

Reply to the letter to the Editor

Answer to Xiaoxian Zhang's comment on "A three-dimensional spatial model for plant competition in an heterogeneous soil environment"

As Zhang points out in his comments, equations similar to the one I used in 3DMIPS (Biondini, 2001) are commonly used in the modeling of soil solute movement. In addition to Zhang's citation (Mitchella and Mayerb, 1998), one can add the Barber and Cushman model (Barber, 1984), widely used in agriculture and soil models described by Campbell (1985) among others (for a full list of citations, see the Biondini, 2001 paper). The reasons why these models use equations for soil solute movement similar to equation 21 of 3DMIPS, rather than Zhang's equation 6, vary so I will go through a few of them in some detail and use that process to answer Zhang's comments.

1. In all of the models in question (including 3DMIPS), the buffer power of the soil (Cl_buffer), which in Zhang's equation 1 is represented by the term $\theta + [B_k K_c Q_c / (1 + K_c c)]$ (even though a more precise representation should be $(\theta/B_k) + [K_c Q_c / (1 + K_c c)]$ since water has to be expressed on a mass base), is always treated as a constant at each Δt step of the numerical integration algorithm, and then recalculated in the next Δt step to account for the pertinent changes in θ and c . Furthermore, in most models, the θ/B_k and $1 + K_c c$ terms are ignored since θ/B_k and $K_c c$ are $\ll 1$, while $K_c Q_c \geq 1$, thus making Cl_buffer a true constant. K_c is generally 10^2 or higher while Q_c is a very small number, *but can not be 0*, otherwise the solid phase of the soil nutrient in question (S) would be 0 and its soluble phase ∞ , since $S = \text{Cl_buffer} \times c$. The assumption of $K_{Cl} = 0$ used by Zhang in equation 2 thus is inaccurate.

Some examples of $K_c Q_c$ are 5.6 for NH_4 , 6.4 for K , and anywhere from 60 to more than 1000 for P .

In 3DMIPS, Cl_buffer is also treated as a constant within each Δt step, and then updated at the next time step to account for variations in θ and B_k (the last one, a result of OM buildup from litter and root decomposition). With these assumptions in mind, then the left hand side of Zhang's equation 1 would be $B_k (\partial S / \partial t) = B_k (\partial \text{Cl_buffer} \times c / \partial t) = B_k \times \text{Cl_buffer} \times (\partial c / \partial t)$.

If one were not to treat Cl_buffer as a constant, then the left hand side of Zhang's equations 1 or 2 should actually be $B_k \partial \{[(\theta/B_k) + (K_c Q_c / (1 + K_c c))]c\} / \partial t$ not $[\theta + (B_k K_c Q_c / (1 + K_c c))] \partial c / \partial t$ or $\partial \theta c / \partial t$ since *neither K_c or Q_c can be 0*. As one can readily see, this equation is much more complicated to solve because of the presence of c in the denominator.

A final point regarding the issue of treating some values as constants for numerical integration purposes. The approach used for solving solute movement equations is not unique, in fact, it is fairly standard when solving similar equations like the heat flow equation. In that equation, the left hand side is usually written as $C_h (\partial T / \partial t)$ even though C_h (the volume specific heat of the soil) is really not a constant but a function of θ and thus should be written as $C_h (\partial T / \partial t) + T (\partial C_h / \partial t)$. Nevertheless, for numerical integration purposes, it is routinely treated as a constant at every Δt step and then recalculated in the next Δt step to adjust if for changes in (see Campbell, 1985, chapter 4).

2. A similar treatment to the one given to Cl_{buffer} is used for f_w . In this case, the water flux vector field (f_x, f_y, f_z) is also treated as a constant at each Δt step of the numerical integration and then recalculated at the next Δt step to take into account the pertinent changes in soil water potential that result from changes in water content, soil temperature, soil evaporation, and plant water uptake. That means that the impact of plant water uptake as well as evaporation *are already included in the calculations of solute movement* at every Δt step of the numerical integration through their effects in the water flux vector field. With this approach, and for numerical integration purposes only, the terms $c(\partial f_x/\partial x)$, $c(\partial f_y/\partial y)$, $c(\partial f_z/\partial z)$, can be dropped.
3. In summary, regarding the first part of Zhang's concerns:
 - a. Equation 21 of 3DMIPS and variations of it are extensively used in calculating soil solute movements because Cl_{buffer} and the water flux vector field (f_x, f_y, f_z) are treated as constants at each Δt step of the numerical integration algorithm and their values updated at the next Δt step. In that fashion, the effects of water uptake in solute movement *are incorporated into the solution* of the solute movement equation on a discrete Δt by Δt step. The use of this approach results in almost negligible if any mass loss and its accuracy has been proven by the extensive simulations validated by actual experiments published by Jungk and Barber (1975), Caassen and Barber (1976), Edwards and Barber (1976), Silberbush and Barber (1983), and Barber (1984) among others.
 - b. Zhang is correct, however, in one point. If one wanted to simultaneously solve the temperature, water, and solute movement system of equations, then treating Cl_{buffer} , C_h , the water flux vector, and other components of these equations as constants would not be appropriate. But if one were to do that many other variables that are treated routinely as constants when solving soil flow equations would also have to be treated as functions and their partial differential equations included in the system. Examples include the soil thermal conductivity (λt) and the solute diffusion coefficients (D_{xx} , D_{yy} , D_{zz}), both of which are functions of soil water content and the water flux vector. The simultaneous solution of these systems of equations would be extremely computationally demanding and needed only when a high level of precision is required. One may need to do that, for example, when modeling water and solute movement at scales of mm or μm , or when directly modeling water and nutrient uptake by individual root hairs. In my model and many of the others Zhang has cited solutions are calculated at scales of cm (1 cm^3 in 3DMIPS).
 - c. Following up on the previous point, the problem gets even more complicated with the addition of plants. In this case, to simultaneously solve the soil equations would also require a simultaneous solution of the plant equations since many soil components which appear as constants (for example, c and w in Zhang's equations 2, 5, and 6) are not. Both c and w are complex functions of, c , root diameter, root length, leaf water potential, root water resistance, soil water resistance, etc. This would be a daunting task mostly because of differences in the formulation and time steps of the soil and plant equations. As a result, in most models, including 3DMIPS, the equations are solved sequentially starting with the plant equations and then followed by the temperature, water, and solute equations. Thus, the need to treat many of the variables we discussed above, Cl_{buffer} , C_h , etc., as constants at each Δt step of the numerical integration and then recalculate them at the next Δt step. A similar approach is used by Campbell (1985) to solve the solute movement equation this time by sequentially solving the soil water equation and then the solute movement equation.
4. The other major point raised by Zhang suggested that the complex root architecture used in 3DMIPS would generate a complicated water flow field and thus require a second-order tensor. Actually this is not applicable to 3DMIPS. Of course, if one were to model individual root hairs in a 3D space, which would be equivalent to modeling water movement "inside" a fractal porous medium, then a tensor would be needed since the roots would be located in various positions, interfere with each other, and thus there would be a requirement of including cross-direction anisotropic dispersion.

3DMIPS, however, does not model individual roots and, therefore, there is no need to incorporate cross-direction anisotropic dispersion. The way 3DMIPS treat roots is as follows:

- a. Root lateral spread, root biomass distribution by depth, and root surface area equations (equations 29–34 in Biondini, 2001) are used to calculate the total amount of root surface area within each of the $\Delta_x \Delta_y \Delta_z$ cubes (1 cm^3) used in the numerical integration algorithms.
- b. 3DMIPS uses total root surface area to calculate the amount of nutrient solute taken by each plant from each $\Delta_x \Delta_y \Delta_z$ integration cube. There is no complicated movement of solutes to individual roots that are located at various angles and that interfere with each other and thus no need for anisotropic dispersion. In the numerical integration algorithms, thus, diffusion and mass flow can be calculated in a standard way strictly along the x , then y , and then z directions.

References

- Barber, S.A., 1984. Soil Nutrient Bioavailability: A Mechanistic Approach. Wiley, New York.
- Biondini, M.E., 2001. A three dimensional spatial model for plant competition in a heterogeneous soil environment. *Ecol. Modell.* 142, 189–225.
- Caassen, N.S.A., Barber, S.A., 1976. Simulation model for nutrient uptake from soil by a growing plant root system. *Agron. J.* 68, 961–964.
- Campbell, G.S., 1985. *Soil Physics with BASIC*. Elsevier, New York.
- Edwards, J.H., Barber, S.A., 1976. Phosphorus uptake rate of soybean roots as influenced by plant age, root trimming, and solution P concentration. *Agron. J.* 68, 973–975.
- Jungk, A.S.A., Barber, S.A., 1975. Plant age and the phosphorus uptake characteristics of trimmed and untrimmed corn root Systems. *Plant Soil* 42, 227–239.
- Mitchella, R., Mayerb, A., 1998. A numerical model for transient-hysteretic flow and solute transport in unsaturated porous media. *J. Contam. Hydrol.* 30, 243–264.
- Silberbush, M., Barber, S.A., 1983. Sensitivity analysis of parameters used in simulating K uptake with a mechanistic mathematical model. *Agron. J.* 75, 851–854.

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