Improving the numerical stability of the MAGIC model

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Abstract: MAGIC is one of the most widely used models for forecasting long-term acidification. The model's code, however, has been experiencing numerical instability, though this might not be widely known to the public users. The major instability comes from the analytical solution to two cubic equations for calculating SO_4^{2-} concentration and the exchangeable fraction of Al on the soils. The mathematical algorithm for calculating the concentration of SO_4^{2-} from a quadratic equation is also found instable. This paper is aimed at improving the instability above through proved numerical algorithms.

Key words: MAGIC model; numerical instability

Introduction

The model of acidification of ground water in catchment (MAGIC) is one of the most widely used models worldwide for predicting catchment acidification and is still under further upgrading (Cosby, 1985; Hinderer, 1995; Cosby, 1995). The model, however, is inherently associated with numerical instability in its original computer codes. The importance of these instabilities cannot be underestimated, as they are unknown to most public users, given the scales, the public acceptability and trustworthiness of the model. Although it is difficult to quantify what consequences these instabilities have caused in practice, it is essential that a model be free from any numerical errors.

1 The numerical instability

There are two numerical instabilities in the MAGIC model. The first one is associated with the solution to a cubic equation for calculating either the SO_4^{2-} concentration in soil water or the exchangeable fraction of Al on the soils. Both SO_4^{2-} and Al are the major components of the MAGIC model in influencing the changes of alkalinity in soil and surface waters. In the numerical codes, this equation is invoked in each iterative time-step, and the associated errors might thus be quickly propagated into other numerical calculations. To be representative, the cubic equation for calculating SO_4^{2-} is used herein as an example to illustrate the instability. Mathematically, the equation can be written as,

$$A_1 \cdot SO_4^3 + A_2 \cdot SO_4^2 + A_3 \cdot SO_4 + A_4 = 0, \tag{1}$$

in which A_1, A_2, A_3 and A_4 are given by

$$A_1 = 4 \cdot KS_2 \cdot Al, \tag{1a}$$

$$A_2 = 2 \cdot (1 + KS_1 \cdot Al + C \cdot KS_2 \cdot Al), \tag{1b}$$

$$A_3 = C + SP \cdot EMX/V - TSO_4/V + C \cdot KS_1 \cdot Al, \tag{1c}$$

$$A_4 = -C \cdot TSO_4/(2V), \tag{1d}$$

where SO_4 is the concentration of sulfate in the soil water; KS_1 and KS_2 are equilibrium constants for the reactions between Al^{3+} and SO_4^{2-}, Al is the concentration of aluminum in the soil, C is the half saturation coefficient of the sulfate adsorption, SP is the soil mass density, TSO_4 is the total amount of sulfate in the soil solution and stream water and V is the volume of soil solution per unit area.

In the original computer program, a traditional analytical method was applied to solve the above equation. The equation is the first divided by A_1 to have the following form,

$$SO_4^3 + P \cdot SO_4^2 + Q \cdot SO_4 + R = 0. \tag{2}$$

Let

$$A = (3Q - P^2)/3 \tag{2a}$$

and

$$B = (2P^3 - 9 \cdot PQ + 27R)/27, \tag{2b}$$

$$CHK = \frac{B^2}{4} + \frac{A^3}{27}. \tag{2c}$$

If $CHK < 0$, the first real root can be solved directly as

$$SO_4 = \left(-\frac{B}{2} + \sqrt{CHK}\right)^{\frac{1}{3}} + \left(-\frac{B}{2} - \sqrt{CHK}\right)^{\frac{1}{3}} - \frac{P}{3}. \tag{2d}$$

The above value is then regarded as the final root of Eq. (1). Otherwise if $CHK < 0$, $\left(-\dfrac{B}{2} + \sqrt{CHK} \right)^{\frac{1}{3}}$ and $\left(-\dfrac{B}{2} - \sqrt{CHK} \right)^{\frac{1}{3}}$ in Eq. (2d) are complex numbers. As the two components are conjugated, SO_4^{2-} in Eq. (2d) will still be a real number.

Let

$$\alpha = a\cos\left(-\frac{B}{2}\sqrt{-\frac{27}{A^3}} \right),$$ (2e)

$$TRM = 2\sqrt{-A/3}.$$ (2f)

Then Equation (2d) is changed into:

$$SO_{4(i)} = TRM \cdot \cos\left(\alpha + i \cdot \frac{2\pi}{3} \right) - \frac{P}{3} \quad i = 0,1,2.$$ (2g)

Here $SO_{4(i)}$ is the ith possible solution to Eq. (1). If $SO_{4(0)} > 0$, then $SO_{4(0)}$ is treated as the final root, otherwise $SO_{4(1)}$ and $SO_{4(2)}$ are checked in the same way until a root is identified. If all the three $SO_{4(i)}$ is less than zero, there is no root to be practically accepted, and the computer simulation will be automatically stopped with an error message.

There are at least two problems to the above analytical solution. First, since KS_2 is rather small at the magnitude of 10^{-8}, A_1 will be very small too and at the same magnitude. When Eq. (1) is divided by it, the error can be significantly enlarged. Second, the above root selection procedure is not at least theoretically sound because there is no evidence to prove that the selected one is the one we need of the three roots.

2   The new algorithm

To avoid the above numerical instability, the well-known Newton iteration method is applied to resolve Eq. (1), the procedure of which can be summarized as follows. First the item $(SO_4)^3$ is omitted from Equation (1) since its coefficient is too small. Thus we have,

$$A_2 \cdot SO_4^2 + A_3 \cdot SO_4 + A_4 = 0.$$ (3)

Because of $A_2 \geqslant 0$ and $A_4 \geqslant 0$, Eq. (3) is sure to have a positive real root, which can be used as the initial estimate for SO_4 by a numerical stable algorithm, i. e.

$$SO_4^{(0)} = -\frac{2A_4}{A_3 + \sqrt{A_3^2 - 4A_2A_4}}.$$ (3a)

The iteration method is then applied to calculate more accurate values for SO_4, i. e. ,

$$SO_4^{(n+1)} = SO_4^{(n)} - \frac{A_4 \cdot [SO_4^{(n)}]^3 + A_3 \cdot [SO_4^{(n)}]^2 + A_2 \cdot SO_4^{(n)} + A_1}{3 \cdot A_4 \cdot [SO_4^{(n)}]^2 + 2 \cdot A_3 \cdot SO_4^{(n)} + A_2}.$$ (4)

Since the initial value of SO_4 is quite close to the real root, which is denoted as $SO_{4(0)}$, the iteration procedure only takes several steps to converge. The CPU time by the Newton iteration method is even less than the one by the analytical method. After finding the first root of Eq. (1), the other two can be solved by the following equation:

$$SO_4^2 + (SO_{4(0)} + P)SO_4 + (SO_{4(0)}^2 + P \cdot SO_{4(0)} + Q = 0.$$ (5)

It is easy to see that there is at most one positive root for Eq. (1) because of the characteristics of its coefficients, i. e. , $A_1 \geqslant 0$, $A_2 \geqslant 0$, $A_4 \leqslant 0$. The only positive root thereafter is the final result. In general, the first root $SO_{4(0)}$ is the needed one.

3   Results and conclusions

The differences of the original and proposed methods are assessed by the data from White Oak Run, based on which the MAGIC model was initially developed (Cosby, 1985). This was achieved by assessing the root differences of the two methods under different concentrations of aluminum. The reason for
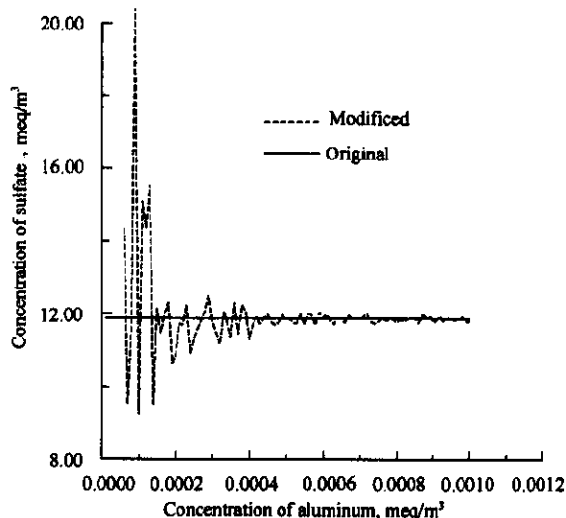

Fig. 1   The numerical stability of different algorithms for Eq. (1)

that is due to the direct sensitivity of aluminum to the coefficients of Eq. (1), especially A_1 and A_2. Fig. 1 showed the SO_4^{2-} concentration by the original method when Al concentration was subject to the range of 0.00001 to 0.001 meq/m^3. It is apparent that the resolved SO_4^{2-} concentration became extremely unstable when the Al concentration was less than 0.00030 meq/m^3. On the contrast, however, the Newton iteration method presented a constant root of SO_4^{2-}.

In addition to the above numerical instability, the following equation, which is to resolve the concentration of SO_4^{2-} in the stream water via total sulfate, is also noted to be numerically problematic,

$$2 \cdot Al \cdot KS_2 \cdot SO_4^2 + (1 + Al \cdot KS_1)SO_4 - TOTS = 0, \tag{6}$$

when resolved through,

$$SO_4 = \frac{(1 + Al \cdot KS_1) + \sqrt{(1 + Al \cdot KS_1)^2 + 8Al \cdot KS_2 \cdot TOTS}}{4 \cdot Al \cdot KS_2} \tag{6a}$$

This is because its denominator is close to zero when Al concentration is low. We thereafter, suggested the following equation to replace Eq. (6a),

$$SO_4 = \frac{2 \cdot TOTS}{(1 + Al \cdot KS_1) + \sqrt{[1 + Al \cdot KS_1]^2 + 8Al \cdot KS_2 \cdot TOTS}}. \tag{6b}$$

Again the numerical instability is eliminated as shown in Fig. 2.

Notation:

C: half saturation constant for the sulfate adsorption isotherm (meq/m^3); EMX: maximum adsorption isotherms (meq/m^3); SP: amount of soil per unit area of watershed (kg/m^2), assuming a specific gravity of 2.65; V: aqueous volume per unit area of watershed (m); Al: aqueous concentrations of the aluminum (millimoles m^{-3}); SO_4: aqueous sulfate concentration (millimoles m^{-3}); $TOTS$: total amount of free aqueous sulfate concentration (millimoles m^{-3}); TSO_4: total catchment sulfate (meq/m^2); KS_1: constant for the aqueous reaction of sulfate with aluminum (millimoles^{-1} m^3), and $KS_1 = \dfrac{[Al(SO_4)_2]}{[Al^{3+}] \cdot [SO_4^{2-}]}$, where [·] means the concentration of the item included in it (millimoles m^{-3}); KS_2: constant for the aqueous reaction of sulfate with aluminum (millimoles^{-2} m^6), and $KS_2 = \dfrac{[Al(SO_4)_2^-]}{[Al^{3+}] \cdot [SO_4^{2-}]^2}$, where [·] means the concentration of the item included in it (millimoles·m^{-3}).
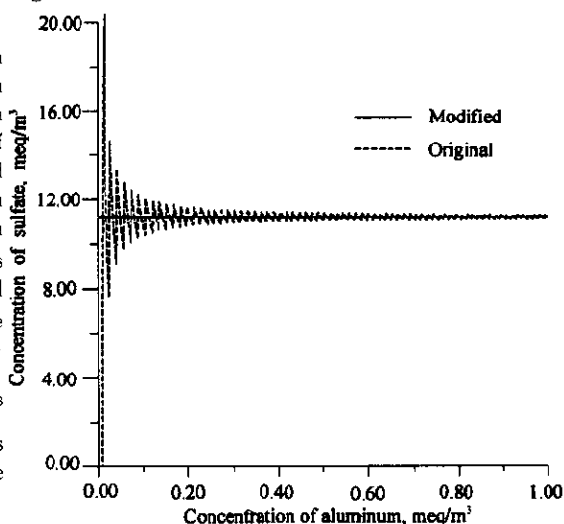

Fig. 2   The numerical stability of different algorithms for Eq. (6)

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