

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 equilibrium 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 processes 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 processes 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 envisaged. 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 $AlOHSO_4$.

- 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 $pAl(OH)_3$ and pH_2SO_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

$$H.Su \frac{dAl}{dt} + H.Al \frac{dSu}{dt} - Al.Su \frac{dH}{dt} = 0 \quad (2.1)$$

$$\text{or } pH = pSu + pAl + d \quad (pH = \log_{10}H) \quad (2.2)$$

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).

$$\frac{dAl}{dt} = -(q + Q_s + Q_r)Al + (q.Al^q + Q_s.Al^i) - P_{Al} - D_{Al} \quad (2.3)$$

$$\frac{dSu}{dt} = -(q + Q_s + Q_r)Su + (qSu^q + Q_s.Su^i) - P_{Su} - D_{Su} \quad (2.4)$$

$$\frac{dH}{dt} = -(q + Q_s + Q_r)H + (qH^q + Q_s.H^i) - P_H - D_H \quad (2.5)$$

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^q , Su^q , H^q are concentrations of Al, Su, H respectively in flow q .

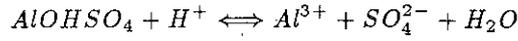
- Al^i , Su^i , H^i are concentrations of Al, Su, H respectively.

- The matter derivative is defined by

$$\frac{d..}{dt} = u \frac{\partial ..}{\partial x} + v \frac{\partial ..}{\partial y} + w \frac{\partial ..}{\partial z} + \frac{\partial ..}{\partial t}$$

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];



so the following relationship can be established:

$$P_{Al} = P_{Su} \quad (2.6)$$

$$P_H + P_{Al} = 0 \quad (2.7)$$

$$D_{Al} = D_{Su} = D_H \quad (2.8)$$

Denote

$$a = H.Su; \quad b = H.Al; \quad c = Al.Su$$

$$\sigma = q + Q_s + Q_r; \quad \Phi_1 = q.Al^q + Q_s.Al^i$$

$$\Phi_2 = qSu^q + Q_s.Su^i; \quad \Phi_3 = qH^q + Q_s.H^i$$

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

$$D_{Al} = L'.Al \quad (L' \text{ is a proportional coefficient}) \quad (2.9)$$

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:

$$\frac{dAl}{dt} = -\sigma.Al + \Phi_1 - P_{Al} - L'.Al \quad (2.10)$$

$$\frac{dSu}{dt} = -\sigma.Su + \Phi_2 - P_{Al} - L'.Al \quad (2.11)$$

$$\frac{dH}{dt} = -\sigma.H + \Phi_3 + P_{Al} - L'.Al \quad (2.12)$$

$$a \frac{dAl}{dt} + b \frac{dSu}{dt} - c \frac{dH}{dt} = 0 \quad (2.13)$$

$$\text{Denote: } L = 2L' \quad (2.14)$$

$$r = a + b + c; \quad \alpha = \frac{a}{R}; \quad \beta = \frac{b}{r}; \quad \tau = \frac{c}{r} \quad (2.15)$$

After some transformations the following equations can be established:

$$\frac{dAl}{dt} = -\sigma_1.Al + F_1 \quad (2.16)$$

$$\frac{dSu}{dt} = -\sigma_2.Su + F_2 \quad (2.17)$$

where:

$$\sigma_1 = \sigma(\alpha + \tau) + \tau L; \quad \sigma_2 = \sigma(\alpha + \tau) + \tau L$$

$$F_1 = \beta\sigma.Su - \tau\sigma.H + (\tau + \beta)\Phi_1 + \tau\Phi_3 - \beta\Phi_2$$

$$F_2 = \alpha\sigma.Al - \tau\sigma.H + (\alpha + \tau)\Phi_2 + \tau\Phi_3 - \alpha\Phi_1$$

From (2.13) the following similar equation for H can be obtained

$$c \frac{dH}{dt} = a.F_1 + b.F_2 - a.\sigma_1.AI - b.\sigma_2.Su \quad (2.18)$$

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

$$pH = d + pAl + pSu \quad (2.19)$$

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 of 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 intergration 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

$$\frac{\partial C_i}{\partial t} + u \frac{\partial C_i}{\partial x} + v \frac{\partial C_i}{\partial y} + w \frac{\partial C_i}{\partial z} = -n.C_i + m \quad (2.20)$$

AI, Su, H correspond to $i = 1, 2, 3$, respectively; n and m are functions of C_i .

We define:

$$\begin{aligned} u &= U + u'; & v &= v'; & w &= w'; \\ C_i &= C_i' + c_i''; & n &= n' + n''; & m &= m' + m'' \end{aligned} \quad (2.21)$$

where

$$U = \frac{1}{A} \int_A u dA \quad \text{and} \quad C_i' = \frac{1}{A} \int_A C_i dA$$

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:

$$\frac{1}{A} \frac{\partial (AC_i')}{\partial t} + \frac{1}{A} \frac{\partial}{\partial x} (AU C_i') + \frac{1}{A} \frac{\partial}{\partial x} \int_A u' c_i'' dA = -n' C_i' + m' + \phi \quad (2.22)$$

where

$$\phi = \frac{1}{A} \int_A (m'' - n'' c_i'') dA$$

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'' 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

$$\int_A u' c_i'' dA = -A.E. \frac{\partial C_i'}{\partial x} \quad (2.23)$$

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

$$\frac{\partial(AC'_i)}{\partial t} + \frac{\partial}{\partial x}(AUC'_i) = \frac{\partial}{\partial x}\left(AE\frac{\partial C'_i}{\partial x}\right) - n'.A.C'_i + m'.A + \phi \quad (2.24)$$

using the following equation of Saint-Venant system

$$\frac{\partial A}{\partial t} + \frac{\partial(AU)}{\partial x} = q + Q_s + Q_r$$

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

$$\frac{\partial C'_i}{\partial t} + \left(U - \frac{1}{A}\frac{\partial(EA)}{\partial x}\right)\frac{\partial C'_i}{\partial x} = E\frac{\partial^2 C'_i}{\partial x^2} - \Theta.C'_i + \delta_i$$

or

$$\frac{\partial C'_i}{\partial t} + U(1 + \mu)\frac{\partial C'_i}{\partial x} = E\frac{\partial^2 C'_i}{\partial x^2} - \Theta.C'_i + \delta_i \quad (2.25)$$

here $\Theta > 0$, μ 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 δ_i 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 Al, Su, ... mentioned above. It is also noted that for hydrogen we can apply (2.25) or use (2.19) in the form:

$$Al.Su = \tau_1.H \quad \text{with} \quad \tau_1 = 10^d \quad (2.26)$$

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

$$Al'.Su' + \varepsilon = \tau_1.H' \quad (2.27)$$

where

$$\varepsilon = \frac{1}{A} \int_A Al''.Su'' dA$$

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

$$\frac{dAl}{dt} = E\frac{\partial^2 Al}{\partial x^2} - \frac{\sigma}{A}Al + \frac{\phi^1}{A} - P_{Al} - D_{Al} + \delta_1 \quad (3.1)$$

$$\frac{dSu}{dt} = E\frac{\partial^2 Su}{\partial x^2} - \frac{\sigma}{A}Su + \frac{\phi^2}{A} - P_{Su} - D_{Su} + \delta_2 \quad (3.2)$$

$$\frac{dH}{dt} = E\frac{\partial^2 H}{\partial x^2} - \frac{\sigma}{A}H + \frac{\phi^3}{A} - P_H - D_H + \delta_3 \quad (3.3)$$

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

$$\frac{d..}{dt} = \frac{\partial..}{\partial t} + U(1 + \mu)\frac{\partial..}{\partial x}$$

Using the symbols:

$$N = Su - Al, \quad S = Su + H$$

$$f_1 = \delta_2 - \delta_1 + (\phi^2 - \phi^1)/A$$

$$f_2 = \delta_2 + \delta_3 + (\phi^2 + \phi^3)/A$$

from (3.1) - (3.3) it follows:

$$\frac{dN}{dt} = E \frac{\partial^2 N}{\partial x^2} - \sigma.N + f_1 \quad (3.4)$$

$$\frac{dS}{dt} = E \frac{\partial^2 S}{\partial x^2} - (\sigma + L).S + f_2 \quad (3.5)$$

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

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

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

$$\frac{df}{dt} = -k_1.f + k_2 \quad (3.7)$$

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

$$C = (CO - k_2/k_1) \exp(-k_2.t) + k_2/k_1$$

where CO is the value of C defined at the previous time step. It is noted that due to $L > 0$, in eq. (3.7) $k_1 \neq 0$.

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

$$\frac{\partial h}{\partial t} = E \frac{\partial^2 h}{\partial x^2} \quad (3.8)$$

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):

$$Al.Su + \varepsilon = \tau_1.H \quad (3.9)$$

using (3.3), (3.9) becomes

$$Su^2 + (\tau_1 - N)Su - \tau_1.S + \varepsilon = 0 \quad (3.10)$$

If $\varepsilon = 0$ (3.10) is an algebraic equation of second order for which it is easy to find solutions of Su and hence, from (3.3), Al 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.

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HỆ PHƯƠNG TRÌNH CƠ BẢN TRONG MÔ PHỎNG NƯỚC CHUA PHÈN TRÊN KÊNH SÔNG

Sự hình thành và lan truyền nước chua phèn trên kênh sông bị chi phối bởi các quá trình hóa lý và sinh học khác nhau như hòa tan, kết tủa, tái, khuếch tán, ... nhưng chúng vẫn tuân theo các luật cân bằng nhất định. Trong nghiên cứu này trình bày cách thu nhận hệ phương trình cơ bản sử dụng để mô phỏng nước chua phèn trong kênh sông với cân bằng Jurbanite là cân bằng chủ yếu cho nước kênh Đồng Tháp Mười đồng bằng sông Cửu Long. Mặc dù sử dụng luật cân bằng nhưng quá trình động học cũng được xem xét. Trong nghiên cứu cũng thảo luận cách giải số cho trường hợp một chiều.