation constant for the electron donor; $[Ae]$ [L^0] is the concentration of electron acceptors; g_{Ae} [L^0] refers to the half-saturation constant for the electron acceptors; and μ_{dec} [T^{-1}] denotes the die-off rate. Subscript 0 is adopted for the main acceptor, while subscripts $1,\ldots,N_{SEC}$ refer to the N_{SEC} optional limiting secondary acceptors. $\delta_{\phi\phi crit}$ is a step function defined by:

$$\delta_{\phi\phi crit} = \begin{cases} 0 & if\ \phi > \phi_{crit} \\ 1 & if\ \phi < \phi_{crit} \end{cases} \tag{3}$$

SENSITIVITY ANALYSIS

A summary of the sensitivity of the model parameters is presented for the two cases that were cited in the Introduction: biological clogging in a sand column (vertical flow) and clogging by suspended sediments under field conditions (radial flow). The analysis is limited to the kinetic parameters.

The biological clogging case

A real situation where lake water was infiltrated through a sand column was modelled with CLOG. Some simplifications had to be assumed, including the following:

- simulation for constant infiltration rate; the column was under aerobic conditions during this period (Albrechtsen *et al.*, 1999),
- assumption of constant input concentration of oxygen and organic carbon,
- clogging due to growth of heterotrophic aerobic bacteria, whereby oxygen is the electron acceptor and organic carbon is the electron donor and carbon source.

A satisfactory agreement between the observed data and the calculated values was achieved. Also, the model parameters were in good agreement with values usually obtained in the wastewater treatment by activated sludge (Pérez-Paricio & Carrera, 1999d).

Figure 1 compares the behaviour of the so-called optimum configuration (simulation S0) with six different situations in which one parameter was increased and decreased with respect to the optimum value. Table 2 collects the adopted values for each simulation, where the varying parameters are: maximum growth rate, bacterial mass per biofilm volume (not described above, relates porosity to the concentration of growing bacteria), die-off coefficient, initial bacterial concentration, the Monod half saturation constant, and specific yield (linking changes of bacterial concentration with use of nutrients).

The response suggests that the first two parameters are more important, but both the Monod constant and die-off coefficient also play a significant role. In general, it is evident that the parameters appearing in the kinetic expression are very influential.

Table 2 Configurations for the bacterial clogging case. The simulations are based on the optimum set of parameters (S0), i.e. the combination that led to a satisfactory agreement with the measurements. The results of these configurations are shown in Fig. 1.

	Units	S0	S1	S2	S3	S4	S5	S6	S7	S8	S8	S10	S11	S12
μ_{max} (1.0×10^{-6})	s^{-1}	1.2			0.9	1.5								
μ_{dec} (1.0×10^{-8})	s^{-1}	3.7					4.6	2.8						
$^{*}\delta_{bio}$	kg m^{-3}	4.7							5.9	3.5				
g_{DO} (1.0×10^{-6})	mg l^{-1}	25									31	19		
g_{CH2O} (1.0×10^{-6})	mg l^{-1}	30												
$^{\dagger}Y_{DO}$	L^0	1.0											1.2	0.7
$^{\dagger}Y_{CH2O}$	L^0	2.0												
$X(t=0)$ (5.0×10^{4})	L^0	1.0	0.1	10.										

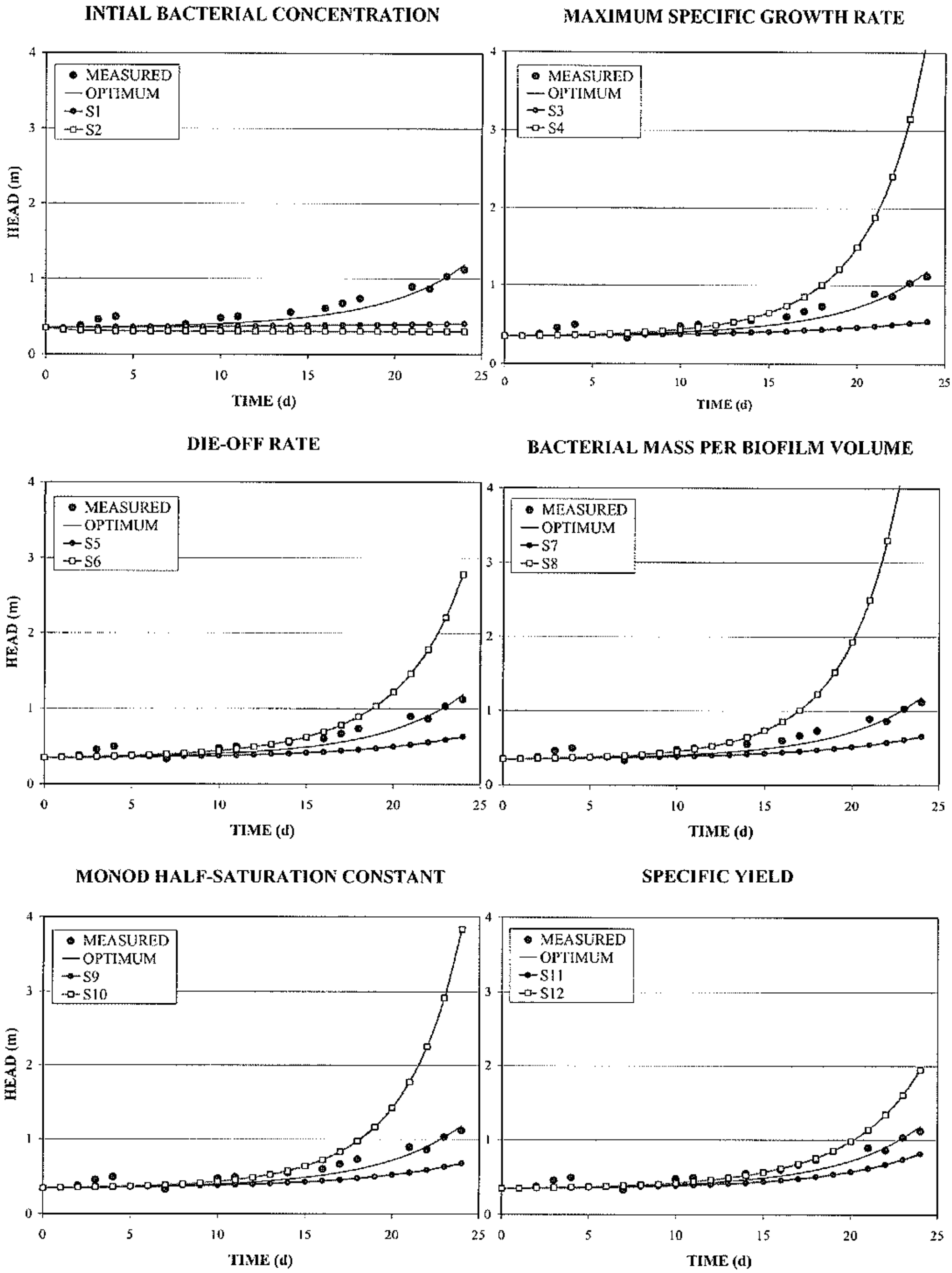
[*] Bacterial mass per biofilm volume. It is assimilable to bacterial density.

[†] Specific yield of dissolved oxygen (DO) and organic carbon (CH2O). They indicate the stoichiometric dependence of the nutrients on the change of bacterial concentration (i.e. how fast they are used).

The physical clogging example

The Langerak field site experienced a (surprising) clogging after 10 months of continuous injection of pre-treated groundwater through a well penetrating a fine sand aquifer. Clogging occurred due to retention of iron flocs generated during aeration of groundwater (Timmer *et al.*, 1999). The concentration of these flocs (suspended particles) was 40 μg l^{-1}, and their size ranged between 20 and 45 μm.

Results obtained with CLOG were satisfactory (Pérez-Paricio & Carrera, 1999c), both in terms of spatial and temporal distribution of clogging. A simple sensitivity analysis was performed too in order to gain insight into the relative importance of the


INTIAL BACTERIAL CONCENTRATION

MAXIMUM SPECIFIC GROWTH RATE

DIE-OFF RATE

BACTERIAL MASS PER BIOFILM VOLUME

MONOD HALF-SATURATION CONSTANT

SPECIFIC YIELD

Fig. 1 Curves that present the sensitivity of the simulations with CLOG to the key model parameters, in terms of the clogging build-up (additional piezometric increase due to clogging) *vs* time. Points indicate the measured values, whereas the maximum, optimum (S0) and minimum configurations are shown with solid lines. The values of the model parameters are shown in Table 1.

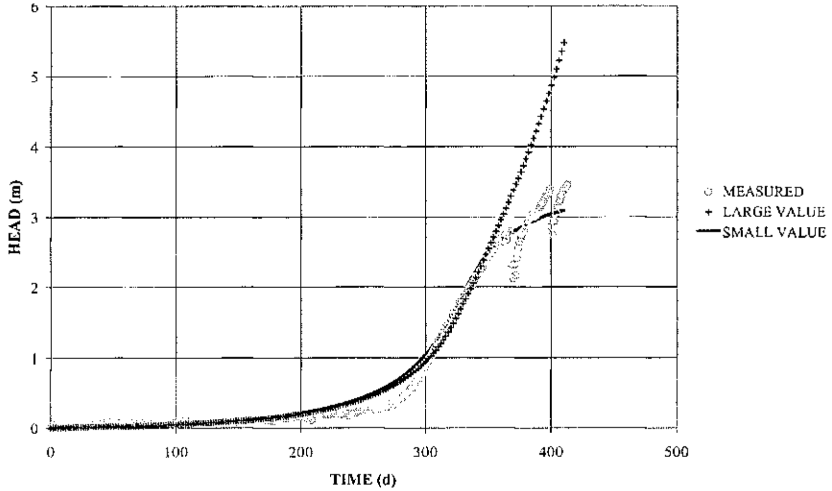


Fig. 2 Sensitivity analysis for the detachment constant, K_{det}. The large value is 1.8×10^{-7}, while the small one is 1.0×10^{-7}, i.e. 20% higher and 33% lower, respectively, than the calibrated parameter.

model parameters. The influence of the parameters that control equation (2) is very high. As an example, Fig. 2 shows the important change that is obtained when the detachment term coefficient is increased (decreased) by 20% (33%) with respect to the optimum configuration. Analogous to the bacterial case, the sensitivity of CLOG is especially high to increases in the attachment parameters, so that great changes can be observed even for relatively small modifications.

CONCLUSIONS

Based on the analysis of two applications of a new integrated clogging model (CLOG) to real data, the validity of the conceptual framework and the mathematical formulation have been confirmed.

However, this paper focused on the sensitivity of CLOG to the model parameters. The response of a system from the point of view of clogging is extremely sensitive to the parameters that intervene in the kinetic expression. Clogging is far more sensitive to increases in the attachment term as compared to changes in the detachment term. As a result, it is not possible to make reliable predictions about the future evolution of a system unless pilot tests are conducted and interpreted with CLOG. But the crucial issue is that *a priori* simulations may be carried out to integrate physiochemical and biological processes in a quantitative tool.

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