A WATER INFILTRATION MODEL: STUDY OF REUSABILITY IN AN ENVIRONMENTAL ENGINEERING PROBLEM

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Abstract

The paper describes a computer simulation, involving a site characterization for the storage of low-level radioactive waste at the Nevada Test Site, in order to highlight the reutilization in that project of skills and tools used in aerospace computing.

paper illustrates this trend by describing a computer simulation in environmental engineering, with emphasis on techniques and tools in aerospace computing used in the project.

Nomenclature

α	soil texture	(1/m)
L_y	half width of ditch	(m)
y, z	spatial coordinates	(m)
$Y = y/L_y$	relative coordinate	
$Z = \alpha z/2$	relative coordinate	
ψ	moisture tension	(m)
$K_{H\pm}$	saturated horizontal conductivity	(m/sec)
$K_{V\pm}$	saturated vertical conductivity	(m/sec)
K	relative hydraulic conductivity	
u	infiltration function	
$\hat{u}$	cosine transform of u	
T_{2p}	2pth order Chebyshev polynomial	
A_k	coefficient of T_{2k-2}	
J_q	qth order first kind Bessel function	

Several areas inside the Nevada Test Site (NTS) have been targeted as repositories for large quantities of low-level radioactive waste such as depleted uranium and thorium. In the interest of obtaining the best management and engineering practice possible, a knowledge of the estimated travel times of water-borne radionuclides to the groundwater is essential. Computer simulation is used to estimate such travel times, based on mathematical models that yield water seepage velocity components.^{2,3,12,13}

Our project deals with modeling of steady-state infiltration of water into desert alluvial soil of type found at waste disposal sites within the NTS. A goal of the project is to understand radionuclide migration around the Cambric Ditch in Area 5 of the NTS. The ditch in question is a 2-m wide and 1600-m-long shallow trench used to conduct water pumped from the water table for about 17 years. Some of the water flowing in the ditch was lost to surface evaporation, some flowed out the end of the ditch to Frenchman playa, some was used by vegetation that grew near the ditch, and the remainder of the water is assumed to have infiltrated into the alluvial soil. A role of the computer model is to provide understanding of the infiltration process.^{4,18} It turns out, however, that the model is also of interest in other applications, for example, in agricultural studies of trickle and drip irrigation.¹⁷

1. Introduction

A reordering of national priorities has resulted in considerable changes in research and development practices of the aerospace community. One trend deals with technology transfer toward applications in energy conservation and environmental pollution control.¹¹ Our

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At this time, the model handles the steady-state case in two-space dimensions, under assumptions of Gardner soil type and anisotropy in conductivity.^{6,17} Instead of discretizing the corresponding boundary value problem, based on the Richards partial differential equation, the model uses an equivalent linear Fredholm integral equation of the first kind in order to accurately capture capillarity and gravitational effects on the boundary.²⁰ The numerical solution of the integral equation is based on the Fourier Cosine Transform followed by a Galerkin method. Parallel processing was used to carry out the intensive computation.

In the sequel, after outlining the model and the corresponding computation, we demonstrate that our simulation possesses remarkable commonality with computing practices in aerospace.

2. The Model

Figure 1 shows a schematic of the long narrow slot infiltrometer. All mathematical symbols are defined in the nomenclature section. For the application involving the Cambric Ditch in the NTS, the porous medium is a gravelly high-desert alluvial soil with characteristics described in Table 1. The methodology used to solve this specific application yields a general solution for a wide range of applications with varying geometry and soil characteristics. This generality is obtained by varying the dimensionless input parameter in the formulation given below.

$$\gamma = \frac{\alpha L_y}{2} \sqrt{\frac{K_{v\phi}}{K_{H\phi}}}$$

Table 1. Input Parameters for NTS Simulation

α	= 5.0	1/m	soil texture property
L_y	= 1.0	m	half width of ditch
$K_{H\phi}$	= 1.0×10^{-4}	m/sec	horizontal saturated conductivity
$K_{v\phi}$	= 1.0×10^{-5}	m/sec	vertical saturated conductivity
γ	= 0.7906		dimensionless parameter

Differential Form

The steady-state flow into the soil from the ditch is modelled by the Richards equation in two space dimensions

$$\frac{\partial}{\partial y} \left(K_H(\psi) \frac{\partial \psi}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_V(\psi) \frac{\partial \psi}{\partial z} \right) - \frac{\partial K_V(\psi)}{\partial z} = 0.$$

Because of symmetry along the vertical plane $y = 0$, only the right half of the ditch needs to be considered.

The assumptions of a Gardner soil, with anisotropy in the conductivity function, and a change to dimensionless independent variables, yield a linearized elliptic partial differential equation

$$\frac{\partial^2 K}{\partial Y^2} + \gamma^2 \left(\frac{\partial^2 K}{\partial Z^2} - 2 \frac{\partial K}{\partial Z} \right) = 0. \quad (1)$$

A well-posed boundary, value problem is obtained by combining this equation with the following boundary conditions:

$$\text{for } Y=0 \text{ and } Z>0, \quad \frac{\partial K}{\partial Y} = 0 \quad (2)$$

$$\text{as } Y \rightarrow \infty \text{ or } Z \rightarrow \infty, \quad K < \infty \quad (3)$$

$$K(Y, 0) = e^{\alpha \psi_0}, \quad 0 \leq Y < 1 \quad (4)$$

$$-K_{v\phi} \left(\frac{1}{2} \cdot \frac{\partial K}{\partial K}(Y, 0) - K(Y, 0) \right) = 0, \quad Y > 1. \quad (5)$$

The goal is to compute within engineering accuracy the relative conductivity $K(Y, Z)$ which satisfies equation (1) together with conditions (2) through (5).

Integral Form

Instead of discretizing the boundary value problem, the model uses an equivalent linear Fredholm integral equation of the first kind in order to capture accurately capillarity and gravitational effects on the boundary. The transformation to an equivalent integral equation uses the Fourier Cosine Transform method applied to the boundary value problem. The result is the integral equation

$$\frac{4\gamma}{\pi} \int_0^\infty \frac{\cos(\xi Y) \hat{u}(\xi)}{\gamma + \sqrt{\gamma^2 + \xi^2}} d\xi = 1, \quad 0 \leq Y < 1, \quad (6)$$

where the unknown function $\hat{u}$ is the cosine transform of the infiltration function u , and the formal solution to the boundary value problem is

$$K(Y, Z) = \frac{4\gamma}{\pi} e^{a\psi_0} \cdot F(\hat{u}; Y, Z) \quad (7)$$

where the functional F is defined by

$$F(f; s, t) = \int_0^\infty \frac{f(\xi) e^{-t\xi^2/\gamma} \left(\gamma + \sqrt{\gamma^2 + \xi^2} \right) \cdot \cos(\xi s)}{\gamma + \sqrt{\gamma^2 + \xi^2}} d\xi \quad (8)$$

The strategy is to approximately solve the integral equation (6) and then substitute the result in (7) in order to evaluate the relative conductivity $K(Y, Z)$ for given coordinates Y and Z .

3. Approximation Method

Equation (6) is a Fredholm integral equation of the first kind. Although such equations often appear deceptively simple, they are rarely solvable analytically and can frequently be difficult to solve numerically because of ill-conditioning, requiring at times tedious regularization techniques.^{8,19} Fortunately, it turns out that equation (6) is numerically tractable without regularization.

We assume that the infiltration function has the form

$$u(s) = w_v(s) \cdot r(s),$$

where $r(s)$ is a smooth and continuous function known to be even, $r(s) = r(-s)$, and where the singular function

$$w_v(s) = (1-s^2)^{-v}$$

represents the effect of capillarity on the sides of the ditch ($s = \pm 1$). The exponent v depends on the input parameter γ and it satisfies $0 < v \leq 1/2$. As $\gamma \rightarrow \infty$, gravity dominates and $v \rightarrow 0$, whereas $\gamma \rightarrow 0$, capillarity dominates and $v \rightarrow 1/2$.

The numerical method used on the integral equation (6) yields an approximate infiltration function

$$u(s) = (1-s^2)^{-1/2} \sum_{k=1}^N A_k T_{2k-2}(s) \quad (9)$$

where T_{2j} are even Chebyshev polynomials.¹ The singular function $w(s) \equiv w_v(s)$ in (9) with $v = 1/2$ was chosen because:

1. It favors the case with marked capillarity (small value of the input parameter γ).

2. It simplifies algorithms because w is the weight function for Chebyshev polynomials.
3. Cases with large γ can be handled by increasing the number of terms N .

To illustrate, engineering accuracy is reached with $N = 1$ when $\gamma = 0.001$ and with $N = 50$ when $\gamma = 100$.

The approximate solution of the integral equation (6) depends on two key analytical properties:

$$\int_0^1 w(t) \cos(st) T_{2p}(t) dt = (-1)^p \frac{\pi}{2} J_{2p}(s) \quad (10)$$

$$\int_0^1 w(t) T_{2p}(t) T_{2q}(t) dt = 0 \quad \text{if } p \neq q \quad (11)$$

where J_m is the m th order Bessel function.¹ Property (10), which shows that the cosine transform of a weighted Chebyshev polynomial is a Bessel function, means that the effects of capillarity represented by the singular weight function w are conveniently absorbed in the transform domain. Property (11) indicates that even Chebyshev polynomials are orthogonal over the interval $[0, 1]$ (as well as the usual interval $[-1, 1]$).

In view of this orthogonality, a Galerkin method is used to get values for the N coefficients A_k in the approximate infiltration function (9). We thus obtain an $N \times N$ linear system of equations

$$[a_{ij}] [x_i] = [b_i] \quad (12)$$

in the N unknowns $x_i \equiv A_i$ where the constant vector is

$$b = (\pi/2, 0, \dots, 0)^t$$

and the matrix elements are given by

$$a_{ij} = (-1)^{i+j} \gamma \pi \int_0^\infty \frac{J_{2i-2}(s) \cdot J_{2j-2}(s) ds}{\gamma + \sqrt{\gamma^2 + s^2}}, \quad (13)$$

where $i, j = 1 \dots, N$. Once the coefficients A_k are known, since we have

$$\hat{u}(s) = \frac{\pi}{2} \sum_{k=1}^N (-1)^{k-1} A_k J_{2k-2}(s),$$

the desired relative conductivity is given by

$$K(Y, Z) = 2\gamma e^{a\psi_0} \sum_{k=1}^N (-1)^{k-1} A_k \cdot F(J_{2k}; Y, Z) \quad (14)$$

where F is the functional defined in (8).

4. Computation

The Galerkin method described above offers several advantages.

1. The coefficient matrix in the system of linear equations (12) is symmetric.
2. Each element (13) of the matrix is independent of the dimension N .
3. The orthogonality relation (11) provides a theoretical structure for analyzing the integral equation (6).

Properties 1 and 2 reduce the workload because only $N(N+1)/2$ elements of an $N \times N$ matrix have to be evaluated and when the size of the matrix needs to be increased only new elements have to be evaluated. We conjecture that the coefficient matrix is in fact positive definite, as supported by numerical evidence, but this has not been established analytically at this time. The positive definiteness would then explain in part the robustness and stability of the numerical procedure. Little is known about the deceptively simple-looking equation (6), but we are hoping that Property 3 will lead to understanding of its spectral properties.

The computation proceeds in three stages:

1. Evaluate the matrix coefficients defined in (13) for $i = 1, \dots, N$ and $j = i, \dots, N$.
2. Solve the $N \times N$ system of linear equations (12).
3. Evaluate the relative conductivity defined in (14) and other engineering parameters.

Stages 2 and 3 are straightforward. The model relies on solving a small dense system of linear equations, for our purposes with $N \leq 100$, in contrast to a large sparse system when finite differences or finite elements are used on the differential problem. The evaluation of the relative conductivity is simplified because of the quickly decaying exponential in the functional F defined in (8).

The numerical difficulty lies in approximating the infinite range integrals in the matrix elements (13). A key aspect of the computation concerns acceleration of the convergence of these quadratures involving slowly decaying and oscillatory integrands. The program uses a step-forward, compound Gauss-legendre rule,

combined with analytical tricks involving Bessel functions and an acceleration scheme based on Euler's transformation.¹⁶

Since the goal is to provide a solution of the infiltration problem for any γ in a wide range of values, $0.001 \leq \gamma \leq 100$, the strategy is to solve the integral equation for each value in a discrete set of γ values (about 90 such γ_k), in order to provide appropriate coefficients,

$$A_j = A_j(\gamma_k), \quad j = 1, \dots, N = N(\gamma_k),$$

for a user-friendly engineering software tool based on spline interpolation. The number $N(\gamma_k)$ of nodes and the location of the nodes γ_k needed to guarantee engineering accuracy in the interpolation were chosen on the basis of a priori knowledge of properties of $A_j = A_j(\gamma)$; see Figures 3 and 4. Typical infiltration curves resulting from the engineering software are shown in Figure 2.

While the engineering tool is targeted for use on conventional desk computers, the off-line computation leading to it requires the throughput of high-performance computing. Since the evaluations of the matrix elements are both intensive and independent of one another, the off-line computation is ideally suited for parallel processing. The issue of throughput becomes critical when the infiltration model is extended to three-space dimensions. The issue is resolved by using the Parallel Virtual Machine (PVM) system, a software framework for concurrent computing that uses a message passing paradigm, in order to combine heterogeneous platforms in a network.⁷ We used the platforms at the National Supercomputer Center for Energy and the Environment (NSCEE), which include multiprocessor CRAY YMP and CONVEX machines, an SGI Crimson station, a SUN Sparc 10 and other workstations. Benchmark timings are given in Table 2.

Table 2. Timing Benchmarks for $\gamma = 1$

N	19 to 1 speedup ratio on production runs	
	PVM	486DX/66
10	3m 36s	6m 57s
20	5m 49s	50m 7s
40	15m 52s	7h 57m 15s
50	51m 36s	16h 45m 11s
80	3h 31m 54s	N/A

5. Reusability

The infiltration simulation outlined above possesses characteristics that show remarkable commonality with computing practices in aerospace:

1. **Mathematical Model.** The nonlinear Richards equation basically couples the conservation of mass law with Darcy's law. As such, it is somewhat analogous to slow fluid flow around a blunt object, the modeling of which occurs in some aerospace phenomena. The nonlinearity and means of dealing with it, in our case via the assumption of a Gardner soil, are characteristics of several problems in computational fluid dynamics (CFD), structures dynamics, and electromagnetic scattering. The transformation of the differential problem via a Green's function to an equivalent integral equation, in order to focus on boundary effects, is commonly used in wing design, radar signature problems, and sometimes in astrodynamics.^{9,15}

2. **Numerical Software.** The use of integral transforms, special functions, orthogonal expansions, and specialized quadratures is made available by software packages in the public domain. Matrix algebraic problems are routinely solved in a wide variety of computers by portable codes such as LAPACK or LINPACK.⁵ The Galerkin and related approximation techniques based on orthogonality are applied in diverse settings. There is considerable synergy in the area of numerical software because experts in one field frequently communicate and exchange software with experts in other fields.¹⁶

3. **Parallel Processing.** This form of supercomputing has become an active area of research in diverse disciplines in aerospace, notably in CFD.¹⁴ The PVM system is an effective means of harnessing and combining the throughput of machines in a network.⁷ The message passing and single master / multiple slaves issues faced in the infiltration model are basically generic to most computations involving a large set of data independent tasks. Dynamic load balancing, fault tolerance, automatic restart, and handling of direct access output files are other common features in that type of computing. The advantages of portability and scalability provided by PVM carry over to diverse applications.

4. **Post Processing.** The design of user interfaces for engineering software tools has been standard fare in aerospace for a long time. The availability and

reutilization of such user interface shells can considerably facilitate the coding of new tools for various engineering problems. The continuing development of visualization tools in the aerospace sector, especially for applications in CFD,¹⁰ is yet another post-processing capability that can be readily transferred to environmental and other engineering applications.

6. Conclusion

We observe that the four aspects of the infiltration model described above indicate significant commonality in mathematical methodology, in software design, and in hardware architecture with aerospace practices in computer simulation.

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9. Figures