A SEMI-DISTRIBUTED MODELLING OF THE EVOLUTION OF GROUNDWATER QUALITY IN FLOODED MINES IN THE LORRAINE IRON BASIN

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ABSTRACT: In Lorraine (France), closure and flooding of ancient mine workings led to a degradation of the groundwater quality, making it unsuitable for human consumption. The two models presented here were developped after the identification of the chemical mechanisms responsible for this phenomenon (Collon et al., 2004) in order to reproduce and predict the evolution of groundwater chemical composition in the Southern part of the lorraine Iron Basin. Based on a Network of Chemical Reactors (NCR) type global approach, two types of modelling are produced: one considers the basin in its totality and calculates the composition of the groundwater only at the overflow point, the other is semi-distributed in order to reproduce the concentrations observed in the four monitoring wells of the basin.

Keywords: Modelling, groundwater quality, mine flooding

RESUME : En Lorraine (France), l'abandon et l'ennoyage des anciens travaux miniers a entraîné une dégradation de la qualité de l'eau souterraine, la rendant impropre à la consommation humaine. Les deux modèles présentés ici ont été développés après la mise en évidence des mécanismes chimiques responsables de ce phénomène (Collon et al., 2004), pour reproduire et prédire l'évolution de la composition chimique de l'eau dans la partie Sud du bassin Ferrifère Lorrain. Basées sur une approche globale de type Réacteurs En Réseau (RER), deux types de modélisation sont réalisées : l'une considère le bassin dans sa globalité et ne calcule la composition de l'eau qu'au point de débordement, l'autre est semi distribuée, de manière à reproduire les concentrations observées dans les quatre puits de contrôle du bassin.

MOTS-CLEFS : Modélisation, qualité de l'eau, ennoyage des mines.

1. Introduction

Mine drainage is one of mining undesirable effects on the environment. In Lorraine, the flooding of the abandonned workings over the past 20 years has led to a degradation of groundwater quality, as indicated by high concentrations of SO_4, Ca, Na, Mg, K, Mn and B, making it unsuitable for human consumption. As this accumulated water in abandoned iron mines will, in the long run, represent a resource of around 300 million m^3 for the Lorraine, it is necessary to predict its future quantitative and qualitative evolution.

Most of the hydro-geochemical model that were applied to simulate the impact of mining on water ressources have been developed for mine tailings, considered similar to porous media (*e.g.*, Elberling *et al.*, 1994; Salomons, 1995; Lin *et al.*, 1997; Bain *et al.*, 2000; Neumann and Sami, 2002). The mine drainage is most often treated either hydrodynamically (*e.g.*, Therrien and Sudicky, 1996; Bochenska *et al.*, 2000; Adams and Younger, 2001; Hauns *et al.*, 2001) or chemically (*e.g.*, Appelo *et al.*, 1998; Brown *et al.*, 1998; Chen *et al.*, 1999; Mayo *et al.*, 2000;

Razowska, 2001; Eary *et al.*, 2003) and only few models couple mine reservoir hydrogeology and chemistry (*e.g.*, Bain *et al.*, 2001).

Based on these studies and on the available poor spatially distributed data, we adopted a Network of Chemical Reactors (NCR) global approach to predict the future evolution of water quality in the Lorraine Iron Basin (LIB).

2. Method

2.1. Principles of the model

The association of reactors in series and parallel was originally developed for process engineering (Villermaux, 1993). Thereafter, it has been used to model the reactive transfer of pollutants in soils (Jauzein *et al.*, 1989; Baranger et Kervévan, 1998), the tailing effluents (Altmann, 1995) and the composition of water discharge from flooded mines (Collon *et al.*, 2003).

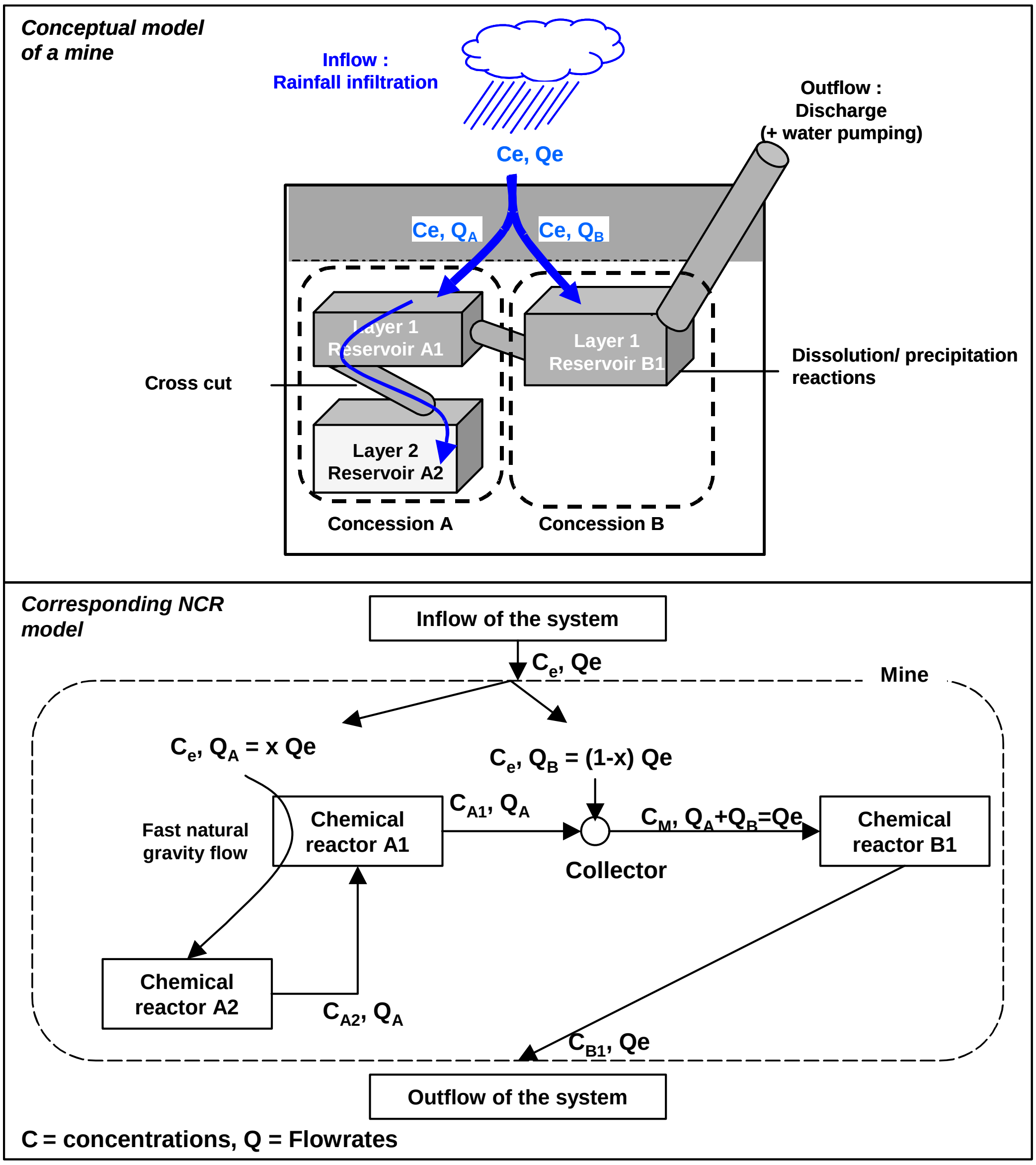

Figure 1. Principle of mine reservoir modelling with a network of chemical reactors – NCR model

Conceptually, the mining system is divided into hydraulically connected concessions or reservoirs (figure 1a). So, by representing each reservoir of this system with a reactor, the mine is represented as a NCR (figure 1b). Only advective mass transfer is taken into account between two reactors. At any time t, each reactor is characterised by an inflow Q_e, an outflow Q_s, a volume of water V that varies with water table fluctuations, and a mass of rock M. Groundwater circulating in a reservoir reacts with the minerals in the reservoir rock and its composition changes. Each reactor is described by the step by step summation of a mass-balance equation that enables to directly express the concentration of any chemical element or compound at time step t:

$$C(t_n)\,V(t_n) = V(t_0)\,C(t_0) + \sum_{i=1}^{n-1}\left[Q_eC_e + V(t_i)\,r(t_i) - QsC(t_i)\right]\Delta t_i \qquad \text{with } n \geq 2 \tag{1}$$

where:

Q_s = outflow rate (l/s)
Q_e = inflow rate (l/s)
C_s = outflow concentration (mol/l)
C_e = inflow concentration (mol/l)
C(t) = concentration in the reactor (mol/l)
V(t) = volume of water in the reactor (l) at time t (hence V_0 = volume of water at time t=0)
r(t) = production or consumption rate (= reaction rate) of a given chemical element or compound (mol/l/s)

The inflow rate Q_e was estimated using rainfall data, the outflow discharge rate and the numerical package TEMPO® based on signal-processing methods (Pinault *et al.*, 2001). This method does not require any hypothesis concerning the internal structure of the reservoir (type of flow, porosity, permeability,...), which is an advantage when no spatially distributed data is available.

A chemical kinetic model, based on the classical approach, is used to estimate the reaction rate r(t). It was built in order to reproduce the water-rock reactions observed in closed reactor tests and leaching column tests that were carried out on rocks of the LIB (Collon *et al.*, 2004). If we consider a dissolution-precipitation reaction of a mineral A_nB represented by the equation:

$$A_nB \leftrightarrow nA^+ + B^{n-} \tag{2}$$

then the rate of reaction is the difference between the dissolution rate (r_{diss}) and the precipitation rate (r_{pcp}):

$$r(t) = r_{diss} - r_{pcp} \tag{3}$$

$$r(t) = (Ctl)\, k_{pcp}\, [K\,(A_nB) - (A^+)^n\,(B^{n-})] \tag{4}$$

where:
K is the equilibrium constant related to the kinetic constants: $K = k_{diss}/k_{pcp}$,
(X) is the activity of X.
The factor (Ctl) enables to introduce the concept of specific surface area into the model:

$$Ctl = Fg\, b_{AnB}\, [m(t)]^{2/3} \tag{5}$$

Where:

$$F_g = \frac{9.756 \quad M_R}{Gr \quad \rho_R}$$

with M_R is the total mass of rock in (kg by litre of water) - 2.04 kg/kg of water in our laboratory experiments -
Gr is the mean grain size of the rock (m)
ρ_R is the mean density of the rock (kg/m^3) - 2.6 10^{-3} kg/m^3 -

The parameter Fg expresses the influence of initial rock granulometry: Fg = 10^6 for the granulometry of 2.5 mm used in the closed reactor tests, and Fg = 0.26 10^6 in the leaching experiments, where the average granulometry is 29 mm.

The coefficient b_{AnB} (dimensionless) represents the accessibility of the mineral AnB in the block of rock; it is a constant specific to each mineral and each sample. It was fitted on experimental results.

The mass of a mineral at time t, *i.e.* $[m(t)]^{2/3}$ (in mol), enables us to take into account the variation of the surface with the available mineral quantity. The initial value m(0) for each mineral in each studied rock sample was evaluated by a mineralogical study (Collon *et al.*, 2004).

The ion activity in water (A^+) and (B^{n-}) was calculated using the Debye-Hückel equation. The activity of the solid (A_nB) and that of water were considered to be 1. The fugacity of the gaseous compounds similar to perfect gases was considered to be equal to their partial pressure.

Equilibrium constant values, K, for mineral dissolution/precipitation reactions (25 °C, 1 bar), ion complexation reactions in water, and O2 and CO2 gas exchange reactions at the water-air interface, were taken from the PHREEQC database (Parkhurst and Appelo, 1999).

In our model, ion complexations are described by kinetic reactions, with the kinetic constants being set arbitrarily to account with their fast rates compared to those of mineral dissolution and precipitation. The kinetic constants were defined on the basis of experimental laboratory results: different scenarios were tested by modifying them. The best agreement with experimental data from the closed reactor tests was obtained with a model based on 12 chemical elements (Al, C, Ca, Fe, K, H, Mg, Na, O, S, Si and Sr), 19 mineral dissolution and precipitation reactions, 25 aqueous speciation reactions, O_2 and CO_2 dissolution and degassing, and 4 cationic exchange reactions (Collon *et al.*, 2004; Collon *et al.*, in press).

Table 1 gives an example of each type of reaction considered in the model (dissolution/precipitation, aqueous complexation, dissolution/degassing and cationic exchange).

Table 1. The kinetic model of five types of chemical reactions

Type of Reaction	Reaction	Rate
Dissolution/ precipitation	$CaSO_4 ,2H_2O \leftrightarrow$ $Ca^{++} + SO_4^{--} + 2\ H_2O$	$r(t) = (Ctl)\ k_{pcp\text{-}gyps}[K - (Ca^{++})(SO_4^{--})]$
Dissolution/ precipitation	$FeS_2 + 3.75\ O_2 + 3.5\ H_2O \leftrightarrow 4\ H^+ + Fe(OH)_{3aq} + 2\ SO_4^{2-}$	$r(t) = (Ctl)\ k_{pcp\text{-}pyr}[K\ (O_2) - (H^+)(SO_4^{--})(Fe(OH)_{3aq})]$
Aqueous complexation	$H_2O \leftrightarrow H^+ + OH^-$	$r(t) = k_{pcp\text{-}H2O}[K – (H^+)\ (OH^-)]$
Dissolution/ degassing	$CO_{2(g)} \leftrightarrow CO_2$	$r(t) = k_{pcp\text{-}CO2}\ [K\ P_{CO2} – (CO_2)]$ *
Cationic exchange	$X\_Na + 0.5\ Ca^{++}$ $\leftrightarrow Na^+ + X\_Ca_{0.5}$	$r(t) = (Ctl)\ k_{pcp\text{-}XNa}[K\ (X\_Na)(Ca^{++})^{0.5} - (Na^+)(X\_Ca_{0.5})]$

* P_{CO2} is the partial pressure of $CO_{2(g)}$

The NCR numerical simulators were built using Matlab® software and its graphic interface, Simulink® (Collon *et al.*, in press). The mining system is represented as an assemblage of reactors in series and parallel (figure 2) where the reactors determine the concentrations in each part of the reservoir and the masses extracted at a given time. To create the network, a distributor and a collector are required. These are characterised by:

$$\text{Distributor} \qquad Qe\ Ce = (\Sigma Qe)\ Ce$$

$$\text{Collector} \qquad \Sigma(Qe\ Cs) = (\Sigma Qe)\ Cs$$

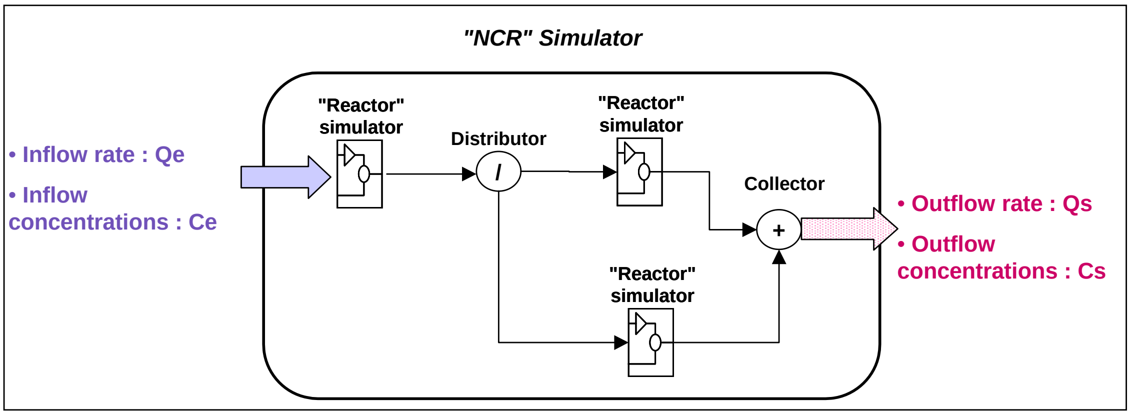

Figure 1. Flow chart of a network of chemical reactors (NRC)

2.2. *Site description*

Located along the eastern edge of the Paris Basin (France), the Lorraine iron-ore deposit extends from the Luxembourg border and the Moselle area to the Woëvre area in the West. The Pont-à-Mousson anticline causes a disruption in the mineralisation, thus creating two basins of unequal size: (i) the Briey-Longwy Basin to the North and (ii) the Nancy Basin to the South. Faults subdivide the Briey-Longwy Basin into three major structural units: the North, the Central, and the South Basins (figure 3). At the moment, the modelling is carried on the South Basin, whose mines were closed in 1995. The gradual flooding of the mine workings ends with the beginning of the overflow at the Tunnel of Moyeuvre in October 1998. Four mine shafts and the overflow point constitute a surveillance system set up for quantitative and qualitative groundwater monitoring. Thus, modelling results would be compared to *in situ* measurements.

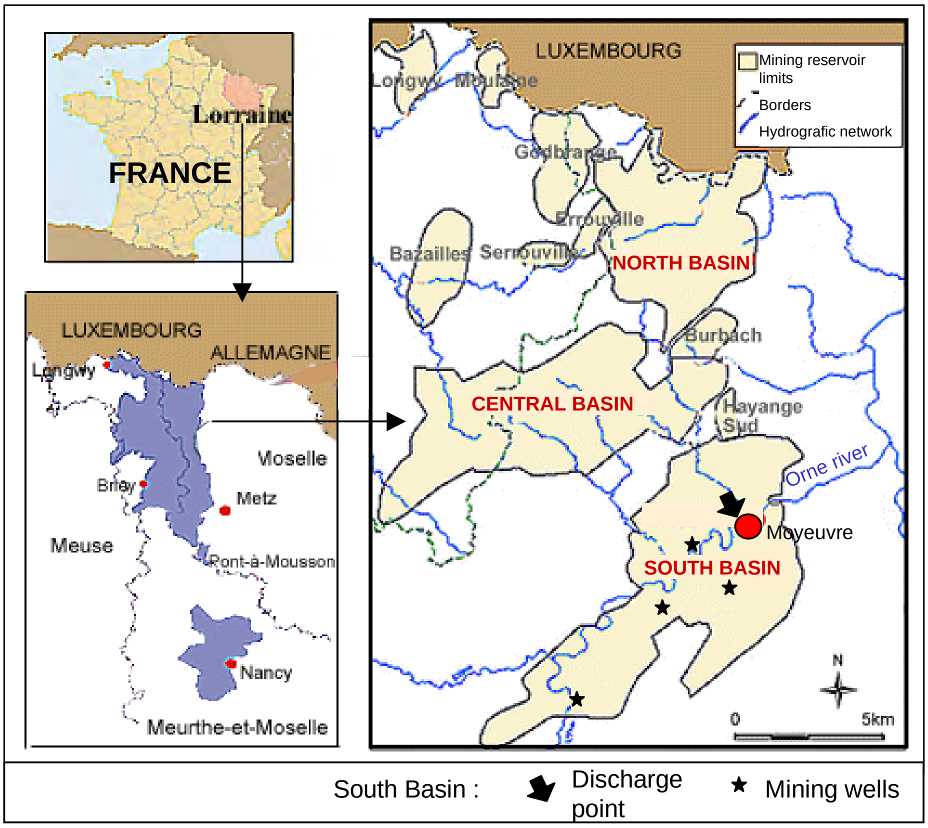

Figure 3. Geographic location of the Lorraine Iron Basin

Dated as Aalenian (Late Lias) the iron-bearing formation overlies Early and Middle Toarcian impermeable deposits. The Lorraine iron-bearing deposit is composed of alternating marly levels (intercalations) and ferruginous limestone (mineralised intervals) corresponding to a regressive sequence. Its thickness varies from 0 to 65 m with an average of 40 m. Nine mineralised intervals, distinguished by their colour, are recognised in the LIB, although generally no more than two were mined in a single concession. In the South basin, five mineralised layers have been mined, named from the bottom up as the green, brown-black, grey, yellow and red layers. The transition from a marly facies to an overlying mineralised facies is gradual via a metre-scale intermediate or "basal" layer. On top of the grey and yellow layers, *i.e.* in the hanging wall, transition into the next overlying marl intercalation occurs via a coarse-grained shelly limestone level known locally as '*crassin*'. The iron-bearing formation is overlain by about 5 m of micaceous marl, followed by a Dogger (Bajocian) limestone succession, some 50-60 m thick, which constitutes a major karstic aquifer. Mining has caused the fracturing and partial destruction of the impermeable level, enabling water from the Dogger limestone aquifer to infiltrate into the mine galleries.

Based on a mineralogical study and tests in closed reactors carried out on rock samples from the North Basin, which is still being mined, three groups of rocks have been differentiated according to their composition and their chemical reactivity in contact with water (Collon, 2003; Collon *et al.*, 2004):

(i) "shelly limestone" or "*crassin*",

(ii) "marly intercalations",

(iii) and "marly hanging wall".

The *crassin* group is composed of the rocks with the lower reactivity - producing less than 200 mg/l of sulphate when in contact with water -: the hanging-wall rocks of the grey and yellow layers and the iron ore. They are both made up of carbonates, quartz and goethite, but in different proportions.

The marly intercalations are characterised by their strong reactivity with water. In addition to the same minerals that make up the *crassin*, they contain pyrite, sulphate (mostly gypsum), phyllosilicates (ferriferous chlorite, illite, kaolinite, and mica), plagioclase and microcline. It is these minerals, and notably gypsum, that explain the degradation of the water quality observed on site (Collon *et al.*, 2004).

The marly hanging walls group is constituted by the hanging walls of the green, brown-black and red layers. Containing smaller quantities of the same minerals as the marly intercalations, they have a slightly lower chemical reactivity.

Two types of mined zones can be distinguished in the South Basin where the room and pillar method was used: the "gallery zones", where the pillars are still standing, and the "collapsed zones" where the pillars have been pulled. In the collapsed zones, the water is in contact with marly intercalations rocks, while it reacts only with *crassin*-type rocks in the galleries in grey and yellow layers. In the green, brown-black and red layers, the hanging-wall rocks react like the marly hanging walls, while the iron ore and basal layer react like the *crassin*. Based on the average dimensions of the galleries we estimate that, in these zones, water is in contact with a "mixed rock" composed by 34% marly hanging wall and 66% *crassin*.

Thus, three types of kinetic chemical reactor have been built. Each of them represents one of the three types of exploited areas encountered in the mine, in which the water reacts with a type of rock:

(i) "crassin" in the galleries zones (grey and yellow layers),

(ii) "marly intercalations" in the collapsed zones,

(iii) "mixed rock" in galleries within marly hanging wall zones.

There are distinguished by the parameters depending on the composition of the rocks which were estimated by laboratory experiments and mineralogical studies (Collon *et al.*, 2004; Collon et al., in press).

2.3. Non-distributed model

In a first step, the South Basin can be considered as a single unit of three parallel reactors, each corresponding to one of the mine zones; i.e. "collapsed" zone, "*crassin* gallery" zone and "gallery with marly hanging wall" zone (figure 4).

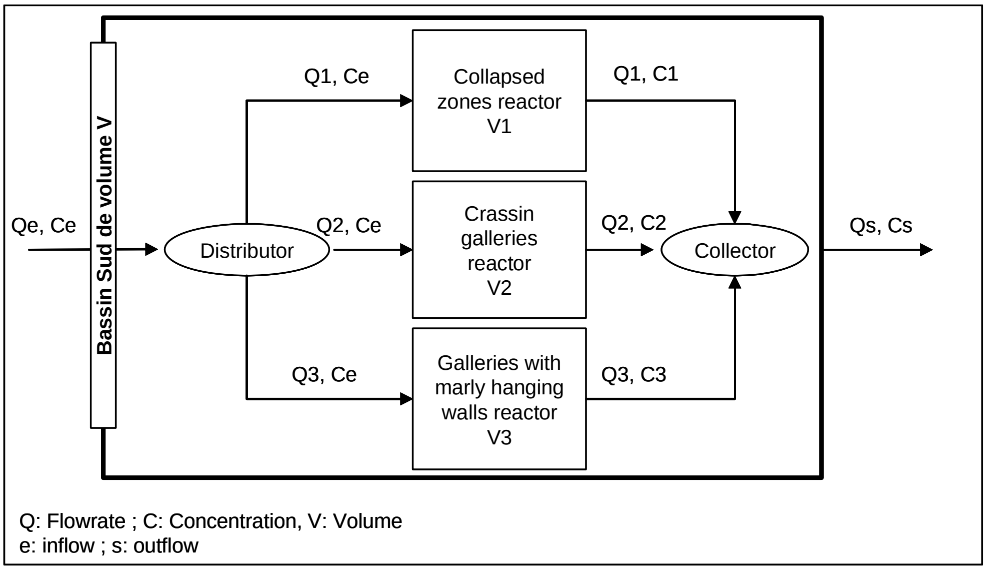

Figure 4. Flow chart of the reactor model of the South Basin

The hydrological model mentioned previously is used to estimate the total volume of water contained in the South Basin ($V = 230\ 10^6\ m^3$) and the total recharge Qe, calculated from 1995 using a daily time step (figure 5a), when the water overflowed through the Moyeuvre tunnel (altitude = 172.5 m above NGF datum). Dewatering water having a composition similar to that of Dogger water, the total inflow Qe entering the system with a concentration Ce is defined as:

$$Qe = Q_{recharge} - Q_{dewatering} \qquad (6)$$

where $Q_{recharge}$ is the estimated recharge and $Q_{dewatering}$ is the dewatering rate measured on site.

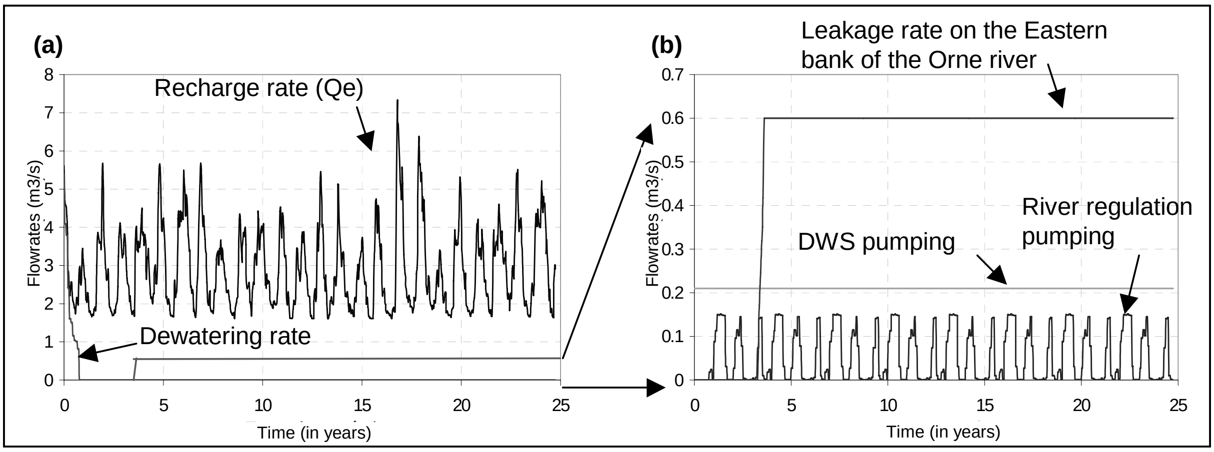

Figure 5. (a) Estimated recharge of and measured dewatering pumping rate in the mine reservoir
(b) Fixed outflow rates : river regulation, leakage, drinking water supply (from Vaute et al., 2004)

Since dewatering has stopped, water is pumped for drinking water supply and river regulation from the flooded parts of the mine. As opposite to the dewatering water, this water is highly mineralised. Thus, it is considered as “outflow” with fixed flow rates in the model. Leaks have also been observed in the alluvial plain below the level of the Moyeuvre tunnel overflow, and they have been estimated at 0.6 m^3/s (Vaute *et al.*, 2004). So, the total outflow rate of the system is defined as:

$$Q_{dis} = Qe - (Q_{DWS} + Q_{reg} + Q_{leak}) \qquad (7)$$

Where Q_{dis} is the discharge rate, Q_{DWS} is the drinking water supply rate, Q_{reg} is the river regulation rate and Q_{leak} is the leakage rate (figure 5b).

For each ore-bearing layer, the zones mined in the galleries and the collapsed zones were digitized with MapInfo® from mine plans of each South Basin concession. Based on these maps, the total mined surface has been estimated to be equal to 138.6 km² comprising 53.6 km² of "*crassin* galleries" (38.7%), 26.5 km² of "galleries with marly hanging walls" (19.1%), and 58.5 km² of "collapsed zone" (42.2%). The volume V_n and the inflow Q_n of each reactor “n” are assumed to be directly proportional to its relative area, *e.q.*: $V_1 = 42.2\%$ V and $Q_1 = 42.2\%$ Q.

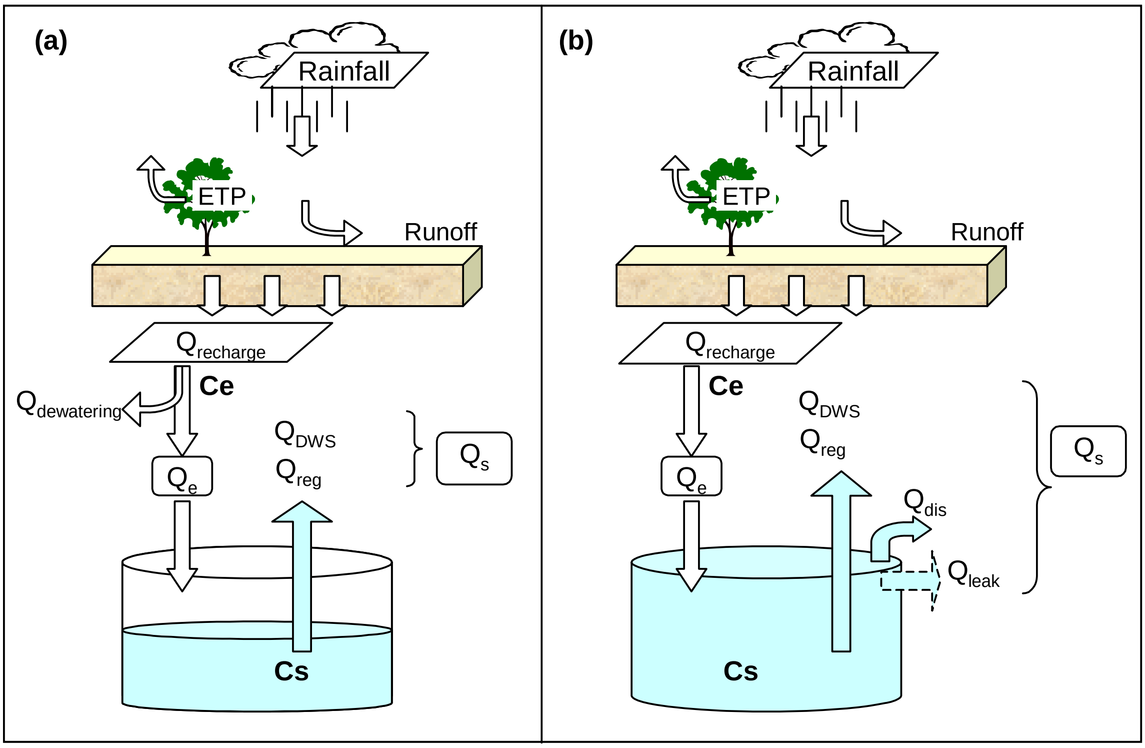

Figure 6. The two phases of hydrological functioning of the reservoir:
(a) filling and (b) overflow (Ci = inflow concentration, Co = outflow concentration)

The flooding of the South Basin mines began on 20/5/1995, date taken as time t = 0. Two phases can be distinguished in the model of the hydrological functioning of the reservoir (figure 6). Indeed, the flooding of the mine workings with no overflow constitutes a transient regime representing the first phase. It ends when the mine workings are full. Then starts the second phase where the mine system overflows.

2.4. Semi-distributed model

The non-distributed model makes it possible to predict the evolution of water quality observed at the overflow point, in the Tunnel of Moyeuvre. But, it gives no information on the spatial distribution of the chemical concentrations in the Basin groundwater. As chemical monitoring of water quality is available at four wells of the South Basin, we developed a semi-distributed model to evaluate the accuracy of the NCR in accounting for the spatial variability of the concentrations.

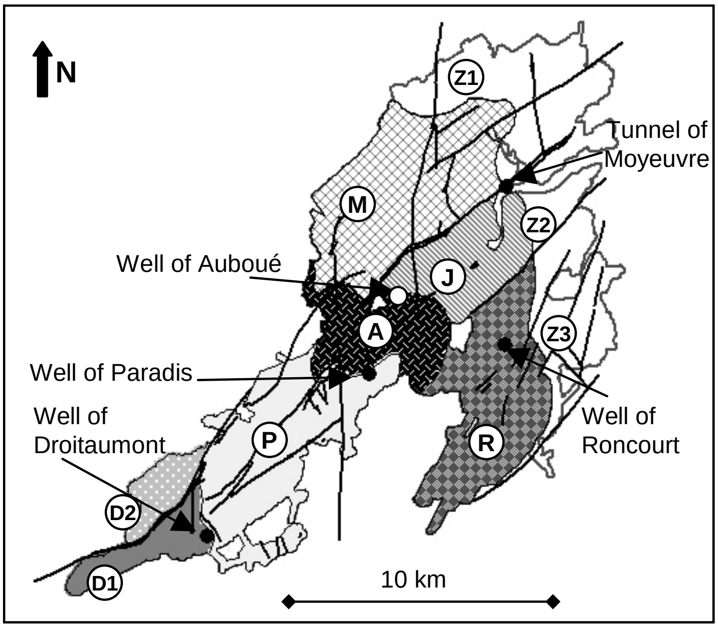

Figure 7. Breakdown of the South Basin into sectors: (D1) Droitaumont 1, (D2) Droitaumont 2, (P).Paradis, (A) Auboué, (R) Roncourt, (J) Joeuf, (M) Moyeuvre; Z1, Z2 and Z3: non-flooded areas.

Seven sectors have been delimited in the South Basin: Droitaumont 1 and 2, Paradis, Auboué, Roncourt, Joeuf and Moyeuvre (figure 7). For three sectors - Droitaumont 1, Paradis and Auboué – the geographical limits have been established in accordance with the mine topography. Major structural faults delimit the other zones, while the overflow level separate the Z1, Z2 and Z3 sectors, located above, from Roncourt, Joeuf and Moyeuvre, located below.

Table 2. Characteristics of the seven areas (S_{basin} = 159 km²)

Sectors	**Symbol**	**S_{rel} (%)**	**V_{sector} (m^3)**
Droitaumont 1	D1	4.2 %	8.46 10^6
Droitaumont 2	D2	3.0 %	6.24 10^6
Paradis	P	16.8 %	4.16 10^7
Auboué	A	8.3 %	2.44 10^7
Roncourt	R	14.6 %	4.8 10^7
Joeuf	J	8.5 %	3.68 10^7
Moyeuvre	M	19.2 %	7.17 10^7
Z1		14.2 %	non-flooded*
Z2		2.3 %	non-flooded*
Z3		8.9 %	non-flooded*

* Located above the overflow altitude (172 m NGF), these zones will never be flooded.

Considering that the inflow rate Qe is the result of the rain flow infiltration through the Dogger limestone, the total recharge in each sector is supposed to be proportional to its relative surface area S_{rel} (table 2): $Q_{sector} = S_{rel} \times Qe$. The volume in each sector is assumed to be proportional to the distribution of total exploited surface area (E_{total} = 139 km²) in each sector (E_{sector}): $V_{sector} = E_{rel} \times V$ (table 2).

Each sector is represented as a unit of three parallel reactors (one reactor for each type of mining zone), similar to those used for the non-distributed model.

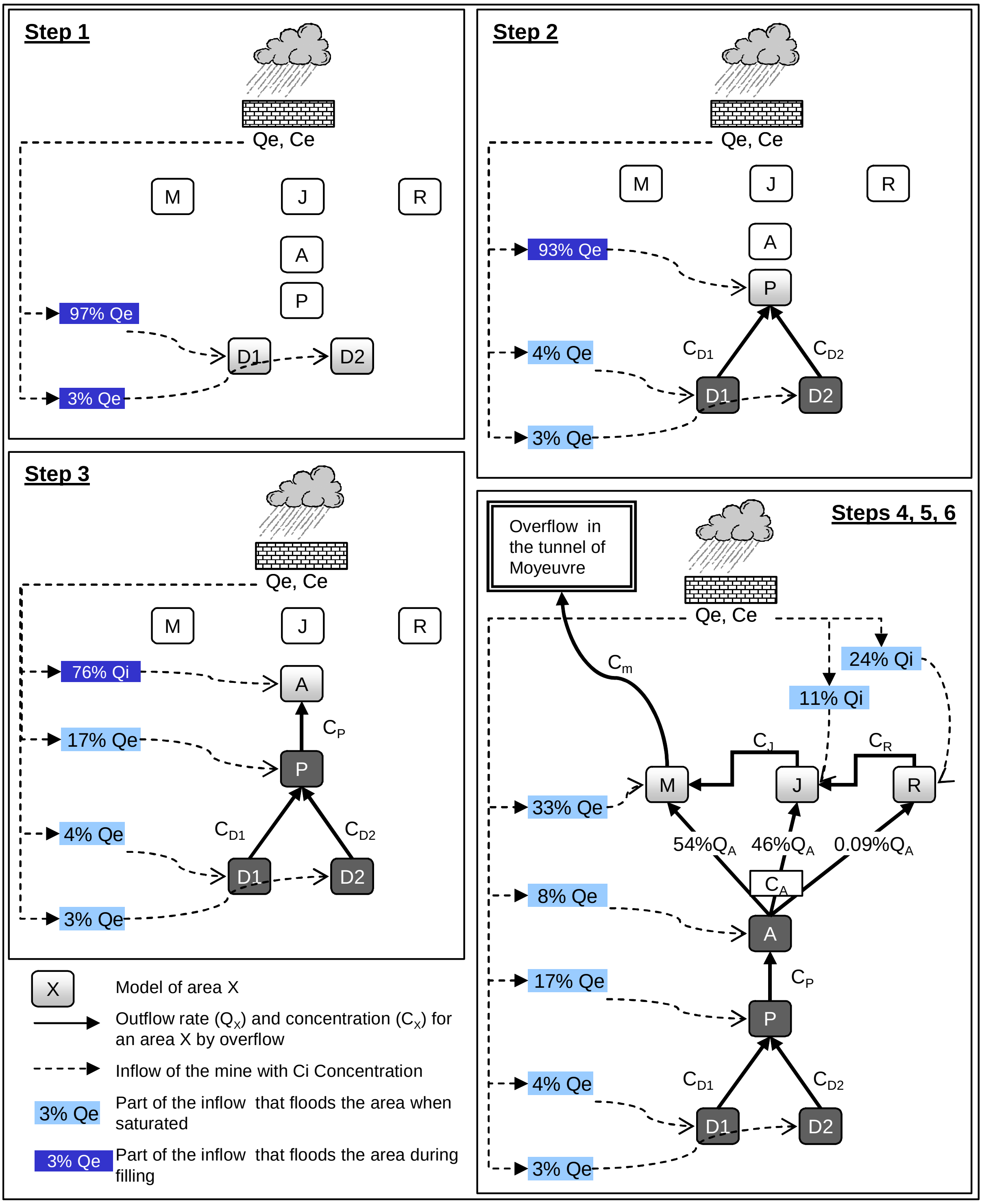

Figure 8. Schematic diagram of the hydraulic flow in the South Basin (Collon *et al.*, 2005)

The hydrological functioning of the mine is split into six phases detailed in the figure 8. Considering gravity, the rainfall water is assumed to be drained by the upper sectors towards the lower sectors. Due to the short transfer times, the initial chemical composition is not modified and remind close to the Dogger water. Thus, in the first phase Droitaumont 1 receives 97% of the inflow rate, while Droitaumont 2, less hydraulically connected to the fellow sectors, is only recharged by the rainfall on its surface area (3%Qe). Once a sector N is flooded, it overflows in the upper sector with a new composition C_N. The flooded sectors only receive the rainfall water in proportion to their relative surface area, while the sector in “the flooding phase” drains the upper sectors. Located at the same depth, Moyeuvre, Joeuf and Roncourt start to fill up at the same time, when Auboué is saturated. They receive a part of Auboué overflow that is proportional to the surface contact they share with this sector. The water drained by the unflooded upper zones - Z1 for Moyeuvre, Z2 for Joeuf and Z3 for Roncourt – adds to the rainfall water that fall on their surface and recharges this sectors. The observed leakage rate is included as an imposed outflow rate for the Moyeuvre sector.

3. Results and discussion

At mine scale, the reference rock mass M_R (on the basis of 1 litre of associated water) and the average granulometry G_R of the rocks are unknown. Depending only on the mining method used, these two parameters are assumed to be identical for both the "crassing galleries" and the "galleries with marly hanging walls". They were determined by fitting the SO_4 concentration simulated with the non distributed model to the SO_4 concentration measured during the first three years at the overflow (table 3).

Table 3. Rock mass, M_R, and average granulometry, G_R, determined by fitting of simulated SO_4 concentrations and those measured at the overflow

	G_R (m)	M_R (kg)
Galleries	0.2	3.5
Collapsed zones	0.4	4

The concentrations simulated with the non-distributed model are in good agreement with the evolution observed at the Tunnel of Moyeuvre of the Na, Ca, Mg and HCO_3 concentrations, the pH, and the SO_4 concentration after the first three years used for fitting (figure 9). These results show that the non-distributed model can predict the evolution of water quality observed at the overflow of the South Basin for the major elements SO_4, Na, Ca, Mg and HCO_3 with a precision of ± 10% and it provides an order of magnitude for minor elements such as K. Thus, as observed in the older abandoned iron-ore mines of the LIB, it appears that the quality of the water at the overflow point will progressively improve with the leakage of the rocks, and will reach again, after several years, the authorized concentrations for human consumption.

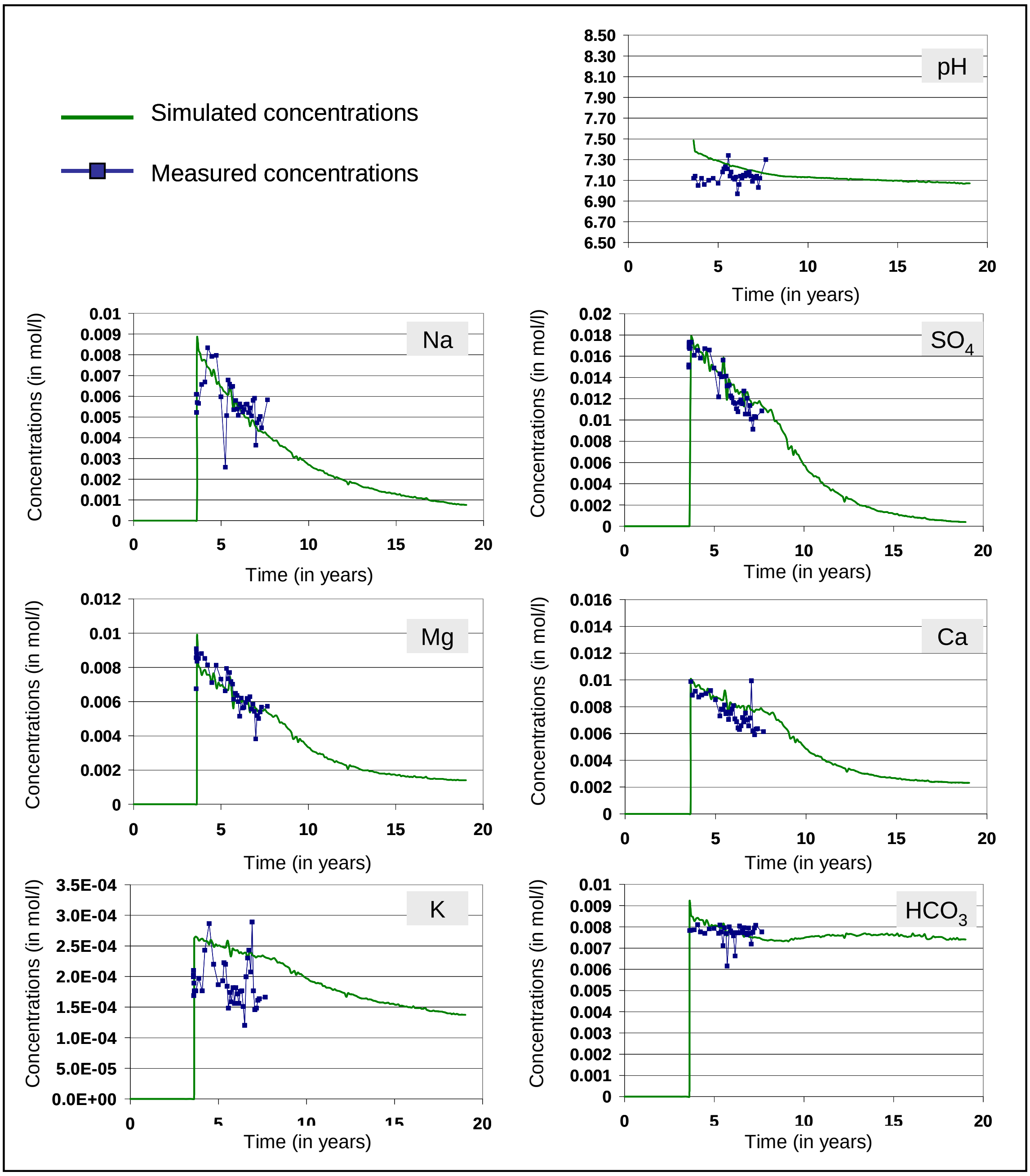

Figure 9. Simulated and measured concentrations at the overflow of the South Basin

The results of the semi-distributed model are more variable (figure 10). The evolution of pH and HCO_3 are always well reproduced, probably due to the buffer action of the CO_2 pressure and the presence of carbonates. Furthermore, the simulated concentration of minor elements such as K falls always within the range of possible maximum and minimum concentrations calculated by our model. Considering the major elements SO_4 (figure 10), Ca, Mg and Na, the concentrations are well reproduced in Roncourt, Auboué and at the overflow point in Moyeuvre. In Auboué, the high fluctuations of the observed concentrations correspond to important rainfall and could be explained by a poor impermeability of the well. The delay between the increase of calculated and observed concentrations in Roncourt is due to an artefact. Indeed, as the well is located in the middle-level, the sector starts to fill up and shows positive concentrations, even though the well is still above the water level. For the others sectors, the wells are located at the outflows of the sectors and the concentrations are represented when the sectors are flooded. In Droitaumont and in Paradis, the observed concentrations are a lightly underestimated. Despite the orders of magnitude of the observed concentrations being correctly reproduced, this shows the limits of the approach: the positions of the wells and the effective hydraulic connections have not been taken into account. Indeed, the well of Paradis is located in a collapsed zone where three layers have been exploited, but only one (the grey layer) is connected with surrounding concessions. This can produce a hydraulic confinement of the well, not taken into account in the model.

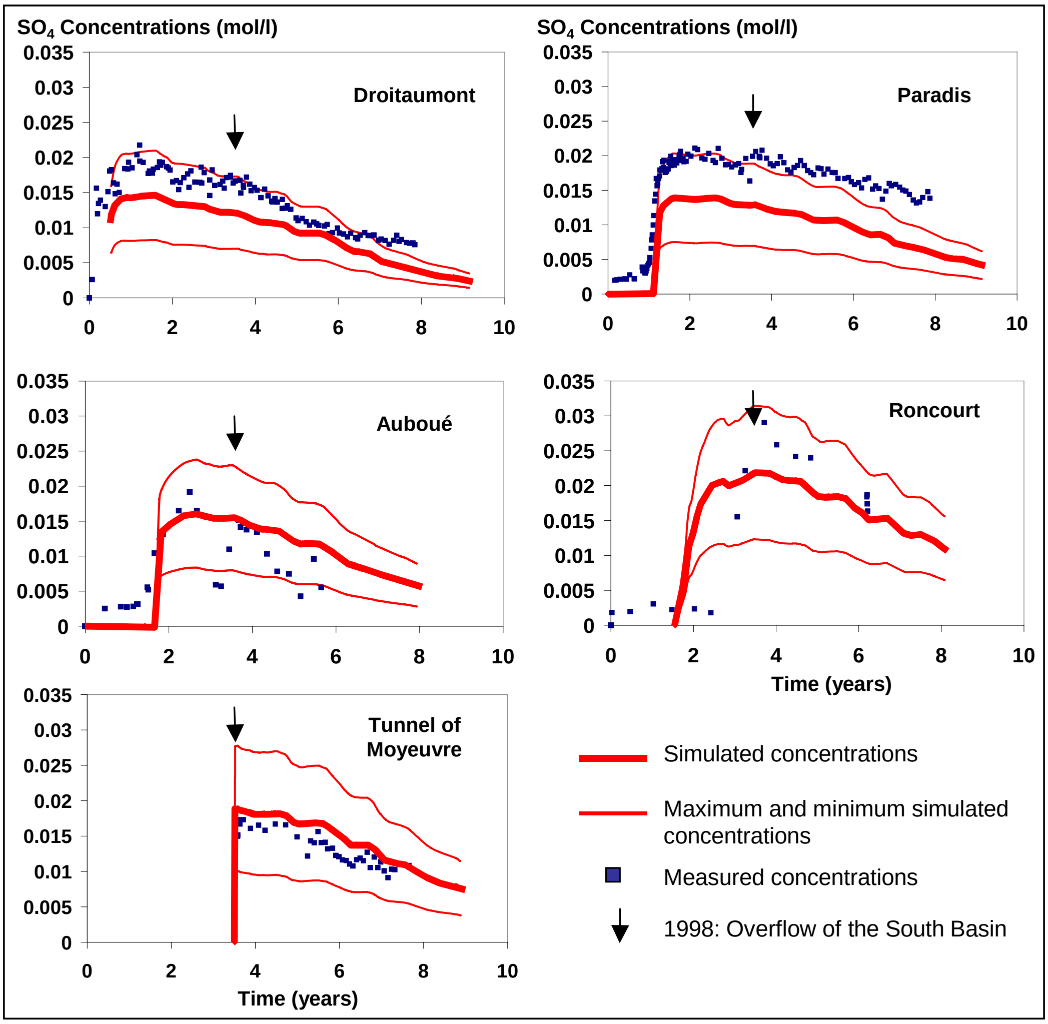

Figure 10. Measured and simulated SO_4 concentrations in the four wells and at the overflow point of the South Basin.

Thus, the global modelling based on a NCR approach (Network of Chemical Reactors) is an interesting approach to predict the evolution of water quality at the overflow. It accounts for the large-scale homogeneity of the South Basin, and characterises the convergence towards the overflow of the water coming from different areas of the mine workings and its mixing near this point. Although encouraging, the results of the semi-distributed model show the need to specify the spatial organisation of water flow in the reservoir in order to reproduce the evolution of chemical concentrations in the different monitored wells.

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