

CHAPTER VI

DISCUSSION AND CONCLUSIONS

« The human brain is a magnificent invention. It works from birth until the moment when one has to stand up and deliver a speech. »

By MARK TWAIN

The results of individual examples presented in Chapter V are jointly discussed here. First, model parameters are compared. This is used to evaluate the consistency of model parameters and the whole conceptual framework. Second, the *a priori* characterisation of other model variables –not calibrating parameters, but more elemental properties of the porous medium and the infiltrating water- is analysed in more detail. Following such discussion, some general conclusions of this work are drawn.

6.1. ON THE MODEL PARAMETERS

Table 6.1. summarises the model parameters used for each simulation. The main interest is placed in kinetic parameters, because only these were modified to calibrate the model. The rest of parameters were fixed based on the information from the experiments and/or values adopted from the literature. The characterisation of some of these empirical parameters is briefly discussed in section 6.2.

6.1.1. PHYSICAL CLOGGING

6.1.1.1. Attachment and Detachment velocities

The velocity of attachment, λ'_{att} , is relatively homogeneous among the different examples. There is not a direct dependency on the size of the suspended particles, although the calibrated value for the *STEPH* example (colloidal-sized particles) is one order of magnitude smaller than in the rest of cases (intermediate and large particles). It is interesting to note that this parameter is approximately similar to the infiltration rate, except in the *STEPH* example, where the influence of other clogging processes can not be overlooked.

Detachment velocity is expressed by parameter λ'_{det} in the numerical model. This parameter is much more variable than λ'_{att} . Table 6.1. shows that it ranges between 0.5 ‰ (*LANG*) and 160 ‰ (*KWAD*) of the attachment velocity parameter. Previous studies confirm that the detachment coefficient is several orders of magnitude smaller than the attachment coefficient (HERZIG ET AL., 1970; ADIN & REBHUN, 1987).

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Table 6.1. Summary of the test cases interpreted with CLOG that are presented in this chapter.
All of them consisted in transient flow and transport problems with different clogging processes incorporated.

CASE [infiltration rate, in $\text{m}\cdot\text{s}^{-1}$]	PHYSICAL CLOGGING				CHEMICAL CLOGGING		BIOLOGICAL CLOGGING				CLOGGING FACTOR $\Phi_m = \beta_m \cdot [\rho_{m1}]^{-1}$ (m^3kg^{-1})					
	ATTACHMENT		DETACHMENT		MODEL	EMPIRIC	GROWTH			DECAY						
	λ'_{att} $\cdot 10^{-5}$ ($\text{m}\cdot\text{s}^{-1}$)	m_{int}	λ'_{det} $\cdot 10^{-7}$ (s^{-1})	ϕ_{crit}/ϕ (%)	a_s (m^{-1})	R^{mj} (s^{-1}) $\cdot 10^{-7}$	μ_{max} $\cdot 10^{-6}$ (s^{-1})	g^{ea} ($\text{mg}\cdot\text{L}^{-1}$)	g^{ed} ($\text{mg}\cdot\text{L}^{-1}$)	μ_{dec} $\cdot 10^{-8}$ (s^{-1})						
LANG [$25\cdot 10^{-5}$]	10	1.0	0.5	50	-	-	-	-	-	-	$\beta_s = 30.0$					
KWAD											5 ppm	10 ppm	20 ppm	30 ppm	40 ppm	60 ppm
	A [$85\cdot 10^{-5}$]	50	1.0	600	70	-	-	-	-	-	25.	19.	15.	11.5	10.	8.5
	B [$85\cdot 10^{-5}$]	50	1.0	600	70	-	-	-	-	-	-	200.	160.	-	-	-
C [$367\cdot 10^{-5}$]	50	1.0	600	70	-	-	-	-	-	-	25.	19.	15.	11.5	10.	8.5
DANE [$1.1\cdot 10^{-5}$]	-	-	-	-	-	-	1.2	8.0	9.0	3.5	$\beta_x \cdot [\rho_x]^{-1} = 4.7$					
STEPH [$12\cdot 10^{-5}$]																
	1	1.0	5	60	0.05	4.6	30	3.2	15.0	400	$\beta_s = 1.0$					
							80	3.2	4.6	300	1) $\beta_x \cdot [\rho_{x1}]^{-1} = 1.0$					
							25	6.2	15.0	450 ⁶	2) $\beta_x \cdot [\rho_{x2}]^{-1} = 0.5$					
											3) $\beta_x \cdot [\rho_{x3}]^{-1} = 2.0$					
											$\beta_m = 1.0$					

6.1.1.2. Other parameters

In principle, the interception exponent [m_{int}] could be variable, but all the model simulations were carried out with a fixed value (1.0) in order to reduce the number of calibrating parameters. Furthermore, m_{int} would be constrained between 0.5 and 2.0, as suggested by BOYD & GOSH (1974).

The last parameter is ϕ_{crit} , i.e. the value of porosity below which hydrodynamic and hydrochemical forces are able to detach particles from the solid matrix. In terms of relative values (ratio of critical to initial porosity), this threshold has been set to values between 50 % and 70 %.

6.1.2. BIOLOGICAL CLOGGING

The specific growth rate for the *DANE* case is one order of magnitude lower than *STEPH* calibrated values. Calibrated parameters are comparable to those commonly presented in the literature of activated sludge technology (Chapter V), despite the conceptual differences between artificial recharge schemes and wastewater treatments. However, as shown in Table 6.2., there is a good correspondence between both of them. From a physical viewpoint, this agreement is important because it is hard to obtain indications about the order of magnitude of kinetic parameters in field and laboratory conditions.

Table 6.2. Comparison of biological kinetic (model) parameters with standard values of the activated sludge technology (after METCALF & EDDY, 1991).

PARAMETER	UNITS	DANE	STEPH			ACTIVATED SLUDGE
			<i>Aerobic</i>	<i>Nitrobacter</i>	<i>Denitrifying</i>	
μ_{max}	d^{-1}	0.1	2.6	6.9	2.2	1.0÷10.0
μ_{dec}	d^{-1}	0.003	0.3	0.3	0.4	0.004÷0.008
g_3	$\text{mg}\cdot\text{L}^{-1}$	8.0÷9.0	3.2÷15.0	3.2÷4.6	6.2÷15.0	15.0÷100.0

As for the die-off rate, *STEPH* values are notably higher than *DANE* ones –this being comparable to activated sludge rates. Although this is not a proof of the credibility of CLOG parameters, at least it is remarkable that the calibrated values can be considered to be ‘realistic’, i.e. they can be constrained based on empirical evidence. The same holds for the half-saturation values shown in Table 6.2.

6.1.3. CHEMICAL CLOGGING

The specific surface area is the only adjustable parameter for true minerals, because the rest of parameters –coefficients determined to describe the reaction rate dependency- are empirically determined by means of laboratory experiments.

The specific surface area of a mineral is critical with regards the velocity of precipitation/dissolution reactions: the higher the surface area the faster the reaction. In this context only one example (*STEPH*) was interpreted with this type of reactions, so that not general results can be obtained. The calibrated value can be considered to be moderately high, but it is comparable with reported hydrochemical modelling (SAALTINK ET AL., 1998b).

6.1.4. POROSITY UPDATE [CLOGGING]

The clogging factor determines the effect of mineral growth on porosity, i.e. it is used to update porosity based on the evolution of the whole system. As explained in CHAPTER III, the clogging factor (Φ_m) is equivalent to the product of the inverse of the mineral density (ρ_m^{-1}) times the apparent clogging factor, (β_m). The former is generally well known, except for bacteria. This is why the calibration process requires adjusting the apparent clogging factor for particles and true minerals, whilst for bacteria it is the clogging factor that is varied –i.e. bacterial density is assumed to be 1.0-.

For the sake of simplicity, the discussion is split up in three groups, depending on the type of generic minerals involved.

6.1.4.1. Particles

Apart from the *STEPH* example, the apparent clogging factor was larger than one. According to HERZIG ET AL. (1970), values between 2.0 and 3.0 could be expected. Taking into account the values compiled in Table 6.1., it can be stated that the model needs to use artificially large β_m values to satisfactorily reproduce clogging. In fact, physical clogging tended to be underestimated in the *STEPH* example (CHAPTER V), which provoked that β_m was smaller than in the rest of examples. A possible explanation for the need of large clogging factors is the inappropriate characterisation of heterogeneity in the simulated cases. As shown in the *Langerak* case (section 5.2.), heterogeneity has a dramatic impact on clogging rate. Consequently, it is not surprising that large β_m values have to be used in order to achieve good calibrations.

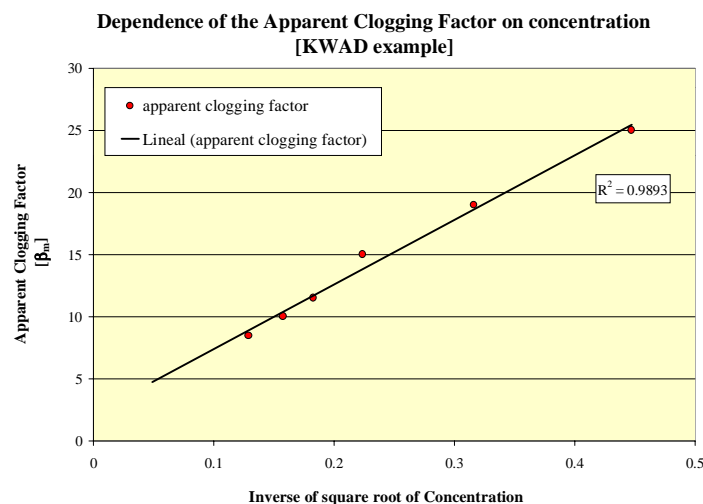


Figure 6.1. A good linear fit results from plotting the value of the apparent clogging factor (β_m) against the inverse of the square root of input concentration of particles [KWAD case].

KWAD simulations provide additional information on this effect, because this is the only dataset where different input concentrations and grain size distribution were compared. A closer investigation of the kinetic model parameters shows that the apparent clogging factor was the only parameter that had to be varied to achieve satisfactory agreements with the measurements for

different input concentrations. If the adjusted values of β_m are plotted against the inverse of the square root of the input concentration value (Figure 6.1.), a straight line is approximately obtained.

Therefore, a unique value can be used for the apparent clogging factor of series A and C, irrespective of the input concentration of suspended solids. It is conjectured that the same would be applicable to series B, because the same effect (reduction of the apparent clogging factor with concentration) can be observed (Table 6.1.).

It is not straightforward to justify the behaviour of the apparent clogging factor. However, it is likely that low concentrations are more 'effective' at reducing the interconnected porosity, whilst larger concentrations are not so prone to obstructing the main porosity conduits as they accumulate much faster in the portions of the porous medium closer to the injection zone. It is well known from filtration theory that the effect of low concentrations of suspended solids can be dramatic when the particles are able to plug the more conductive pathways. However, increasing the input concentration leads always to a faster clogging rate in absolute terms, but not necessarily in terms of actual injected mass.

6.1.4.2. *Bacteria*

In principle, the apparent clogging factor would be around 1.0 for bacteria. According to the calibration results, this was approximately valid for all studied species. Calibrated values ranged between 0.5 (aerobic, *STEPH* case) and 4.7 (*DANE*), i.e. they vary by an order of magnitude.

Other modelling efforts have remarked the sensitivity of the model results to this parameter. HOLM (1999) found that a small value of bacterial density had to be used when calibrating laboratory experiments in sand columns. This was a crucial aspect of the modelling, because it was not straightforward to predict –or, at least, constrain– the value of bacterial density. In the examples presented here, the variability of this parameter is not so high, which can be explained by the homogeneity of the simulated cases and the validity of the proposed conceptual approach.

6.1.4.3. *True minerals*

The reactive surface area of true minerals is the most critical parameter concerning chemical clogging. The rest of parameters involved in precipitation/dissolution reaction formulae can be determined by means of laboratory-controlled experiments. This way, several empirical coefficients can be evaluated. But the value of reactive surface area can not be deduced a priori, because it controls the rate at which heterogeneous chemical reactions will take place. Since it is not immediate to decide whether a given reaction will proceed under kinetic conditions or it will be rate-controlled, this parameter has to be adjusted for each particular case.

6.2. ON THE MODEL VARIABLES

As indicated above, the present section deals with the characterisation of input variables not used for calibration, i.e. the fixed or measurable properties of the aquifer and recharge water

6.2.1. CHARACTERISATION OF GRAIN SIZE DIAMETER

CLOG can be classified as a sphere-in-type-model. The grain size distribution of both aquifer and suspended solids can only be taken into account indirectly, since the code uses a unique value for characterising the grain size diameter.

CLOG takes into account the non-uniformity of the aquifer grains and the suspension, by using the d_{15} value of the aquifer grains and the d_{85} value of suspended solids. Even though such a choice is, in principle, arbitrary, there are numerous filtration studies that use these two values to assess the interception potential of suspended particles in porous media (SHERARD ET AL., 1984; VUKOVIC & SARO, 1992). In this way, CLOG incorporates information about the variability of porous media properties.

6.2.2. FLOW AND TRANSPORT PARAMETERS

In general, flow and transport parameters were characterised during the experiments by means of measuring gauges (piezometers, flowrate control devices, pressure transducers) and in-situ tests (pumping, tracer tests). Quantified parameters include hydraulic permeability, porosity and dispersivity.

Estimates of hydraulic conductivity were directly used in CLOG after converting them into intrinsic permeability values. As for porosity, modelling values are lower than the estimated values, because only the more connected pores are relevant for clogging purposes. In general, initial effective porosities in the models varied between 0.05 (damaged formation in *LANG*) and 0.20 (Table 5.1.). For *STEPH*, input porosity was 0.15 as compared to the estimated porosity of 0.40, which represents a notable reduction. If KOZENY-CARMAN's equation is examined, relative rather than absolute values of porosity are involved. That is, from the viewpoint of clogging it is not very influential whether initial porosity is set at a given value. The influence of absolute porosity is determined by the threshold values of critical (CHAPTER III) and minimum porosity. The lower the initial porosity the faster the minimum value is achieved, which may affect the temporal and spatial evolution of clogging.

As for dispersivity, CLOG parameters tend to be higher than estimated parameters. This has been discussed by other authors (HOLM, 1999) and seems to depend on each particular example. In the cases examined here, aquifers were simply assumed to be homogeneous. Nevertheless, heterogeneity distorts the velocity field, enhancing hydrodynamic dispersion. This is why it is not very surprising that the adopted dispersivities (Table 5.1.) are higher than estimated (or typical) dispersivity values at the scale of study. But it must be highlighted that flow and transport parameters were not modified: the discussion presented in this section is related to the initial parameters that were used in all simulations, not being subject to calibration.

6.3. CONCLUSIONS

Taking into account the description, results and discussion presented in this document, the following conclusions can be drawn:

1. A new, integrated conceptual model has been implemented into a 3-D finite element code (CLOG) that is able to deal with complex real examples involving clogging from different sources: retention of suspended particles, bacterial growth, precipitation of minerals, formation of gas and compaction. Clogging refers to porosity reductions caused by increase in concentration of retained particles, attached bacteria and true minerals –classified as *generic* minerals-.
2. The concept of *generic* minerals is very useful in conceptual and mathematical terms, because the most frequent reactions can be compactly expressed by means of generic equations. The code does not account for heterogeneity of the porous medium in a direct way, but the adoption of granulometric criteria has proven to be very convenient for calibration purposes.
3. The code has been validated against laboratory and field data. Results indicate that it is possible to reproduce satisfactorily the main spatial and temporal trends. Provided that detailed data are available, the fits between measurements and calibration results can be very good.
4. The calibration process is itself hard and difficult when several dissolved species, *generic* minerals and reactions are involved. When different processes are interrelated, then the whole system is inter-dependent and the influence of some species on the rest is considerable. Even though adjusting all the variables (piezometric heads, concentration of various components) is not trivial, and can require lots of CPU and manpower time, CLOG is capable of simulating the response of the system. In other words, the model can determine whether clogging will or not be an issue under particular circumstances.
5. Kinetic parameters have to be calibrated in order to obtain accurate model responses. However, an analysis of calibrating parameters have shown that most of them can be pre-evaluated, or at least constrained, based on physical and empirical arguments. The most uncertain parameter (for particles and bacteria) is the apparent clogging factor, which is used to update the porosity as a function of the current concentration of *generic* minerals. The magnitude of the apparent clogging factor is not easy to determine a priori and makes it difficult to predict clogging response for suspended particles and bacteria, but good initial approximations can be obtained by applying the code.

As for true minerals, the critical parameter is reactive surface area, because it controls the velocity of reaction and this is not known a priori. Empirical determinations of this parameter, under laboratory conditions, are not extrapolable to field conditions.

6. Based on the examples analysed here, clogging by suspended particles in recharge wells can be perfectly simulated when it is limited to the vicinity of the well. When filtration (retention) of particles occurs at the gravel-pack interface, after travelling along the gravel-pack material, the model response is still satisfactory, but there is a tendency to overestimate the clogging impact within the gravel-pack itself.

In the case of bacteria, the spatial distribution of clogging is generally well simulated, even though model results are more uniform (less abrupt changes) than observed data. The distribution of true minerals is controlled by the rest of biochemical variables (pH, redox potential and concentration of catalysts).

7. CLOG has shown that it could be applied to Artificial Recharge projects, at different stages. In the first phase of a recharge project, the code can be used as a preliminary assessment tool of the clogging potential, based on initial estimates of flow, transport and kinetic parameters and data of groundwater, aquifer matrix and recharge water. As the recharge demonstration project evolves, the code is the best way to integrate and interpret all the available data quantitatively. Integrated Mathematical modelling of physical, chemical and biological clogging allows to:
 - 7.1. Integrate all available data in a single decision tool that provides quantitative insight into the importance of the main processes.
 - 7.2. Compare among various starting hypotheses in order to elucidate which are the more likely scenarios. This is also very useful to assess how the system will evolve under the most conservative conditions, i.e. to explore the tightest restrictions that could eventually be imposed on the recharge plant.
 - 7.3. Search for a consistent interpretation of the conceptual mechanisms from a scientific-technical point of view.

In sum, despite the limitations of complicated numerical models (lack of information on parameters, inaccurate characterisation of heterogeneities and most conductive paths, simplifications on the conceptual scheme) it is evident that the use of integrated models such as CLOG is necessary when objective decisions must be made concerning the design and operation of a recharge plant.