GOVERNING EQUATIONS FOR ACID WATER
IN CANALS

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SUMMARY. It is given in this study governing equation system formulation for acid water
movement in canals, especially, in the Plain of Reeds of Vietnam where the jurbanite equilibr ium
is found dominant. It is assumed in the model a chemical equilibrium, however a kinetic treatment
is also used to deal with redissolution of precipitates and sedimentation.

1. INTRODUCTION

An estimated 1.8 million hectares or approximately 45 percent of the Mekong Delta in Vietnam
is covered by acid sulphate soils. It is a problem to put these soils to productive use.

In the parts of Mekong Delta acidity in the surface water is a particular problem at the
beginning of the rainy season. During the dry season acidity is formed in the soils and moves up
to field surface, the first rains of the rainy season wash the formed acidity in high concentrations
to the canal system.

The physical, chemical and biological processes which control the movement of substances in
canals and in soils are many and quite complicated. For canal water, some of the physical proces­
ses involved are longitudinal, lateral and vertical dispersion, advection, sedimentation. Chemical
processes comprise ionic exchange, hydrolysis, oxidation-reduction, precipitation and adsorption.
These processes are all directly or indirectly affected by hydro-meteorological parameters such as
rainfall, run-off, temperature, evaporation and wind etc. Quantitative models for each of the pro­
cesses above are very complex. Therefore there exists a number of approaches using deterministic
and stochastic simulation but the selection will of course depends on the specific application en­
visaged. In spite of the difficulties involved much work has been carried out on the construction of
deterministic canal water quality models because of their usefulness not only as an aid to a better
understanding of the processes involved but also as a practical management tool.

Regarding water quality for the Mekong Delta so far there are two on-going projects and one
major objective of these projects is to develop a mathematical model to simulate and predict the
movement of acid water in the canal network. One important step is to establish the equations
governing the physico-chemical processes of the concerned phenomena. That also is the content of
the study presented below.

2. ACID WATER IN CANALS

Physically, the mechanism of genesis of acidity has been mentioned in many references [1, 12, 13]. Basically, throughout the dry season the products of oxidation of pyrite and movement
of acidity from the subsoil increases the acidity in the topsoil. Moreover, due to agriculture
development a number of new canals or dykes are built. At the beginning of the rainy season
whenever plains are inundated, acid products from the plains or from excavated dykes are released
to canals and spread into other areas. Physico-chemical and biological processes involved in acid water and the role of the different processes varies with each specific situation.

2.1. On characteristic parameters for acid water in the Plain of Reeds of Vietnam

pH of water is used to characterize the acidity situation. Many studies on soil and canal water chemistry show that in the acid water there exists a relationship between pH and some main species such as aluminum, iron, sulphate ... expressed by so-called mass action law for certain equilibria (e.g. jurbanite or gibbsite).

- Based on chemical data analysis of measurement campaigns carried out in 1985-1987 in the Plain of Reeds Tin [4] concludes that pH, Al and SO$_4$ concentrations are in equilibrium with jurbanite Al(OH)$_3$ and pH$_2$SO$_4$.

- From statistical analysis of experimental data collected in Tan Thanh Farm (in the Plain of Reeds) it is also concluded in [5] that there exists a good linear relationship between pH and pH$_{Al(OH)3}$ or pH$_{SO_4}$.

- A linear expression between pH, Aluminum and sulphate have also been found in [1, 2, 3].

It should be noted, however, that regression analyses of relations involving ion activity products must be interpreted with care.

Provided jurbanite equilibrium exists then for the Plain of Reeds the following condition can be used to simulate acidity situation

$$H.Su \frac{dAl}{dt} + H.Al \frac{dSu}{dt} - Al.Su \frac{dH}{dt} = 0$$

or

$$pH = pSu + pAl + d \quad (pH = \log_{10}H)$$

(2.2)

in which $d$ is given constant and actual concentrations of aluminum, sulphate, hydrogen ions at certain point $(x, y, z, t)$ now

2.2. Three-dimensional governing equations

Mass balance for aluminum, sulphate and hydrogen in three-dimensional case yields the following equations (neglecting molecular and turbulent diffusive process).

$$\frac{dAl}{dt} = -(q + Q_s + Q_r)Al + (q.Al + Q_s.Al') - P_{Al} - D_{Al}$$

(2.3)

$$\frac{dSu}{dt} = -(q + Q_s + Q_r)Su + (q.Su + Q_s.Su') - P_{Su} - D_{Su}$$

(2.4)

$$\frac{dH}{dt} = -(q + Q_s + Q_r)H + (q.H + Q_s.H') - P_{H} - D_{H}$$

(2.5)

where:

- $P_{Al}$, $P_{Su}$, and $P_{H}$ are amount of Al, Su, and H respectively, lost or gained by precipitation or redissolution from bottom.

- $D_{Al}$, $D_{Su}$, and $D_{H}$ are amount of Al, Su, and H lost by sedimentation, respectively.

- $q$ is lateral inflow (pumping, drainage etc).

- $Q_s$ is exchange inflow between plain and canal or from underground water.

- $Q_r$ is rainfall.

- $Al'$, $Su'$, $H'$ are concentrations of Al, Su, H respectively in flow $q$.

- $Al^t$, $Su^t$, $H^t$ are concentrations of Al, Su, H respectively .

- The matter derivative is defined by

$$\frac{d}{dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z}$$
where \( u, v, w \) are velocity components in the \( x, y, z \) directions, respectively.

It is understood that in aqueous media the equilibrium equation for jurbanite is as follows [11, 12, 13];

\[
\text{Al(OH)SO}_4 + H^+ \rightleftharpoons \text{Al}^{3+} + \text{SO}_4^{2-} + H_2O
\]

so the following relationship can be established:

\[
\begin{align*}
P_{Al} &= P_{Su} \\
P_H + P_A &= 0 \\
D_{Al} &= D_{Su} = D_H
\end{align*}
\]

Denote

\[
\begin{align*}
a &= H_Su; & b &= H_A; & c &= Al_Su \\
\sigma &= q + Q_s + Q_A; & \Phi_1 &= q \cdot Al^s + Q_A Al^i \\
\Phi_2 &= qS u^s + Q_s Su^i; & \Phi_3 &= q H^s + Q_s H^i
\end{align*}
\]

It is assumed that the rate of loss of the substance by sedimentation is linearly proportional to actual concentration [9, 10],

\[
D_A = L' Al (L' \text{ is a proportional coefficient})
\]

Taking into account (2.6), (2.7), (2.8), and (2.9) with new symbols the equations (2.3) - (2.5) can be rewritten as:

\[
\begin{align*}
\frac{dAl}{dt} &= -\sigma Al + \Phi_1 - P_A - L' Al \\
\frac{dSu}{dt} &= -\sigma Su + \Phi_2 - P_A - L' Al \\
\frac{dH}{dt} &= -\sigma H + \Phi_3 + P_A - L' Al
\end{align*}
\]

\[
\frac{dAl}{dt} + b \frac{dSu}{dt} - c \frac{dH}{dt} = 0
\]

Denote: \( L = 2L' \)

\[
\begin{align*}
\alpha &= a + b + c; & \beta &= \frac{b}{r}; & \tau &= \frac{c}{r}
\end{align*}
\]

After some transformations the following equations can be established:

\[
\begin{align*}
\frac{dAl}{dt} &= -\sigma_1 Al + F_1 \\
\frac{dSu}{dt} &= -\sigma_2 Su + F_2
\end{align*}
\]

where:

\[
\begin{align*}
\sigma_1 &= \sigma (\alpha + r) + rL; & \sigma_2 &= \sigma (\alpha + r) + rL \\
F_1 &= \beta \sigma Su - \tau \sigma H + (\tau + \beta) \Phi_1 + \tau \Phi_2 - \beta \Phi_2 \\
F_2 &= \alpha \sigma Al - \tau \sigma H + (\alpha + \tau) \Phi_2 + \tau \Phi_3 - \alpha \Phi_1
\end{align*}
\]

From (2.13) the following similar equation for \( H \) can be obtained
\[
\frac{dH}{dt} = a.F_1 + b.F_2 - a.A_1 - b.A_2 Su
\]  

(2.18)

Once Al, Su are given by solving (2.16) and (2.17), the pH distribution is then computed by the following furbaneite equilibrium relation:

\[
pH = d + pAl + pSu
\]  

(2.19)

with \( pH = -\log_{10} H \) or \( H = 10^{-pH} \) or using the solution of (2.18) but this procedure will be more complicated and consume the computer time and on the other hand with (2.19) we can consider \( d \) as a model calibration parameter. For the Plain of Reeds, according to the Water Quality Laboratory od Sub-Institute for Water Resources Planning and Management \( d = -2.8 \). Because equilibrium constant is a function of some factors such as temperature, so value of \( d \) must be adjusted according to observed data.

2.3. Governing equations for one-dimensional case

The one-dimensional mass transfer equation can be obtained by direct integration of the three-dimensional equations over a cross-section \( A \) normal to the axis of the canal (see [8] for more details).

Equation (2.16), (2.17) and (2.18) are in the same form of the following partial differential equation

\[
\frac{\partial C_i}{\partial t} + u \frac{\partial C_i}{\partial x} + v \frac{\partial C_i}{\partial y} + w \frac{\partial C_i}{\partial z} = -n.C_i + m
\]  

(2.20)

\( Al, Su, H \) correspond to \( i = 1,2,3 \) respectively; \( n \) and \( m \) are functions of \( C_i \).

We define:

\[
\begin{align*}
    u &= U + u' \quad v = v' \quad w = w' \\
    C_i &= C_i' + c_i'' \quad n = n' + n'' \quad m = m' + m''
\end{align*}
\]  

(2.21)

where

\[
U = \frac{1}{A} \int u dA \quad \text{and} \quad C_i = \frac{1}{A} \int C_i dA
\]

are the real time longitudinal velocity and concentration, respectively, averaged over the cross-section. \( n' \) and \( m' \) are cross-section averaged values of \( n \) and \( m \).

Substituting (2.21) into (2.20), after simplification the one-dimensional equation may be written as:

\[
\frac{1}{A} \frac{\partial (AC_i')}{\partial t} + \frac{1}{A} \frac{\partial (AUC_i')}{\partial x} + \frac{1}{A} \frac{\partial }{\partial x} \int u'c_i'' dA = -n'C_i' + m' + \phi
\]  

(2.22)

where

\[
\phi = \frac{1}{A} \int (m'' - n''c_i') dA
\]

the third term on the left side is usually designated as the longitudinal dispersion. For steady uniform flow, Taylor and Aaris have been shown that the advective mass transport associated with the cross product of \( u' \) and \( c_i'' \) can be expressed as an analogous one-dimensional diffusive transport. On this basis a coefficient of dispersion \( E \) is defined in term of the concentration gradient as

\[
\int_A u'c_i'' dA = -A.E \frac{\partial C_i'}{\partial x}
\]  

(2.23)
The negative sign indicates mass transport in the direction of decreasing concentration. With this definition (2.22) becomes

\[
\frac{\partial (\Delta C'_1)}{\partial t} + \frac{\partial}{\partial x} (AU C'_1) = \frac{\partial}{\partial x} \left( A E \frac{\partial C'_1}{\partial x} \right) - n' A C'_1 + m' A + \phi
\] (2.24)

using the following equation of Saint-Venant system

\[
\frac{\partial A}{\partial t} + \frac{\partial (A U)}{\partial x} = q + Q_s + Q_r
\]

and the expansion of dispersion term, equation (2.24) becomes

\[
\frac{\partial C'_1}{\partial t} + \left( U - \frac{1}{A} \frac{\partial (EA)}{\partial x} \right) \frac{\partial C'_1}{\partial x} = E \frac{\partial^2 C'_1}{\partial x^2} - \Theta C'_1 + \delta_1
\]

or

\[
\frac{\partial C'_1}{\partial t} + U(1 + \mu) \frac{\partial C'_1}{\partial x} = E \frac{\partial^2 C'_1}{\partial x^2} - \Theta C'_1 + \delta_1
\] (2.25)

here \( \Theta > 0, \mu \) is considered as an adjusted parameter during flow calibration. It should be noted that due to the nonlinearity of \( n \) and \( m \) in (2.20), parameter \( \delta_1 \) must be approximately estimated (or linearized) by the previously defined values of concentrations and can be considered as an adjusted parameter during solute calibration. (2.25) is the general form which can be applied to any species \( A_1, S_1, ... \) mentioned above. It is also noted that for hydrogen we can apply (2.25) or use (2.19) in the form:

\[
A_1 S_1 = r_1 H \quad \text{with} \quad r_1 = 10^4
\] (2.26)

if the same average procedure is used then (2.26) becomes

\[
A'_1 S'_1 + \varepsilon = r_1 H'
\] (2.27)

where

\[
\varepsilon = \frac{1}{A} \int_A A_1 '' S_1'' dA
\]

which may not be small in real situation.

3. OUTLINE OF NUMERICAL PROCEDURE FOR THE CASE OF ONE DIMENSION WITH LONGITUDINAL DISPERSION

For simplicity the prime to denote concentrations in case of one dimension will be eliminated. Apply (2.25) for aluminum hydrogen and sulphate the following equations can be obtained

\[
\frac{d A}{d t} = E \frac{\partial^2 A}{\partial x^2} - \frac{\sigma}{A} A + \frac{\phi}{A} - P_{A1} - D_{A1} + \delta_1
\] (3.1)

\[
\frac{d S}{d t} = E \frac{\partial^2 S}{\partial x^2} - \frac{\sigma}{A} S + \frac{\phi}{A} - P_{S1} - D_{S1} + \delta_2
\] (3.2)

\[
\frac{d H}{d t} = E \frac{\partial^2 H}{\partial x^2} - \frac{\sigma}{A} H + \frac{\phi}{A} - P_{H} - D_{H} + \delta_3
\] (3.3)

where \( E \) - longitudinal dispersion; other symbols are similar to those mentioned in (2.3) - (2.5). The matter derivative now is denoted by

\[
\frac{d}{d t} = \frac{\partial}{\partial t} + U(1 + \mu) \frac{\partial}{\partial x}
\]
Using the symbols:

\[ N = S_u - A_l, \quad S = S_u + H \]
\[ f_1 = \delta_2 - \delta_1 + (\psi^2 - \psi^1)/A \]
\[ f_2 = \delta_2 + \delta_3 + (\psi^2 + \psi^3)/A \]

from (3.1) - (3.3) it follows:

\[ \frac{dN}{dt} = E \frac{\partial^2 N}{\partial x^2} - \sigma N + f_1 \]  
(3.4)
\[ \frac{dS}{dt} = E \frac{\partial^2 S}{\partial x^2} - (\sigma + L) S + f_2 \]  
(3.5)

(3.4) and (3.5) are in the general form:

\[ \frac{df}{dt} = E \frac{\partial^2 f}{\partial x^2} - k_1 f + k_2 \]  
(3.6)

which during one time step can be solved by the following fraction step method: firstly the one-dimensional hyperbolic equation:

\[ \frac{df}{dt} = -k_1 f + k_2 \]  
(3.7)

of which the solutions along characteristic lines \( dX/dt = U(1 + \mu) \) are

\[ C = (C_0 - k_2/k_1) \exp(-k_2 \cdot t) + k_2/k_1 \]

where \( C_0 \) is the value of \( C \) defined at the previous time step. It is noted that due to \( L > 0 \), \( k_1 \neq 0 \).

The second step is followed by solving the following pure dispersion:

\[ \frac{\partial h}{\partial t} = E \frac{\partial^2 h}{\partial x^2} \]  
(3.8)

the solutions of (3.8) are the solutions of (3.6) during a time step.

The mass action equation now is used in the form of (2.27):

\[ A_l S_u + \varepsilon = \tau_1 H \]  
(3.9)

using (3.3), (3.9) becomes

\[ S_u^2 + (\tau_1 - N) S_u - \tau_1 S + \varepsilon = 0 \]  
(3.10)

If \( \varepsilon = 0 \) (3.10) is an algebraic equation of second order for which it is easy to find solutions of \( S_u \) and hence, from (3.3), \( A_l \) and \( H \) or \( pH \) can be computed.

4. DISCUSSIONS

Above are main points of governing equation formulation for mathematical simulation of acid water in canal or river under different meteo-hydrological conditions. It should be noted that some assumptions are made in deriving the equations. Although a number of studies on mineral equilibria and solute transport in soil columns has been carried out but the considerations of acid water in canals are still too few. The above mentioned points are first attempts to account the influence of precipitation, redissolution and settling due to sedimentation on the processes taking
place in the acid water. It is also obvious that, physically, acid water is a quite complex process, more man power, material and much effort need to be invested for this problem.

ACKNOWLEDGEMENTS

This study was founded in part by the Fundamental Research Program under code 2.2.1. Author wishes to express his gratitude to Prof. Erik Eriksson from AB Hydroconsult, Sweden for his oriented guidance on water chemistry and helpful discussions. Thanks are due to Dr. N.V.Gia for his useful comments and anyone, unnamed here, who has directly or indirectly helped the author in carrying out this study.

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Received October 30, 1993

HỆ PHƯƠNG TRÌNH CƠ BẢN TRONG MÔ PHƠNG NUOC CHUA PHEN TRÊN KENH SÔNG

Sự hình thành và lan truyền nước chưa phân trên kênh sông bị chi phối bởi các quá trình hóa lý và sinh học khác nhau như hóa tan, kết tủa, tảo, khuyêch tan,... những chúng vận chuyển theo các lưu cạn bằng nhat nhất. Trong nghiên cứu này trình bày cách thu nhận hệ phương trình cơ bản sự dụng để mô phỏng nước chưa phân trong kênh sông với căn bằng Jurbanite là căn bằng chất yêu cho nước kênh Đồng Tháp Mười dòng bằng sông Cửu Long. Mặc dù sự dụng lưu cạn bằng những quá trình dòng hộc cũng được xem xét. Trong nghiên cứu cũng thảo luận cách giải số cho trường hợp một chiều.