

## A different approach to the modified Picard method for water flow in variably saturated media

P.Galvao<sup>a</sup>, P. Chambel Leitao <sup>a</sup>, Ramiro Neves<sup>a</sup> and Paulo Chambel Leitao <sup>b</sup>

<sup>a</sup>Technical University of Lisbon, Instituto Superior Tecnico - MARETEC Environment and Energy Section - Mechanical engineering Department  
Av. Rovisco Pais 1049-001 Lisboa Portugal

<sup>b</sup>HIDROMOD,  
Taguspark Nucleo Central, 349 2780-920 Oeiras Portugal.

Celia et al. (1990) identified a lack of mass conservation when a cross derivative  $\frac{\partial \theta}{\partial h} \frac{\partial h}{\partial t}$  was used in Richards Equation (RE) (which originates the  $h$  based RE). According to the same author a perfectly mass conservative algorithm can be derived by expanding a Taylor series with respect to  $h$  instead of using cross derivatives. This originated the "h-modified Picard method" (as it was called in Pan and Wierenga (1995)). This transformation is widely used in variable saturated flow models, namely Hydrus and Mohid model.

On the other hand the use of cross derivatives  $\frac{\partial h}{\partial \theta} \frac{\partial \theta}{\partial z}$  in RE (which originates the  $\theta$  based RE), also causes problems in heterogeneous soils and saturation conditions. This can be solved using the same principle as the one used by Celia et al. (1990) but in the right side of RE, applying a Taylor series expansion with respect to  $\theta$ . This produces " $\theta$ - biased modified Picard method", since  $\theta$  is the dependent variable. This transformation is used in Mohid model.

Similar results were obtained for "h -modified Picard method" and " $\theta$  -modified Picard method". However in some situations " $\theta$  -modified Picard method" as revealed to be more robust than "h -modified Picard method".

This paper reports the advantages and disadvantages of " $\theta$  -modified Picard method". It also compares it with a recent approach to RE transformation and with Hydrus. Some additional results show the influence of using absolute convergence criteria and the criteria proposed in Huang et al. (1995).

Applications included schematic situations and yearlong simulations of a soil in Alvalade, Portugal where actual data exists (Neves 2002).

### 1. Introduction

Commonly, Richards' equation that derives from mass conservation and Darcy Buckingham flux law is used to calculate flow in these mediums.

$$\frac{\partial \theta}{\partial t} = \nabla \cdot K(h) \nabla h - \frac{\partial K}{\partial z} \quad (1)$$

Where  $\theta$  and  $h$  are volumetric water content and pressure head ;  $K$  is the hydraulic conductivity (considered constant in saturated soils, but has strong dependence on water content on unsaturated soils). Since 2 variables are present in this equation, a relation between water content and head is needed to obtain a closed system. These relations are known as retention curves, for instance Van Genuchten (1980).

The nonlinearity of such relations leads to difficulties in using Richard's equations, from time expensive calculations to mass balance errors.

## 2. Background

The traditional method for solving Richards equation is based on a substitution of either the head or the water content variable by the relation between them (ex: Van Genuchten(1980)). This leads to the theta and head form of Richards equation, both these forms together with Picard or Newton iterations have been described by many authors with various degrees of success (Davis and Neumann, 1983; Hills et al., 1989; Kirkland et al. 1992, etc).

Both approaches have advantages and disadvantages. For instance the head form is known to create mass balance errors, while the theta form has shown bad performance in layered soils.

The approach used in both methods is quite similar: since we know the analytical form of  $\theta(h)$  the derivative  $\frac{\partial\theta}{\partial h}$  is also known. As so we can rewrite Richards equation as:

$$\frac{\partial\theta}{\partial h} \frac{\partial h}{\partial t} = \nabla \cdot (K(h) \nabla [h + z]) \quad (2)$$

$$\frac{\partial\theta}{\partial t} = \nabla \cdot \left( K(h) \frac{\partial h}{\partial\theta} \nabla [\theta + z] \right) \quad (3)$$

When solving these equations with an implicit algorithm and the finite volume method one would obtain (for one-dimensional situation):

For the  $h$  form:

$$\begin{aligned} \left( \frac{\partial\theta}{\partial h} \right)_{ijk} \frac{h_{ijk}^{dt+1} - h_{ijk}^{dt}}{\Delta t} = & + \frac{1}{V_{ijk}^{dt}} A_{ij} K \left( h_{ijk+\frac{1}{2}}^{dt+1} \right) \left[ \frac{h_{ijk+1}^{dt+1} - h_{ijk}^{dt+1}}{ZCC_{ijk+1} - ZCC_{ijk}} + 1 \right] \\ & - \frac{1}{V_{ijk}^{dt}} A_{ij} K \left( h_{ijk-\frac{1}{2}}^{dt+1} \right) \left[ \frac{h_{ijk}^{dt+1} - h_{ijk-1}^{dt+1}}{ZCC_{ijk} - ZCC_{ijk-1}} + 1 \right] \end{aligned} \quad (4)$$

For the  $\theta$  form.

$$\begin{aligned} \frac{\theta_{ijk}^{dt+1} - \theta_{ijk}^{dt}}{\Delta t} = & + \frac{1}{V_{ijk}^{dt}} A_{ij} K \left( \theta_{ijk+\frac{1}{2}}^{dt+1} \right) \left( \frac{\partial h}{\partial\theta} \right)_{ijk+\frac{1}{2}}^{dt+1} \left[ \frac{\theta_{ijk+1}^{dt+1} - \theta_{ijk}^{dt+1}}{ZCC_{ijk+1} - ZCC_{ijk}} + 1 \right] \\ & - \frac{1}{V_{ijk}^{dt}} A_{ij} K \left( \theta_{ijk-\frac{1}{2}}^{dt+1} \right) \left( \frac{\partial h}{\partial\theta} \right)_{ijk-\frac{1}{2}}^{dt+1} \left[ \frac{\theta_{ijk}^{dt+1} - \theta_{ijk-1}^{dt+1}}{ZCC_{ijk} - ZCC_{ijk-1}} + 1 \right] \end{aligned} \quad (5)$$

Where  $dt$  is the time level,  $i, j, k$  are the cell location ( $k$  for vertical coordinate),  $ZCC$  is the center of each cell  $A_{i,j}$  is the area where the flux occurs.

The truth is that neither of these new equations looks that good, they still are not linear due to the conductivity  $K(h)$  or  $K(\theta)$  and the new derivative terms, so an iterative

process is still needed. However, both these coefficients can be "lagged" (ie. Evaluated at the previous iteration), so we would obtain ( $it$  is the iteration level) for the  $h$  form.

$$\begin{aligned} \left(\frac{\partial \theta}{\partial h}\right)_{ijk}^{dt+1,it} \frac{h_{ijk}^{dt+1,it+1} - h_{ijk}^{dt}}{\Delta t} = & + \frac{1}{V_{ijk}^{dt}} A_{ij} K(h_{ijk+\frac{1}{2}}^{dt+1,it}) \left[ \frac{h_{ijk+\frac{1}{2}}^{dt+1,it+1} - h_{ijk}^{dt+1,it+1}}{ZCC_{ijk+1} - ZCC_{ijk}} + 1 \right] \\ & - \frac{1}{V_{ijk}^{dt}} A_{ij} K(h_{ijk-\frac{1}{2}}^{dt+1,it}) \left[ \frac{h_{ijk}^{dt+1,it+1} - h_{ijk-1}^{dt+1,it+1}}{ZCC_{ijk} - ZCC_{ijk-1}} + 1 \right] \end{aligned} \quad (6)$$

And for the  $\theta$  form:

$$\begin{aligned} \frac{\theta_{ijk}^{dt+1,it+1} - \theta_{ijk}^{dt}}{\Delta t} = & + \frac{1}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk+\frac{1}{2}}^{dt+1,it}) \left(\frac{\partial \theta}{\partial h}\right)_{ijk+\frac{1}{2}}^{dt+1,it} \left[ \frac{\theta_{ijk+\frac{1}{2}}^{dt+1,it+1} - \theta_{ijk}^{dt+1,it+1}}{ZCC_{ijk+1} - ZCC_{ijk}} + 1 \right] \\ & - \frac{1}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk-\frac{1}{2}}^{dt+1,it}) \left(\frac{\partial \theta}{\partial h}\right)_{ijk-\frac{1}{2}}^{dt+1,it} \left[ \frac{\theta_{ijk}^{dt+1,it+1} - \theta_{ijk-1}^{dt+1,it+1}}{ZCC_{ijk} - ZCC_{ijk-1}} + 1 \right] \end{aligned} \quad (7)$$

A Picard like iterative process would replace the new calculated values of either  $h$  or  $\theta$ , for all variables calculated in ( $it$ ), and repeat all calculations. This process would continue until consecutive values of the main variable doesn't vary more than a given values. More complex and efficient convergence criteria can be used Huang *et al.*(1995).

In 1990 Celia *et. all* has shown a method to derive a perfectly mass conservative solution for Richards equation, that also performed well in layered soils. Using a Taylor series to expand  $\theta^{dt+1,it+1}$  about  $h$  in the original form of Richards equation.

Many developments have followed Celia original article Huang *et al.*(1995). However the original head form of Richards equations shows bad performances for the same reason that the  $\theta$  form, the cross derivatives representation of  $\frac{\partial \theta}{\partial t}$  or  $\frac{\partial h}{\partial z}$  create problems. This article attempts the same formulation but expanding in Taylor series the left side of 1.

### 3. Proposed Method

The modified Piccard method shown in Celia et al. 1990 solved the mass conservation problems that were raised from the use of the standard  $h$ -form of the Richards equation. This procedure is similar to the "quasy-Newton" method used by Allen et al., and displays good mass balance (Celia 1990).

Instead of replacing  $\frac{\partial \theta}{\partial t}$  with  $\frac{\partial \theta}{\partial h} \frac{\partial h}{\partial t}$ , the mixed form is used. When this equation is discretized, besides the variable for which the system will be solved ( $h^{dt+1,it+1}$ ), another variable appears  $\theta^{dt+1,it+1}$

$$\frac{\theta^{dt+1,it+1} - \theta^{dt}}{\Delta t} = f(h^{dt+1,it+1}) \quad (8)$$

But a Taylor series with the expansion of  $\theta^{dt+1,it+1}$  about  $h$  can be used to replace this variable.

$$\theta^{dt+1,it+1} = \theta^{dt+1,it} + \left. \frac{\partial \theta}{\partial h} \right|^{dt+1,it} (h^{dt+1,it+1} - h^{dt+1,it}) \quad (9)$$

This variable change is performed and the iterative process continues. This method is reported in Celia 1990 as perfectly mass conservative. This "modified method" was implemented in most of the available software that is used today to predict flow in variable

saturated media (HYDRUS, RZWQM). However and following the ideas of Pan and Wirenga (1995) the correct term should be "h-modified Picard", which leads to the idea of applying this method to obtain a " $\theta$ -modified Picard" form of Richards equation.

The "core" of the modified Picard is the use of a Taylor series, about the expansion point  $h^{dt+1,it}$  so for the water content formulation of Richards equation the same expansion is performed about  $\theta^{dt+1,it}$ :

$$h^{dt+1,it+1} = h^{dt+1,it} + \left. \frac{dh}{d\theta} \right|^{dt+1,it} (\theta^{dt+1,it+1} - \theta^{dt+1,it}) + 0\delta^2 \quad (10)$$

Describing the vertical water flux, using the finite volume formulation:

$$\frac{V_{ijk}^{dt+1}\theta_{ijk}^{dt+1} - V_{ijk}^{dt}\theta_{ijk}^{dt}}{\Delta t} = -A_{ij}F_{i,j,k+\frac{1}{2}} + A_{ij}F_{i,j,k-\frac{1}{2}} \quad (11)$$

Where  $F$  is the water flux in each of the faces bounding the control volume.

Since the explicit approach proves to be too restrictive in terms of space and time discretization, an implicit approximation is preferred, and as so both the fluxes on the right hand side must be evaluated at  $dt + 1$ . Assuming that no control volume changes occur:

$$\begin{aligned} \frac{\theta_{ijk}^{dt+1} - \theta_{ijk}^{dt}}{\Delta t} = & + \frac{1}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk+\frac{1}{2}}^{dt+1}) \left[ \frac{h_{ijk+1}^{dt+1} - h_{ijk}^{dt+1}}{ZCC_{ijk+1} - ZCC_{ijk}} + 1 \right] \\ & - \frac{1}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk-\frac{1}{2}}^{dt+1}) \left[ \frac{h_{ijk}^{dt+1} - h_{ijk-1}^{dt+1}}{ZCC_{ijk} - ZCC_{ijk-1}} + 1 \right] \end{aligned} \quad (12)$$

The " $\theta$ -modified Picard", replaces the unknown value of  $h^{dt+1}$  as a function of  $\theta^{dt+1}$  maintaining an implicit approach and good mass balance.

$$h^{dt+1,it+1} = de\theta^{dt+1,it+1} - de\theta^{dt+1,it} + h^{dt+1,it} \quad (13)$$

Where  $de = \left. \frac{dh}{d\theta} \right|^{dt+1,it}$  Replacing 13 in 12

$$\begin{aligned} \frac{\theta_{ijk}^{dt+1,it+1} - \theta_{ijk}^{dt}}{\Delta t} = & + \frac{1}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk+\frac{1}{2}}^{dt+1}) \left[ \frac{(de_{ijk+1}\theta_{ijk+1}^{dt+1,it+1} - de_{ijk+1}\theta_{ijk+1}^{dt+1,it} + h_{ijk+1}^{dt+1,it}) - (de_{ijk}\theta_{ijk}^{dt+1,it+1} - de_{ijk}\theta_{ijk}^{dt+1,it} + h_{ijk}^{dt+1,it})}{ZCC_{ijk+1} - ZCC_{ijk}} + 1 \right] \\ & - \frac{1}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk-\frac{1}{2}}^{dt+1}) \left[ \frac{(de_{ijk}\theta_{ijk}^{dt+1,it+1} - de_{ijk}\theta_{ijk}^{dt+1,it} + h_{ijk}^{dt+1,it}) - (de_{ijk-1}\theta_{ijk-1}^{dt+1,it+1} - de_{ijk-1}\theta_{ijk-1}^{dt+1,it} + h_{ijk-1}^{dt+1,it})}{ZCC_{ijk} - ZCC_{ijk-1}} + 1 \right] \end{aligned} \quad (14)$$

Equation 14 solves the problems that arise from cross derivative  $\frac{\partial h}{\partial \theta} \frac{\partial \theta}{\partial z}$ , however 14 is not linear due to the dependence of the conductivity on the water content. Since the iterative process is set up, we will simply lag the conductivity coefficients to the last iteration values.

Creating a matrix for the system in the form:

$$\begin{bmatrix} E & F & 0 \\ D & E & F \\ 0 & D & E \end{bmatrix} [\theta] = [Ti] \quad (15)$$

$$D_{coef} = -\frac{\Delta t}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk-\frac{1}{2}}^{dt+1,it}) \left[ \frac{de_{ijk-1}}{ZCC_{ijk} - ZCC_{ijk-1}} \right] \quad (16)$$

$$E_{coef} = 1 + \frac{\Delta t}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk+\frac{1}{2}}^{dt+1,it}) \left[ \frac{de_{ijk}}{ZCC_{ijk+1} - ZCC_{ijk}} \right] \\ + \frac{\Delta t}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk-\frac{1}{2}}^{dt+1,it}) \left[ \frac{de_{ijk}}{ZCC_{ijk} - ZCC_{ijk-1}} \right] \quad (17)$$

$$F_{coef} = -\frac{\Delta t}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk+\frac{1}{2}}^{dt+1,it}) \left[ \frac{de_{ijk+1}}{ZCC_{ijk+1} - ZCC_{ijk}} \right] \quad (18)$$

$$Ti_{coef} = \theta_{ijk}^{dt} \\ + \frac{\Delta t}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk+\frac{1}{2}}^{dt+1,it}) \left[ \frac{de_{ijk}\theta_{ijk}^{dt+1,it} - de_{ijk+1}\theta_{ijk+1}^{dt+1,it}}{ZCC_{ijk+1} - ZCC_{ijk}} \right] \\ - \frac{\Delta t}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk-\frac{1}{2}}^{dt+1,it}) \left[ \frac{de_{ijk-1}\theta_{ijk-1}^{dt+1,it} - de_{ijk}\theta_{ijk}^{dt+1,it}}{ZCC_{ijk} - ZCC_{ijk-1}} \right] \\ - \frac{\Delta t}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk-\frac{1}{2}}^{dt+1,it}) \left[ \frac{h_{ijk}^{dt+1,it} - h_{ijk-1}^{dt+1,it}}{ZCC_{ijk} - ZCC_{ijk-1}} + 1 \right] \\ + \frac{\Delta t}{V_{ijk}^{dt}} A_{ij} K(\theta_{ijk+\frac{1}{2}}^{dt+1,it}) \left[ \frac{h_{ijk+1}^{dt+1,it} - h_{ijk}^{dt+1,it}}{ZCC_{ijk+1} - ZCC_{ijk}} + 1 \right] \quad (19)$$

## 4. Numerical Experiments

### 4.1. Schematic Situations

The first tests that were performed used a one-dimensional model for a soil column with 20 cells (numbered from bottom to top). Each cell has a height of 5 cm and 1m width. In order to evaluate the convergence power of each method, a large step gradient was imposed in the top boundary, a water content value of 0.3 was imposed in the top cell while the rest of the soil was in a dry situation (0.007). Soil hydraulic parameters (according with Van Genuchten(1980) model) used in these simulations were identical to the parameters measured in the surface layer of a soil in Alvalade - Portugal (table 1).

Table 1  
Alvalade Soil Parameters Goncalves *et al.* 2003

$\theta_r$	$\theta_s$	$\alpha$ 1/dm	n dm/day	$K_s$ dm/day	L
0	0.3727	0.395	1.154	2.13	-6.913

Since the top node is nearly saturated, this creates a massive head gradient of 1.86E11[m].

The initial time step used was of 1E-5 seconds with a max iteration attempts fixed at 200 (after that value time step is reduced). The maximum possible time step was 200 seconds. The time step was allowed to increase if the number of iterations necessary to converge was inferior to 6 iterations. The convergence criterion used proposed by Huang *et al.* 1995.

Both Theta and head based modified Picard methods were applied in this situation. 2 summarizes the necessary iterations to overcome the initial gradient.

Table 2  
Iterations necessary to converge

Elapsed Time	$\theta$ -base modified Picard	$h$ -base modified Picard
0.00001	7	19
0.00001	7	5
0.00002	5	4
0.00003	5	4
0.00004	5	4
0.00005	4	4
0.00006	4	4
0.00007	4	3
0.00008	4	3
0.00009	4	3
0.0001	4	3
0.00011	4	3
0.00012	4	3
0.00013	4	3
0.00014	4	3
0.00015	4	3
0.00016	4	3
0.00017	4	3
0.00018	4	3
0.00019	4	3
0.0002	4	3
0.00021	4	3
0.00022	3	3
0.00023	3	3

For that point on nothing interested occurred, the time step increased and only two iterations were needed to converge. The final results were equivalent with both methods.

The  $h$ -modified Picard method has converged with less iterations for the initial time interval (7 iterations against 19). However after this initial difficulty is overcome, the theta-modified Picard form seems to converge faster reaching five, four and three iteration steps earlier. Overall the head based method performed only less 10 iterations that the theta based form.

Looking at the modified Picard  $\theta$  and  $h$  form variations for the first time step (19 and 7 iterations respectively):

The fact is that in the " $\theta$ -modified Picard" the large water flux registered on the frontier between the 19 and 20 node over saturates cell 19, leading to an impossible water content value of  $2.2 \left[ \frac{m^3_{H_2O}}{m^3_{soil}} \right]$ .

This presents a problem, the first iteration predicts an over saturated value for water content. Water retention curves do not supply values for over saturated or negative (physically impossible) water content values. So when second iteration starts, no derivative

Figure 1. Soil water content variations for the first time step in the head form (initial condition and iterations 1,5,7)

Figure 2. Soil water content variations for the first time step in the theta form (initial condition and iterations 1,4,12,13,17)

or head values are available to use in 20

$$\frac{\theta^{dt+1,it+1} - \theta^{dt}}{\Delta t} = f(h^{dt+1,it+1}) \quad (20)$$

However the derivative can be approached by a Taylor series 21, if we prolong the retention curve as a constant line for over saturated values and negative water contents, the iterative process can continue.

$$\left. \frac{dh}{d\theta} \right|^{dt+1,it} = \frac{h^{dt+1,it} - h^{dt}}{\theta^{dt+1,it} - \theta^{dt}} \quad (21)$$

The reason no over saturated values are predicted by the head form can be explained by looking at the descretization obtained using this method (in the form  $AX=B$ , where  $A$  is the coefficient matrix):

$$D_{coef} = -\frac{\Delta t}{V_{ijk}^{dt}} \frac{A_{ij}K(\theta_{ijk-\frac{1}{2}}^{dt+1,it})}{ZCC_{ijk} - ZCC_{ijk-1}} \quad (22)$$

$$E_{coef} = de_{ijk} + \frac{\Delta t}{V_{ijk}^{dt}} \frac{A_{ij}K(\theta_{ijk-\frac{1}{2}}^{dt+1,it})}{ZCC_{ijk} - ZCC_{ijk-1}} + \frac{\Delta t}{V_{ijk}^{dt}} \frac{A_{ij}K(\theta_{ijk+\frac{1}{2}}^{dt+1,it})}{ZCC_{ijk+1} - ZCC_{ijk}} \quad (23)$$

$$F_{coef} = -\frac{\Delta t}{V_{ijk}^{dt}} \frac{A_{ij}K(\theta_{ijk+\frac{1}{2}}^{dt+1,it})}{ZCC_{ijk+1} - ZCC_{ijk}} \quad (24)$$

$$Ti_{coef} = de_{ijk}h_{ijk}^{dt+1,it} - \theta_{ijk}^{dt+1,it} + \theta_{ijk}^{dt} + \frac{\Delta t}{V_{ijk}^{dt}} A_{ij}K(\theta_{ijk+\frac{1}{2}}^{dt+1,it}) - \frac{\Delta t}{V_{ijk}^{dt}} A_{ij}K(\theta_{ijk-\frac{1}{2}}^{dt+1,it}) \quad (25)$$

No matter how high the pressure head is on the upper node, Dcoef will always create a positive value when multiplied by that pressure head. The same occurs with Ecoef. The Ticoef will never predict a positive value, so no positive values of  $h$  can ever be predicted (unless source terms are included).

On the other hand the Ticoef for the theta -modified Picard (19) can predict over saturated values due to the fluxes calculated at the previous iteration.

Repeating this rehearsal but with an initial time step of 100 second:

This time even though the "modified Picard h form" converges faster than the "modified Picard theta form" in the first iteration (18 iterations against 30), the theta form in the final performs less 97 iterations in a total of 5135 against the 5232 performed by the head form.

Additional test were performed in layered soils again with equivalent results from both forms.

#### 4.2. Field validation

After analysis on schematic test runs, the modified Picard theta form was tested with field data. Gonalves et al. (2003) made a one-year period of field water contents measures in three monoliths of a Eutric Fluvisol. Each monolith was a parallelepiped with an area of approximately 1.1x1.1 meter and a depth of 1 meter. The water content measuring devices (TDR probes) were installed in monoliths at 10, 30, 50 and 70 cm depth. The hydraulic properties were measured by Gonalves et al. (2003), for the three soil layers.

Table 3  
Alvalade hydraulic properties for three profiles

Depth	$\theta_r$	$\theta_s$	$\alpha$ 1/dm	n dm/day	$K_s$ dm/day	L
0-48	0	0.427	0.292	1.208	1.82	-4.391
48-85	0	0.4275	1.083	1.161	9.94	-5.909
>85	0	0.3727	0.395	1.154	2.13	-6.913

Hydrus was used has a "h modified Picard" benchmark software. After a calibration process based on water content measured until end of September 2001, the model was validated against values of water content collected until May 2002. A simulation was made using rainfall measures and ETo calculations. Figure 1 shows the water content prediction (with Mohid and Hydrus models).

Figure 3. Water content evolution: simulated (with calibration) and measured values at 10, 30, 50 and 70 cm.

Figure 4. Water content evolution: simulated (with new options included in MOHID) and measured values at 10, 30, 50 and 70 cm.

In the Figure 3 is possible to see that both Mohid and Hydrus models give the same results. However the models were not validated because of differences between simulated values and data measured between November and February, which corresponds to the none calibrated period. This results show that some simplifications considered in the calibration (using the inverse method) were not accurate. One simplification was that soil water content did not significantly influence evaporation. The other one was considering that macropores were implicitly simulated in soil hydraulic properties.

New options were introduced to Mohid which allowed: i) calculating evaporation as a function of soil water content and ii) considering the hysteretic effect of macropores in vertical soil water conductivity. For evaporation it was used the FAO method for a bare soil. For hysteretic effect of macropores a numerical solution was found. It was considered that the conductivity calculated in the faces was the maximum of adjacent cells for downward flow and average for upward flow.

This new options in Mohid improved results (Figure 4). However it was concluded that numerical macropore simulation was not enough to simulate completely the effect of macropores (Chambel-Leitao et al., 2003). Because of that is currently under development a module to simulate macropores in Mohid.

## 5. Summary and Conclusion

Theta -modified Picard form is a valid alternative to the traditional h -modified Picard. The main advantage of this formulation is its ability to recover from negative or over saturated water content predictions using an approximation to the derivative of the water retention function. The traditional modified Picard head form has show better performances at localized events with hight gradients. However the iteration process used by this method can predict positive head values for negative water contents, a situation from which is no possible recovery, leading to a decrease in the time step. The new approach still suffers from problems in saturated media. A mixed process solving either the modified Picard head or the modified Picard theta form could present some advantages.

## REFERENCES

1. J. Bear. Intruduction to Modeling transport Phenomena in Porous Media. Kluwer academic Publishers (1991)
2. M.A. Celia, E. T. Bououtas and R. L. Zarba. A general mass-concervative numerical solution for the unsaturated flow equation. *Water Resour. Res.*, 26, 1496, (1990).
3. K. Huang, B.P. Mohanty and M.Th. van Genuchten. A New Convergence Criterion for Modified Picard Iteration to Solve Variably-Saturated Flow Equation. *Journal of Hydrology*. 178, 69-91, (1996)
4. R.G. Hills, I. Porro, D. B. Hudson and P.J.Wierenga. Modeling one-dimensional infiltration into very dry soils. 1. Model development and evaluation, *Water Resources Research*,25(6), 1259-1269, (1989).
5. M. R. Kirkland, R. G. Hills, and P. J. Wierenga. Algorithms for solving Richards equation for variably saturated soils, *Water Resources Research*, 28(8), 2049-2058, (1992).
6. L.Pan, and P. J. Wierenga. A transformed pressure head-based approach to solve

- Richards equation for variably saturated soils, *Water Resources Research*, 31(4), 925-931, 1995.
7. K. Rathfelder and L. M. Abriola. Mass conservative numerical solutions of the head-based Richards equation, *Water Resources Research*, 30(9), 2579- 2586, (1994).
  8. P. Chambel-Leitao, M.C. Goncalves, R. Neves, P. Galvao, M.E. Mesquita. Modelling soil dynamic of solutes and water. *Revista de Ciencias Agrarias* (submitted for publication) (2003).
  9. M. C. Goncalves, J. C. Martins, A. Oliveira, F. P. Pires, A. R. Goncalves, J. Bica and M. Bica. Preliminary study about evolution of the salinisation and alkalisation of a Fluvisol, irrigated with different quality waters, in Alvalade Sado (Alentejo). *Revista de Ciencias Agrarias* (in press) (2003).