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ON SOLUTION FOR THE PROBLEM OF SPREADING OF ACID WATER IN CANALS

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ABSTRACT. It is dealt with in this study a one-dimensional mathematical and statistical model for acid water transport in canals including a case study in the Saigon river with data provided by Environment Protection Centre - HCM city. It is shown that based on statistical analysis of data collected in the field the computation will be improved in sense of making their solutions more reliable.

1. Introduction

Pollution of water and solid environment is of critical importance, because it is difficult to control the signs of pollution and recovering time normally is very long. The effect of acid water plays an important role in many environmental problems, especially in living and agricultural activities.

The main sources of acid water are: oxidation of reduced S in acid sulfate soils and discharged from coal mine operations; production of H_2CO_3 - the reactions of atmospheric CO_2 with rain water; acid rain - the reaction of SO_2 and reactive nitrogen gases NO_x produces H_2SO_x and HNO_3 ; decomposition of litter and plant residues resulting in the formation of organic acids; mineralization of natural organic products in soil and litter. The formulation of these sources are concerned in modeling and solving acid - water problem in the southern areas of Vietnam, especially in canals and rivers.

The mechanism of acidity genesis has been presented in [1-5]. Using the jurbanite equilibrium, the governing equations for acid water in canals have been derived in [6, 7] and applied to compute the acidity for the Plain of Reeds of Vietnam. But in some extent, the assumption of jurbanite equilibrium is not strictly satisfied so statistical tests must be used before application.

This paper presents an adapted solution in solving the problem of spreading of acid water in canals in combination with statistical tests. It is also presented a cases study of the Saigon river between Ben Than - Thu Dau Mot.

2. Transport mechanism and modeling

2.1. During the dry season, water in surface soil layers gradually evaporates. The ground water table is dropped and the soil dries, a certain amount of oxygen entering to subsurface soil layers oxidizes pyrite and the acid product is formed. At the beginning of the rainy season, the first rains will wash these formed acid quantities to canals and rivers. Beside this phenomenon, due to agriculture development, new dikes or canals are constructed and some acid products are also formed by these processes. They are, under the first rains, also released from exacavated dikes to canals, etc.. These are the main sources producing acidity in surface water.

The acid water spreads to other zones, in dissolved form, so the phenomena such as advection, dispersion, sorption, chemical and biological transformation,... will strongly influence on the spreading of acid water. Understanding of the various mechanisms will help us to illustrate the conceptual complexities of acid transport and its distribution.

The acidity in the acid water environment is characterized by $pH = -\log(H)$. According to Van Breeman N. [1], Tin N. T. [2], Phien H. N. [3], and Erikson E. [4] if jurbanite equilibrium is dominant, a relation between pH, aluminum and sulfate is established in the following form:

$$pH = -d + pAl + pSu, \tag{2.1}$$

where d is constant, $pAl = -\log(Al)$, $pSu = -\log(Su)$, and H, Al and Su are hydrogen, aluminum and sulfate concentrations, respectively, measured by mol per liter. Using this chemical mechanism, the acidity in canals is estimated by the transport model introduced in [6, 7]. In practice the collected data sometimes do not strictly confirm the relation (2.1), so some hypotheses must be made based on marking regression such as:

$$pH = a + b_1 pAl + b_2 pSu \tag{2.2}$$

with (2.1):

$$a = d$$
 and $b_1 = 1, b_2 = 1.$ (2.3)

In practice the jurbanite assumption is too strong and must be tested, as a necessary condition, before applying the governing models in [6, 7]. To distinguish, it is suggested to define the following concepts:

- The jurbanite equilibrium is verified, when the jurbanite hypothesis is accepted at level of alpha and beta errors [8], in the tests of significance not exceed 5%.

- The jurbanite equilibrium is weakly verified, if the jurbanite hypothesis is accepted at alpha error not exceed 5%, but beta greater than 5%. In this case, (2.1) can be considered as an operating hypothesis, but needed more observations to have a strong conclusion.

- The jurbanite equilibrium is not verified, if there exists one of the hypothese in (2.2) and (2.3) is rejected at significant level of the tests less than 5%.

2.2. Mathematical models of the acid transport in canals and rivers are attractive and effective because they offer an inexpensive and rapid way to assess potential hazard during process development. Furthemore, the absence of reliable monitoring data makes mathematical modeling a useful tool to access complex environment events, but it should be stated that due to inadequate monitoring studies, data required for model validation are lacking.

Considering advection, dispersion, sorption and the jurbanite equilibrium mechanisms for flow, the one dimensional mass transport equations have been obtained by the method of direct integration over a cross-section area from the equations in three dimensions [7]:

$$\frac{\partial C_i}{\partial t} = D_h \frac{\partial^2 C_i}{\partial x^2} - \alpha v \frac{\partial C_i}{\partial x} - \varsigma C_i + \eta_i \quad i = 1, 2, 3$$
(2.4)

where C_i stand for the concentrations of Al, Su and H, respectively, D_h is dispersion coefficient, $\alpha \ge 1$ is an adjusted parameter, ς and η are coefficients. Using the jurbanite equilibrium, the above non-linear partial differential equations can be combined into following system to solve for $S_1 = Su - Al$ and $S_2 = Su + H$ as follows:

$$\frac{dS_i}{dt} = D_h \frac{\partial^2 S_i}{\partial x^2} - \sigma S_i + \delta \quad i = 1,2$$
(2.5)

in which σ and δ are parameters. Finally, the acidity pH can be computed from S_1, S_2 and (2.1).

2.3. It should be noted that computed pH strongly depends on *d*-value from (2.1). If the jurbanite is an operating hypothesis, *d* can be estimated by the observed mean \underline{D} from the sample of *n* observations D_i , (i = 1, ..., n) of the random variable D = pAl + pSu - pH. According to the chemical mechanism of each area, several values of *d* have been introduced in [1-5]. To accept one of the priori *d*-values, the Student test must be used.

Comparing the various used d-values, in the following case study, (2.2) gives a minimal loss function value [8], less than any one from (2.1). This shows that using (2.2) to estimate pH is better than (2.1). After partitioning the various sources

of variation, the χ^2 - theorem allows to determine the distribution of a, b_1 and b_2 in (2.2) so the confidence intervals (pH_L, pH_U) are obtained for the predicted pH-values at a certain values of pAl_* and pSu_*

$$pH_U = pH_* - tS_{pH}$$
 $pH_L = pH_* + tS_{pH}$ (2.6)

where t is the 97.5% - percentile of the Student distribution with a degree of freedom n-3 and pH_* is computed by (2.2) and pAl_* , pSu_* , S_{pH} the standard deviation of the model (2.2) - is a quadratic from of pAl and pSu, determined by observed data as follows:

$$S_{pH}^{2} = s^{2} \left\{ \frac{1}{n} + \left[(pAl - \underline{pAl})^{2} SSD_{pSu} + (pSu - \underline{pSu})^{2} SSD_{pAl} - 2SPD_{pAlpAl}(pAl - \underline{pAl})(pSu - \underline{pSu}) \right] / Dt \right\}$$

in which SSD_x , SPD_{xy} denoted sum of derivations of x, sum of product of derivations of x, y - observations around their sample means: \underline{x} , \underline{y} , respectively, and s^2 is the total variance of observed pH-values $s^2 = SSD_{pH}/(n-1)$, $Dt = SSD_{pSu}SSD_{pAl} - SPD_{pAlpSu}^2$.

3. Case study

From collected data it is seen that spreading of acid water strongly affects water quality in the Saigon river. The area, in figure 1, from Thi Tinh to Binh Phuoc in the Saigon river and the five canals Thai My, Rach Tra, Trung Uong, An Ha, Ben Cat with the total length of 130 kilometers are selected as a case study.

The acid water on these areas of river and canals is under the influence of the tide regime from Vam Co Dong and Saigon river, especially under the acid water generating regions of 200 ha in the Cu Chi, Binh Chanh districts. Additionally, in the flood season, passing through canals the acid water from the Plain of Reeds is also flowing to these areas and increasing the acidity on these canals and Saigon river.

Data collected on Nov. '98, provided by Environment Protection Centre, have been statistically analyzed and the above model has been used to simulate the problem of acid water spreading on the canals and river. The model consists of 281 branches and 734 cross-sections. The sources of acid water from Cu Chi, An Ha, the Plain of Reeds and the tide regime of the Saigon and Vam Co Dong rivers have been used as boundary conditions.

According to the statistical analysis [9], the jurbanite equilibrium tested with data on Apr. and on Jul. '98 in the region of case study is weak. But the

jurbanite hypothesis has been rejected when unifying data on both of these months to analyze. This conclusion requires separate models for each months. The two linear regression for acidity are given as follows

Apr.

$$pH_{PRE} = 3.54 + 0.27 pAl - 0.01 pSu$$

Jul.

$$pH_{PRE} = 2.95 + 0.20pAl - 0.06pSu \tag{3.1}$$

The confidence limits are determined by (2.6) and the corresponding standard deviations S_{pH} are

For Apr.

$$S_{pH}^{2} = 36.164 - 3.874pAl - 3.633pSu + 0.924pAlpSu + 0.610pAl^{2} + 0.876pSu^{2}$$
(3.2)

For Jul.

 $S_{pH}^{2} = 21.117 - 8.512pAl - 7.628pSu - 0.555pAlpSu + 1.548pAl^{2} + 0.581pSu^{2}$ (3.3)

The *d*-values minimizing the loss functions of (2.1) and accepted by the Student test on April and July data, figure 2, are 3.5 and 2.9, respectively. They were used in calculating the acidity from (2.5). It is also noted that these minimal values are still greater than the ones of (2.2).

A computer program for acid water computation has been developed and coupled with the model to simulate the concentration of Al, Su and pH. Some computed results during time periods in the simulation areas between Thi Tinh and Binh Phuoc such as Thi Tinh (TT), Thu Dau Mot (TDM), Rach Tra (RT), Binh Phuoc (BP) and some other locations, the Vam Co Dong (VCD) and Saigon (SG) rivers are shown in the following tables.

Table 1. Distribution of acid water from Thi Tinh to Binh Phuoc in the Saigon river

Location	TT		TDM		RT	_	1-	BP
Dist. in km	0.0	5.2	11.1	15.7	20.	24.9	29.8	34.7
Apr. pH. max	5.29	5.29	5.29	5.27	5.27	5.39	5.39	5.39
Apr. pH. ave	4.34	4.35	4.35	4.33	4.33	4.45	4.45	4.45
Apr. pH. min	4.31	4.30	4.31	4.28	4.27	4.40	4.40	4.40
Jul. pH. max	5.19	5.19	5.19	5.17	5.17	5.29	5.29	5.29
Jul. pH. ave	4.26	4.26	4.26	4.24	4.25	4.36	4.37	4.38
Jul. pH. min	4.21	4.20	4.22	4.18	4.18	4.3	4.3	4.3

Location	VCD					Confluence		SG
		111.1	Upril 18	11 11 7	1-			
Dist. in km	0	5	17	29	35	45	48	52
Apr. pH. max	5.49	5.49	5.49	5.49	5.49	5.09	5.09	5.09
Apr. pH. ave	4.31	4.31	4.42	4.50	4.53	4.14	4.14	4.15
Apr. pH. min	4.07	4.23	4.36	4.46	4.48	3.98	4.02	4.05
Jul. pH. max	5.14	5.14	5.14	5.14	5.14	4.94	4.94	4.94
Jul. pH. ave	4.18	4.17	4.19	4.18	4.18	3.97	3.99	4.01
Jul. pH. min	3.98	4.11	4.15	4.14	3.98	3.98	3.91	9.93





4. Conclusion and recommendation

1. The governing equations (2.5) and their numerical solution strongly depend on the jurbanite equilibrium, so before application, this hypothesis must be significantly tested by the meaning (2.2) and (2.3). In the case when the jurbanite hypothesis is not accepted, it is necessary to recreate the new system of governing equations.

2. The loss function value of (2.2) is lowest in comparison with the one of (2.1) at the *d*-value minimizing this one's function. When computing, (2.2) should be taken into account.

3. When the jurbanite equilibrium is accepted as an operating hypothesis, the *d*-value used in computing the acidity pH from (2.5) must be tested by a sample of observations. It is also noticed that the *d*-value and the estimation *a* in (2.2) are seemly approximate.

4. The limits at the confidence level of 95% in (2.6) should be used in prediction of the acidity pH to obtain the compatibility with experimental observations.

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VỀ LỜI GIẢI CỦA BÀI TOÁN LAN TRUYỀN AXIT TRONG KÊNH SÔNG

Bài báo này trình bày những bổ sung trong phương pháp tính toán độ axit với điều kiện có cân bằng jurbanite trên các kênh sông theo mô hình đã giới thiệu trong [6, 7]. Qua kết quả thu được khi tính toán lan truyền phèn tại những vùng giữa Bến Than và Thủ Dầu Một trên sông Sài gòn trong các tháng 4 và 7/98, cần thiết phải kiểm định giả thiết cân bằng jurbanite và xác định ước lượng d trong (2.1). Những tính toán cho thấy tổn thất khi dùng (2.1) để tính độ axit thường cao hơn so với dùng (2.2). Bài báo này cũng đề nghị nghiên cứu cải tiến mô hình cho cân bằng jurbanite yếu hoặc chỉ có cân bằng tuyến tính giữa pH và pAl, pSu.

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