

A MODEL FOR SIMULATION OF ACID WATER IN CANALS AND LINKAGE TO ACID SULPHATE SOIL MODEL

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Abstract: *It is given in this paper an attempt to consider the problem of canal acid water in linkage to the ground acid water with the presence of the alunite and jurbanite in the soil. 1D model is applied for canals while 2D depth-average model is used to simulate the processes occurred in the soil. Data of 1995 collected at Tan Thanh farm, in the Plain of Reeds of the Mekong Delta in Vietnam, are used as a case study.*

Keywords: *Acid water in soil and canal, modeling, spreading of acid water*

1. INTRODUCTION

It is mentioned in [11] that for the Mekong Delta, acidity in the surface water is a particular problem at the beginning of the rainy season. Much effort has been made to mathematically simulate the processes occurred in both canals and soils [1,10,11,14,18].

It is given here an attempt to numerically simulate the physical and chemical dominant processes in the canals and in the soil and their interaction with the assumption that the canal water is governed by jurbanite equilibrium and the alunite and jurbanite are present in the soils.

2. ACID WATER MODEL FOR CANALS

In canals, the dominant process is longitudinal so one-dimensional model is practically useful for consideration and the governing equations in this case can be obtained by direct integration of the three-dimensional equations over cross-section normal to the axis of the canal. In [11] three-dimensional mass balance law is written for aluminum, sulphate and hydrogen in which the precipitation/redissolution and sedimentation processes

have been taken into account. After integration over canal cross-section the following governing equations for one-dimensional case with jurbanite equilibrium are obtained

$$\frac{\partial C_i}{\partial t} + U(1+\varepsilon)\frac{\partial C_i}{\partial x} = E\frac{\partial^2 C_i}{\partial x^2} - \phi_i \cdot C_i + \varphi_i \quad (1)$$

$i=1,2,3$ corresponding to Aluminum, Sulphate and Hydrogen concentrations averaged over canal cross-section. $\phi_i > 0$ and φ_i are given parameters; ε is considered as an adjusted parameter during calibration; U is average flow velocity over cross-section; E is dispersion coefficient.

3. MODELS FOR SOILS

The physical and chemical mechanism of acidity in the soils has been discussed in many studies [14], [19], [20]. Some simple mathematical models have been also found in [4], [5], [10], [15], [17]. The basic governing equation of these models is:

$$\frac{\partial C}{\partial t} + \frac{\rho}{\theta} \frac{\partial S}{\partial t} + U \frac{\partial C}{\partial z} = D \frac{\partial^2 C}{\partial z^2} + \frac{-R \cdot C + Q^*}{\theta} \quad (2)$$

where C and S are concentrations of any constituent in the solution and adsorption phases, respectively; ρ : soil bulk density; θ : volumetric moisture; D : dispersion coefficient; U is flow rate (Velocity); R : water taken by roots; and Q^* : source/sink term.

Receipt Date: August 01th, 2022

Review Approval Date: September 14th, 2022

Publish Approval Date: October 05th, 2022

SCIENCE AND TECHNOLOGY (S&T) JOURNAL OF HO CHI MINH CITY ASSOCIATION FOR SCIENCE AND ENGINEERING OF WATER RESOURCES (HCAEW) - ISSN: 2525-1247 (Print) / 2525-1255 (Online) - Volume 14, Number 10, October 2022

The difference between these models can be found in the relationship between C and S . For instantaneous linear model the relationship is

$$S = K.C \quad (3)$$

K is called the distribution coefficient and is the slope of the isotherm curve. The Langmuir equation is one kind of (3).

There are some even more complicated models. In general, all the models try to reflect the structure of the physical phenomenon to be modeled. But the more detailed the model is, the more coefficients need to be determined and sometimes this makes the model unrealistic.

It can be seen that (3) is the simplest in terms of model development and only one coefficient K needs to be determined by experiment. Moreover, the number of equations like (2) to be included in the model is equal to the number of constituents in the simulation. E.g. If jurbanite equilibrium in canal water is used in simulation then only sulphate, aluminum and hydrogen in the soil are necessary in the simulation. So it is suggested to use (2) and (3) for simulation of solute transport in a soil column and to generalize these equations for the large-scale area of the Plain of Reeds (or even for the Long Xuyen Quadrangle) in the Mekong Delta, Vietnam.

In order to simulate acid water in canals and solute transport in soil in Tan Thanh farm, a master model may consist of two submodels: one for processes in the canal and another for processes in the soil.

3.1. Submodel for canal

To simulate processes taking place in the canal, it is customary to use an one-dimensional model and the movement of water is described by the Saint-Venant system of equation.

For solute transport it is assumed that in the Plain of Reeds canal water is governed by jurbanite equilibrium [13], so the pH can be calculated by (see [11])

$$pH = -d + pAl + pSu \quad (4)$$

where: H , Al and Su are Hydrogen, Aluminum and Sulphate concentrations, respectively; $pH = -\log_{10}(H)$; $pAl = -\log_{10}(Al)$; $pSu = -\log_{10}(SO_4)$; d is a constant. Concentrations of aluminum and sulphate satisfy the following transport-dispersion equation

$$\frac{\partial C_i}{\partial t} + U \frac{\partial C_i}{\partial x} = E \frac{\partial^2 C_i}{\partial x^2} + \frac{Q_{is} - q \cdot C_i}{A} \quad (5)$$

where C_i ($i=1,2$) are aluminum and sulphate concentrations, respectively.; E : dispersion coefficient; U : flow velocity; Q_{is} : source/sink term coming from plains, underground water-table, pumping, rainfall, settling and interaction between the components; q : lateral flow; A : cross-sectional area; E : dispersion coefficient.

Eq. (5) with suitable boundary and initial conditions is numerically solved for aluminum and sulphate and then (4) is used for the calculation of the pH. Data of flow are provided from solving flow equations. The linking terms Q_{is} will be dealt with in the next paragraph.

3.2. Submodel for soil

For a soil column it is suggested to use (2) and (3) for each constituent concerned. For a large area some extensions should be made so that the model can simulate the change of flow in different directions. In the groundwater table the flow is essentially horizontal and thus the groundwater motion is described by the equation

$$\mu \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left(T \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial H}{\partial y} \right) + \omega \quad (6)$$

where μ denotes the storage coefficient; $H(x,y,t)$: groundwater head; ω : (source or sink term) exchange flow between the canal and water-table or interchange with the unsaturated zone; t : time; x, y : the horizontal coordinates of the water-table; T is the transmissivity and practically can be defined by.

$$pH = 2.3 - \frac{1}{3} \text{Log}(Al / 3000) \quad (13)$$

The distribution coefficient, K_s , for sulphate can be estimated from the Langmuir equation after carrying linearization:

$$K_s = \frac{A_m \cdot b}{(1 + b \cdot Su)^2} \quad (14)$$

where A_m , b are experimental coefficients (Langmuir isotherm constants); Al and Su are aluminum and sulphate concentrations, respectively. Thus it remains to determine only one distribution coefficient K_a for aluminum, of which the magnitude is about 0.001 to 0.1 [10]. If additional constituents need to be considered (e.g., Nitrogen N, phosphorous P,...), some more distribution coefficients must be determined and additional equations of type (12) must be included in the model.

4. NUMERICAL SCHEME

The numerical procedure for flow and mass transport in canals has already mentioned in many studies, e.g. see [11, 21].

$$\sum_j^M \iint_A \left\{ \mu \frac{dH_j}{dt} N_j N_i - \left[\frac{\partial}{\partial x} \left(T \frac{\partial H_j}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial H_j}{\partial y} \right) \right] N_i - \omega N_i \right\} dx dy = J1 - J2 - J3 = 0$$

$$i = 1, 2, \dots, M$$

$$(16)$$

where A is a triangular element with three vertices (i, j, k). Upon application of Green's theorem the integral $J2$ for an element becomes

$$J2 = \iint_A \left[\frac{\partial}{\partial x} \left(TN_i \frac{\partial H_j}{\partial x} \right) + \frac{\partial}{\partial y} \left(TN_i \frac{\partial H_j}{\partial y} \right) \right] dx dy - \oint N_i \mathfrak{R}_n d\Gamma \quad ; i = 1, 2, \dots, M \quad (17)$$

$$= J21 - J22$$

$$\text{where } \mathfrak{R}_n = \left(T \frac{\partial H_j}{\partial x}, T \frac{\partial H_j}{\partial y} \right)_n$$

The integral $J22$ is taken along three sides of each element and is the contribution (or extraction) from the boundary or from canals inside region to the soil. The integrals in (16)

4.1. Numerical computation of water movement in the soil

At this stage, equation (12) is numerically solved to give hydraulic head and flow rate at every point in considered area. For good representation of the complexity of the boundary and the bathymetry of the region, the FEM (Finite Element Method) with triangular elements is used in this model. According to FEM [12] a system of coordinate or basis functions N_k ($k=1,2,\dots, M$ with M is number of grid points) is chosen. Any function $f(x,y,t)$ defined in the considered region can be approximated by :

$$f(x, y, t) \approx \sum_j^M f_j(t) \cdot N_j(x, y) \quad (15)$$

Where $f_j(t)$ is the value of f at node j and at time t . Eq. (15) is substituted into (12) and resulting equations are made orthogonal to N_j according to Galerkin's procedure. The equations that result are

are calculated and assembled in the following matrix form:

$$\mathbf{M} \frac{d\mathbf{H}}{dt} + \mathbf{D} \cdot \mathbf{H} = \mathbf{P} \quad (18)$$

where \mathbf{M} , \mathbf{D} , \mathbf{P} are sparse coefficient matrices; \mathbf{H} is column matrix with components H_i ,

H_2, \dots, H_M ; matrix P characterizes for exchange flow with outside domain (canals,

air,..). If the Preissmann scheme for time derivative is applied eq. (18) becomes:

$$\left(\frac{M}{\Delta t} + \theta D \right) H = \left(\frac{M}{\Delta t} + \theta D \right) H^0 - D H^0 + P \quad (19)$$

where H^0 is values of H at time $n \Delta t$.

The coefficient matrices in (19) are sparse, so the *SOR* method (Successive Over Relaxation) can be applied to (19). In fact *SOR* is iterative method applied to sparse matrix and

its size is not expandable during elimination.

4.2. Numerical computation of solute transport in the soil

If Darcy's law (8) is used we can rewrite (12) in the form

$$R_{ei} \frac{\partial C_i}{\partial t} - \frac{K_s}{g} \left(\frac{\partial H}{\partial x} \frac{\partial C_i}{\partial x} + \frac{\partial H}{\partial y} \frac{\partial C_i}{\partial y} \right) = \frac{\partial}{\partial x} \left(T \frac{\partial C_i}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial C_i}{\partial y} \right) + \omega C_i^b - \omega C_i \quad (20)$$

where C_i^b is concentrations in the source/sink flow.

The same FEM procedure as mentioned above is also applied to (20). It is interesting to note that by the application of FEM and the direct coupling of Darcy's law in one equation (10) we can use directly hydraulic head values at

grid point but not its gradient so can avoid numerical error coming from differencing calculation of velocity field.

For each triangular element, Galerkin's procedure is applied to (20) and Preissmann is also used for time derivative we can obtain the following matrix equation:

$$\left\{ \frac{MI}{\Delta t} + \theta (D - K_p H) \right\} C_i = P_i + \left\{ \frac{MI}{\Delta t} + (\theta - 1)(D - K_p H) \right\} C_i^0 \quad (21)$$

where MI , D , P_i are coefficient matrices ; H is also a given matrix coming from hydraulic head calculation; C_i^0 are concentrations at previous time step and P_i is mass flux of exchange flow (e.g. from canal or to canal); K_p is average over element value concerning hydraulic conductivity; θ is weighting coefficient.

Eq. (21) is put together over all elements and the resulting equation is also solved by *SOR* method.

5. OUTLINES OF APPLICATION OF THE DEVELOPED MODEL TO THE AREA OF TAN THANH FARM

To illustrate the use of the developed model and to evaluate the validity of the model's conceptual basis, the model is applied to Tan Thanh area with data set collected in March 1995. During five days, from 17 to 22 March, a measurement campaign was carried out in Tan Thanh and covered about 250 ha (the schematization of the master model for Tan Thanh farm consists of two submodels, one-dimensional for canals and two-dimensional for the soil. The two-dimensional region is divided into 42 triangular elements with 32 nodes. The one-dimensional schematization contains 10

canal branches and 36 grid points). The collected data consist of four types:

- + physical data in three surrounding canals and in two ditches inside the area.
- + chemical data collected in canals.
- + ground water level (physical data) collected in the soil.
- + and chemical data collected at some nests in the soil.

From data analysis it is suggested to use the following values for parameters in the test runs of the model : storage : $\mu = 0.002$ & 0.014 ; moisture θ : from 0.60 to 0.75 ;

effective porosity: 0.75 ; thickness of ground table: 1.2m . The Langmuir isotherm average constants: $A_m = 12.38$; $b = 1.28\text{E}-2$; horizontal conductivity hydraulic varies from 1m/day to 5m/day .

It is also noted that it is difficult to correctly create a relation between pH, Aluminum and Sulphate in the soil. Look into the below table we can see one value of pH can correspond to some values of Aluminum and Sulphate. For example, from the first two rows and (pH = 4.02) and the rows 5 and 6 (pH= 3.52 and 3.53) it seems pH does not depend on Aluminum concentrations.

Date	Time	Nest	pH	Al ⁺³ (mg/l)	SO ₄ ⁻² (mg/l)
03/17	19	F1	4.02	20.30	429
03/17	23	F1	4.02	10.07	429
03/18	3	F1	4.01	5.94	446
03/19	1	F1	3.53	16.36	534
03/19	3	F1	3.52	12.02	515
03/19	17	F1	3.53	9.56	515
03/18	15	F8	3.52	14.19	784
03/20	1	F8	3.53	12.86	679
03/21	1	F8	3.52	11.68	693
03/17	21	F10	3.52	4.79	342
03/18	1	F14	3.51	5.85	335
03/18	9	F11	3.50	10.01	869

So we can conclude that the relation $\text{pH} = 2.3 - \text{Log} (\text{Al}/3000)/3$ mentioned in [1] is not suitable for simulation of pH in the soil of Tan Thanh area. So, data of March 1995 have been used only for the test runs.

6. REMARK AND CONCLUSION

Some first test runs mentioned above show that physically the developed model can be

used for real-life simulations of large-scale problems. The chemical equilibrium formulated by previous studies, mainly for soil column, seems to be suitable for a limited range of simulations. In order to correctly reproduce chemical processes in the soils or in canals and their interactions further more studies must be carried out.

REFERENCES

- [1] Erik Erikson (1992), Modelling flow of water and dissolved substances in acid sulphate soils, Selected Papers of the Ho Chi Minh City Symposium on Acid Sulphate Soils, Ho Chi Minh City, Vietnam, March 1992, Ed. by D.L. Dent and M.E.F. van Mensvoort, Publication 53.
- [2] J. Rubin (1968), Theoretical Analysis of Two-Dimensional, Transient Flow of Water in Unsaturated and Partly Unsaturated Soils, Proceedings Soil Science Society of America, vol 32, No.5.
- [3] L.M. Dudley, R.J. Waenert and J.J. Jurinak (1981), Description of Soil Chemistry Transient Solute Transport, Water Resources Research, Vol 17, No. 5.
- [4] D.R. Nielsen, M.Th. van Genuchten and J.W. Biggar (1986), Water Flow and Solute Transport Processes in the Unsaturated Zone, Water Resources Research, Vol. 22, No.9.
- [5] C.W. Miller and L.V. Benson (1983), Simulation of Solute Transport in a Chemically Reactive Heterogeneous System: Model Development and Application, Water Resources Research, Vol.19, No.2.
- [6] H.M. Selim and R.S. Mansell (1976), Analytical Solution of the Equation for Transport of Reactive Solutes Through Soils, Water Resources Research, Vol.12, No.3.
- [7] Davis J. Kirkner and Howard Reeves (1988), Multicomponent Mass Transport With Homogenous and Heterogeneous Chemical Reactions : Effect of the Chemistry on the Choice of Numerical Algorithm, 1. Theory, Water Resources Research, Vol. 24, No.10.
- [8] Peter J. Ross and Keith L. Bristow (1990), Simulating Water Movement in Layered and Gradational Soils Using the Kirchoff Transform, Proceedings of Soils Science Society of America, Vol. 54.
- [9] Nicholas Jarvis (1994), The MACRO Model (version 3.1), Technical Description and Sample Simulation, Swedish University of Agricultural Sciences, Department of Soils Sciences.
- [10] Bernard Tychon (1993), Etude du Transfert d'Eau et d'Azote dans les Soils d'un Micro-Bassin Agricole, Dissertation pour l'Obtention du Titre de Docteur en Sciences de l'Environnement, Fondation Universitaire Luxembourgeoise.
- [11] T.V. Truong, N.T.Dac and H.N.Phien (1996), Simulation of Acid Water Movement in Canals, Journal of Hydrology 180, pp 361-371.
- [12] George F. Pinder and William G. Gray (1977), Finite Element Simulation in Surface and Subsurface Hydrology, Edt. by Academic Press.
- [13] 13.Tin, N.T.(1990), Chemical equilibrium in acid water in the Plain of Reeds of Vietnam, Report on the Water Quality Monitoring Network Project.
- [14] Van Breemen, N. (1973), Soil forming processes in acid sulphate soils, Proceedings of the International Symposium 13-20 August 1972, International Institute for Land Reclamation and Improvement, Publ. 18:1.
- [15] 15.Brusseau M.L. et all (1989), Modeling the Transport of Solutes Influenced by Multiprocess Nonequilibrium, Water Resources Research, Vol.25, No. 9.

- [16] 16. Ne-Zheng Sun, William W.-G. Yeh (1983), A Proposed Upstream Weight Numerical Method for Simulating Pollutant Transport in Groundwater, Water Resources Research, Vol. 19, No. 6.
- [17] 17. David J.Kirkner and Howard Reeves (1988), Multicomponent Mass Transport with Homogeneous and Heterogeneous Chemical Reactions : Effect of the Chemistry on the Choice of Numerical Algorithm, 1. Theory, 2. Numerical Results , Vol. 24, No. 10 .
- [18] 18. Erik Erikson, Vo Khac Trí, Phan Thi Binh Minh, Nguyen Tan Danh, Ngo Dang Phong (1994), Modelling of water movement and solute transport in acid sulphate soils. Application to Tan Thanh farm, Plain of Reeds, Vietnam, MASS project (in Vietnamese).
- [19] 19. Dost H. And Van Breemen N. (1982). Proceedings of the Bangkok Symposium on Acid Sulphate Soils, January 1981. ILRI Publ. 31, International Institute for Land Reclamation and Improvement, Wageningen, Netherlands.
- [20] 20. Dent D.L. (1986). Acid Sulphate Soils. ILRI Publ. 39, International Institute for Land Reclamation and Improvement, Wageningen, Netherlands.
- [21] 21. Dac N.T., (1987). Unsteady one-dimensional mathematical model for tide movement and salinity intrusion in river network. Doctoral Thesis, Hanoi (in Vietnamese).