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# Initial results in the development of a near-surface component for use in a performance assessment model for the geological disposal of nuclear waste

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**ABSTRACT**

The proposed method of geological disposal for the UK's nuclear legacy waste creates a need for performance assessment models which can guide decisions about the suitability of sites for waste repositories. These models are typically run several times with multiple scenarios and simulate processes occurring over 100 million years. Even with modern computing technology, this can present impractically long run times. Therefore there is a need for fast, reliable and accurate numerical solutions to the nonlinear Richards equation, which describes flow, and the governing equations for contaminant transport. The initial results from the modelling efforts to produce a one dimensional flow model are presented in this paper. The limited results show the potential advantages of implicit finite difference methods of solving Richards' equation, as well as the need for further work in implementing a well-established method with an user-specified accuracy criterion.

## INTRODUCTION

In their recommendations to government, the Committee on Radioactive Waste Management (CoRWM, 2006) endorsed geological disposal as a long term strategy for UK nuclear legacy waste. Another facet of their recommendations was that site selection be made on the basis of community 'volunteerism', a scheme which would involve the government working in close partnership with communities who express a willingness to host repositories. Both the severity of the risk associated with radionuclide contamination of the biosphere and the high levels of public involvement in the site selection process make the development of robust, defensible and transparent performance (or risk) assessment models very important.

Performance assessment models numerically solve the governing equations for physical and chemical processes involved in radionuclide transport. They predict the temporally and spatially varying distribution of radionuclide contaminants from their source (at the underground repository) via their pathway (the subsurface) to a receptor of interest. In more recent research, interest in endpoint receptors has expanded from humans only to biota more generally (e.g. *Patton et al.*, 2000). The aim of this project is to develop the near-surface component of the performance assessment model, dealing specifically with the influence of soil heterogeneity on flow and transport processes in the unsaturated zone and hence on dose rates to plant receptors.

*Wheater et al.* (2007) recently published the results of nearly 20 years of experiments conducted by Imperial College quantifying the uptake of radionuclides grown in lysimeters at Silwood Park. Early modelling efforts to simulate the results of this field work have been documented in *Butler et al.* (1999). More recently, *Mathias et al.* (2008) developed a method of finding the optimal upscaled parameters for the plant solute and water uptake response of a heterogeneous field. In their model of the unsaturated zone, horizontal heterogeneity is incorporated as a series of parallel, internally homogenous soil columns, flow in each of which the flow is independent (the 'streamtube' assumption, see *Vereecken et al.*, 2007). Each column is assigned different soil properties from one of 105 uniformly distributed points, triangle-shaped range on the soil texture triangle which incorporates the actual range of soil textures found in the lysimeters at Silwood. Using a Nash Sutcliffe efficiency criterion, they identified a single set of soil hydraulic parameters which best represented the combined response, with a view to using these as 'field-scale' parameters to reduce the computational burden for a regional scale performance assessment model. Their results showed a highly non-linear relationship between the upscaled parameter values and their effectiveness in acting as surrogates for the heterogeneity of the model, particularly in cases where the water table was significantly below the root tips.

*Mathias et al.* (2008) used the MATLAB ode15s stiff solver to perform the numerical time integration in the solution of the flow and transport equations. This method is not suitable for multiple runs in three dimensions because the internal precision of the algorithm makes it slow. While the precision is a benefit in some sense, it has been argued that the inherent uncertainties in soil hydraulic parameters and the sometimes poor representation of physical and chemical processes in the governing equations mean the extra computational time required is not consistent with the nature of the problem (e.g. van Genuchten, 1982). With this in mind, the first step in building on the work of *Mathias et al.* (2008) is to implement a fast and robust numerical method, for which accuracy can be specified by the user.

Richards' equation (*Richards*, 1931) describes flow in unsaturated porous media. The numerical solution to Richards' equation is a well-explored area of academic research because of its central importance in numerous hydrological flow problems. One of the most well known and widely used methods for solving Richards' equation was developed by *Celia et al.* (1990). Their finite difference method uses a linearised, mixed form of the Richards' equation which minimises error by iterating within time steps. They have shown that the solution is mass conservative, and free from numerical oscillations. It has proved to offer an attractive combination of accuracy, numerical stability and simplicity to code in comparison to alternative methods (*Paniconi et al.*, 1991 and *Paniconi and Putti*, 1994). Other researchers have effectively modified the form presented by *Celia et al.* (1990) increasing its efficiency (e.g. *Huang et al.*, 1994; *van Dam and Feddes*, 2000). An interim goal of this project is to implement the *Celia et al.* (1990) method in three dimensional problems.

## GOVERNING EQUATIONS

The continuity equation for one dimensional flow through an unsaturated porous media is:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial t} \tag{1}$$

Where $\theta$ (-) is moisture content, $t$ (s) is time, $q$ (cm/d) is water flux and $z$ (cm) is depth measured downwards from the top of the soil column.

To solve the continuity equation the following equations are also needed:

$$\frac{\partial \theta}{\partial t} = \left(S_e S_s + \frac{\partial \theta}{\partial \psi}\right)\frac{\partial q}{\partial t} \tag{2}$$

and

$$q = -K(\psi)\left(\frac{\partial \psi}{\partial t} - 1\right) \tag{3}$$

Where $S_e$ (-) is the effective saturation, $S_s$ ($cm^{-1}$) is the specific storage term and $K$ (cm/d) is the unsaturated hydraulic conductivity of the soil. $K$ has been found from the van Genuchten-Mualem relationship (*van Genuchten*, 1980; *Mualem*, 1976):

$$K = K_s S_e^{\eta}\left[1 - \left(1 - S_e^{\frac{1}{m}}\right)^m\right]^2 \tag{4}$$

with

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left(\frac{1}{1 + |\alpha\psi|^n}\right)^m \tag{5}$$

$\theta_r$ (-) and $\theta_s$ (-) are the residual and saturated moisture contents respectively, $K_s$ (cm/d) is the saturated hydraulic conductivity and $\alpha$, $\eta$, $n$ and $m=1 -1/n$ are empirical parameters.

This is often presented in the form of Richards' equation (*Richards*, 1931):

$$C(\psi)\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z} - 1\right)\right] \tag{6}$$

where the specific capacity, $C$ ($cm^{-1}$) is given by:

$$C(\psi) = \frac{\partial \theta}{\partial \psi} \tag{7}$$

## MODEL DESCRIPTION

A model to simulate one dimensional flow in a single porous medium has been developed (Figure 1). The soil column has a total length of 100 cm and is discretised using $N$ block-centred nodes. Space and time stepping may be distributed evenly or logarithmically. The boundary and initial conditions for all the results in Table 1 were:

$$\begin{array}{lll} \psi = -500cm & 0 \le z \le 100cm & t = 0 \\ \psi = -500cm & z = 100cm & t > 0 \\ q_0 = 24cm/d & z = 0 & t > 0 \end{array} \tag{8}$$

Where $\psi$ is the pore water pressure head, $z$ is the depth, measured from the top of the column and $q_0$ is the flux at the boundary.

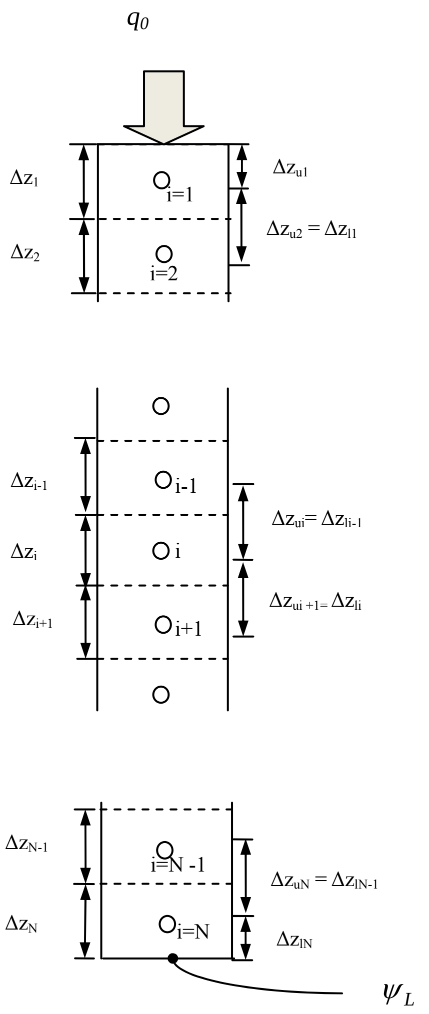


**Figure 1** Model diagram showing method of spatial discretisation and boundary conditions

## NUMERICAL METHOD

Although the intention of this research was to implement the *Celia et al.* (1990) discretisation immediately, coding difficulties arose in implementation of the iteration process. As a stage within the model building process, a non-iterative method, simple implicit method (referred to hereafter as SIM) was used to solve Richards' equation instead. As with *Celia et al.* (1990), this method uses a backward difference approximation in time and the hydraulic properties at each time step are found from the heads at the previous time step. However, the iterative procedure of *Celia et al.* (1990) has several advantages over SIM, namely:

- it works to a specified tolerance, which can be set either on head or moisture content (*Huang et al.*, 1996);
- it is more efficient (faster for a given level of precision), performing more iterations in regions of the solution space where change is occurring rapidly in time; and
- it can be set up to reduce the time-step size in the cases where a prescribed maximum number of iterations has been reached, but the accuracy criterion was not satisfied.

By contrast, SIM will often fail to produce the desired level of accuracy, and can diverge greatly from the true solution. The experience of the author is that error introduced in the time stepping process, and can usually be solve by re-running the simulation with more time nodes (see table 1). The 'trial and error' nature of this procedure is obviously undesirable, and increasingly so as simulations become more intensive and take longer to run.

Manipulation of Richards' equation leads to the following discretised form:

$$C(\psi_i)\frac{\psi_i^n}{\Delta t_n} + \frac{K^n_{i+\frac{1}{2}}}{\Delta z_i} - \frac{K^n_{i-\frac{1}{2}}}{\Delta z_i} = \frac{K^n_{i-\frac{1}{2}}}{\Delta z_i \Delta z_{Ui}}\psi^{n+1}_{i-1} + \left(-\frac{C(\psi_i)}{\Delta t_n} - \frac{K^n_{i+1/2}}{\Delta z_i \Delta z_{Li}} - \frac{K^n_{i-1/2}}{\Delta z_i \Delta z_{Ui}}\right)\psi_i^{n+1} + \frac{K^n_{i+1/2}}{\Delta z_i \Delta z_{Li}}\psi^{n+1}_{i+1} \qquad (9)$$

where,

$$K^n_{i+\frac{1}{2}} = \frac{K^n_{i+1} + K^n_i}{2} \quad ; \quad K^n_{i-\frac{1}{2}} = \frac{K^n_i + K^n_{i-1}}{2} \qquad (10), (11)$$

The subscript index, *i*, indicates the spatial node, and the superscript index, n, indicates the time step. Note that the hydraulic conductivity and the specific capacity terms have superscript *n*, indicating that they are evaluated using the pressure heads found at the previous time step (the linearization process). Note also that implicit solves for all spatial nodes simultaneously at each, bringing in the boundary conditions to match the number of knowns and unknowns (the known terms are grouped on the left hand side here).

## RESULTS

In order to compare the performance of SIM with MATLAB's ode15s, the run times of the two models have been compared using different time and space steps. Both codes were tested against the freely available USEPA software CHEMFLO-2000 (*Nofziger and Wu*, 2003) for verification. Excellent agreement was found.

Table 1 shows the results of the performance. All tests were performed with even space and time steps, on the model soil column, using the conditions in (8). The infiltration, $q_0$, was set to 24 *cm/d*. The following soil parameter values were used for all tests: $\theta_r$=0.08, $\theta_s$ =0.43, $K_s$= 48 cm/d,

$\alpha$=0.015 $cm^{-1}$, $n$= 1.875, $\eta$ = 0.5 and $S_s$= $10^{-5}$ $cm^{-1}$. The simulation was performed for 1 day.

The error term has been calculated as follows:

$$\varepsilon_r = \frac{\sum_{i=1}^{N} \left| \frac{\psi_i^e - \psi_i^{SIM}}{\psi_i^e} \right|}{N} \times 100 \qquad (12)$$

Where $\psi_i^e$ is the 'exact' pressure head at node $i$ calculated at time one day by the MATLAB ode15s integrator and $\psi_i^{SIM}$ is the pressure head at node $I$ calculated at time one day by SIM algorithm. Note that the reference pressure head $\psi_i^e$ varies with the spatial step size, $dz$.

**Table 1** Run time comparison of ode15s and SIM using different time and space step sizes

| Space step *dz* (cm) | time step, *dt* (d) | ode15s run time (s) | SIM run time (s) | SIM time as % ode15s time | $\varepsilon_r$ |
|---|---|---|---|---|---|
| 2 | 1/500 | 1.13 | 0.15 | 13.7% | 6.41% |
| 2 | 1/1000 | 1.22 | 0.33 | 26.9% | 3.20% |
| 2 | 1/2000 | 1.25 | 0.67 | 53.8% | 1.59% |
| 2 | 1/5000 | 1.34 | 1.64 | 122.0% | 0.61% |
| 1 | 1/500 | 4.18 | 0.26 | 6.1% | 13.26% |
| 1 | 1/1000 | 4.08 | 0.48 | 11.9% | 4.02% |
| 1 | 1/2000 | 4.13 | 0.99 | 24.0% | 1.99% |
| 1 | 1/5000 | 4.22 | 2.45 | 58.1% | 0.77% |
| 0.2 | 1/500 | 237.56 | 0.92 | 0.4% | 32.78% *(did not converge)* |
| 0.2 | 1/1000 | 241.22 | 1.80 | 0.7% | 8.48% |
| 0.2 | 1/2000 | 241.76 | 3.61 | 1.5% | 6.33% |
| 0.2 | 1/5000 | 243.67 | 9.24 | 3.8% | 1.03% |
| 0.2 | 1/20000 | 245.52 | 36.79 | 15.0% | 0.25% |

## DISCUSSION

The run time of ode15s is independent of time step size, because the algorithm uses its own time step size adaption. The results suggest that for models involving a fine resolution in space, implicit methods such as SIM offer significant time savings over adaptive time step methods such as ode15s, whilst maintaining an acceptable level of accuracy, given the inherent uncertainties in the problem. Time savings are still present but less marked for lower spatial resolutions ($dz$=2cm, $dt$=1/100d). The results also indicate that there is a cross-over point at which using ode15s becomes both quicker and (it is assumed here) more accurate. However, for finer spatial resolutions, there is no justification for using ode15s as even a crude method such as SIM can achieve acceptable accuracy at much lower run times (e.g.$dz$=0.2cm, $dt$=1/20000d). Figure 1 illustrates that SIM exhibits the stability and 'front-smearing' properties observed in implicit methods used by several other authors, (*van Genuchten*, 1982; *Celia et al.*, 1990).

However, it is not possible to control the accuracy of the SIM solution without a reference solution to compare it against. This can be found from in some cases this could be from an analytic or semi-analytic solution to the Richards equation, or from the ode15s solution. The production of a reference solution requires inconvenient extra programming effort and processing time. Where the time step size becomes too large (e.g. $dz$ = 0.2, $dt$ = 1/500), the SIM solution fails to converge because of increased error introduced into the linearised, time-varying $K$ and $C$ terms.

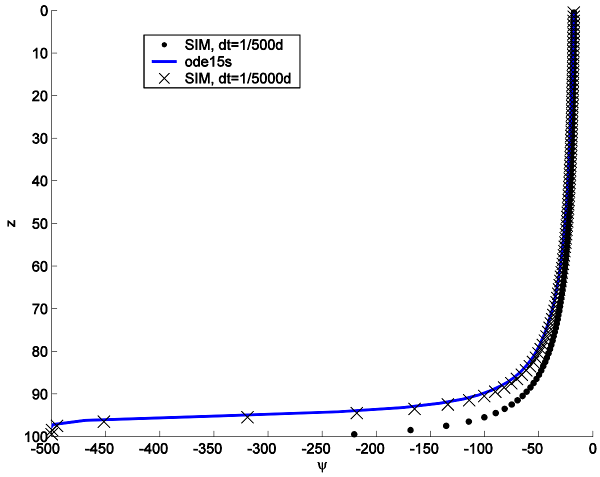


**Figure 2** Comparison of pressure head predictions after one day using ode15s and SIM with two different time-step sizes (dz = 1cm).

## CONCLUSIONS AND FURTHER WORK

The results show the need to control accuracy independent of a reference solution which takes a long time to run. They also show promise that the *Celia et al.* (1990) method, which can be viewed as an extension of the SIM method, will be able to produce much faster simulations than the integrators available in MATLAB. It is expected that for comparable run times *Celia et al.* (1990) will be able to produce more accurate results by focussing computational effort on the nonlinear regions of the problem. By using an error criterion on moisture content as opposed to pressure head, it is hoped that the run times will be even further reduced and solution convergence will be much more regular than with the 'trial and error' approach of SIM (*Huang et al.*, 1996).

For this modelling work to develop into a useful tool for performance assessment the method of *Celia et al.* (1990) must be implemented for both flow and radionuclide contaminant transport. A root extraction model then be added. Following this, the model must be extended to 3 dimensions. The final stage will be to incorporate soil heterogeneity, ensuring that the model could be parameterised cost-effectively using data from currently available site investigation techniques.

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