EVALUATION OF THE NON-ISOTHERMAL / THERMAL UNSATURATED / SATURATED FLOW AND TRANSPORT (NUFT) CODE USING ANALYTICAL SOLUTIONS

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ABSTRACT

The Non-isothermal / Thermal Unsaturated / Saturated Flow and Transport (NUFT) code is a suite of 3-D multi-phase, multi-component models for numerical solution of non-isothermal flow and transport in porous media. These distinct models are imbedded in a single code in order to utilize a common set of utility routines and input file format. One of the first stages in testing such a computer program is to examine the performance of the numerical solutions by comparing them to analytical solutions. This paper describes test problems for unsaturated flow and two-phase flow and how well NUFT modeled them.

INTRODUCTION

The Non-isothermal / Thermal Unsaturated / Saturated Flow and Transport (NUFT) code (Nitao 1995) is a suite of 3-D multi-phase, multi-component models for numerical solution of flow and transport in porous media. It also has the perfect gas law modified by a z factor, steam tables, and the energy balance equation to model steam injection. These distinct models are imbedded in a single code in order to utilize a common set of utility routines and input file format. NUFT is a structured integrated finite difference (finite volume) code that has several differencing and upwinding type options. One of the first stages in testing such a computer program is to examine the performance of the numerical solutions by comparing them to analytical solutions. The objective of this paper is to describe the performance of NUFT with regard to test problems for unsaturated flow and two-phase flow.

UNSATURATED FLOW

There are only a few analytical solutions of unsaturated flow because of the nonlinear nature of the governing equations. However, those that have been developed (Segol 1993 and Tracy 1995) can be used for testing numerical codes like NUFT.

GOVERNING EQUATIONS

1-D unsaturated flow in the vertical z direction with constant fluid density and dynamic viscosity is governed by

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(k\frac{\partial h}{\partial z}\right) + \frac{\partial k}{\partial z} \tag{1}$$

where θ is the moisture content, k is the hydraulic conductivity, h is the pressure head, z is the positive vertical direction, and t is the time. k and h are typically some nonlinear function of the moisture content θ.

DESCRIPTION OF PROBLEM

The problem consists of 1-D unsaturated flow in a vertical column of homogeneous soil of length L, hydraulic conductivity k, and a residual moisture content θ_n that is initially dry until water is introduced at the top of the column at a constant rate of infiltration R as shown in Figure 1. This problem represents a sharp front, and the goal is to see

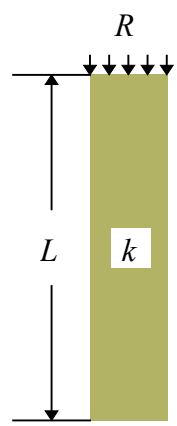

Figure 1. Downward unsaturated flow example

how well the pressure head front is captured by NUFT. Hydraulic conductivity varies in this problem as follows. First define dimensionless quantities as

$$z^* = \frac{z}{\lambda_s} \qquad h^* = \frac{h}{\lambda_s} \qquad t^* = \frac{t}{t_s} \qquad k^* = \frac{k - k_n}{k_s - k_n}$$
$$\theta^* = \frac{\theta - \theta_n}{\theta_s - \theta_n} \qquad \frac{\lambda_s}{t_s} = \frac{k_s - k_n}{\theta_s - \theta_n} \qquad R^* = \frac{R - k_n}{k_s - k_n} \tag{2}$$

where λ_s is a characteristic length, t_s is a characteristic time, k_s is the saturated hydraulic conductivity, k_n is the hydraulic conductivity at residual moisture level, and θ_s is the saturated moisture content. Using a parameter C, dimensionless hydraulic conductivity is modeled as

$$k^* = \frac{(C-1)\theta^{*2}}{C-\theta^*} \tag{3}$$

ANALYTICAL SOLUTION

The solution procedure is to start with values for the constants and selected z and t, and find a ζ from iteratively determining the root of the following equation:

$$C(L^* - z^*) - (\rho^2 + \rho)\tau - (2\rho + 1)\varsigma + \ln u = 0 \tag{4}$$

$$m = 4C(C-1) \qquad \rho = \frac{R^*}{m} \qquad \tau = mt^* \tag{5}$$

$$u = \frac{1}{2}\mathrm{e}^{-\left(\frac{\varsigma^2}{\tau}\right)}\left[2\,\mathrm{e}^{\frac{(\varsigma+\rho\tau)^2}{\tau}} + f(T_1) - f(T_2) + f(T_3) - f(T_4)\right] \tag{6}$$

$$f(x) = \mathrm{e}^{x^2}\mathrm{erfc}(x) \qquad \mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty \mathrm{e}^{-y^2}\,dy \tag{7}$$

$$T_1 = \frac{\varsigma - \sqrt{\rho^2+\rho}\tau}{\sqrt{\tau}} \quad T_2 = \frac{\varsigma - \rho\tau}{\sqrt{\tau}} \quad T_3 = \frac{\varsigma + \sqrt{\rho^2+\rho}\tau}{\sqrt{\tau}} \quad T_4 = \frac{\varsigma + \rho\tau}{\sqrt{\tau}} \tag{8}$$

Dimensionless moisture content can then be computed directly from

$$\theta^* = C\left(1 - \frac{1}{2\rho + 1 - \frac{1}{u}\frac{\partial u}{\partial \varsigma}}\right) \tag{9}$$

where from Equation 6

$$\frac{\partial u}{\partial \varsigma} = \mathrm{e}^{-\left(\frac{\varsigma^2}{\tau}\right)}\left[2\rho\,\mathrm{e}^{\frac{(\varsigma+\rho\tau)^2}{\tau}} - \sqrt{\rho^2+\rho}\,f(T_1) + \rho f(T_2) + \sqrt{\rho^2+\rho}\,f(T_3) - \rho f(T_4)\right] \tag{10}$$

Finally, from the definition of the two constants

$$a = \frac{1}{2}\frac{k_n}{(k_s - k_n)(C-1)} \qquad b = \sqrt{2aC - a^2} \tag{11}$$

pressure head is

$$h = \frac{\lambda_s}{C}\left[\ln\frac{C-1}{C-\theta^*} + \frac{1}{2}\ln\frac{\theta^{*2} - 2a\theta^* + 2aC}{1-2a+2aC} - \frac{a-C}{b}\left(\tan^{-1}\frac{\theta^*-a}{b} - \tan^{-1}\frac{1-a}{b}\right)\right] \tag{12}$$

NUFT SOLUTION

A NUFT data set was created with the following data: L = 100 m, R = 2.01 m/d, k_n = 0.01 m/d, k_s = 10.01 m/d, θ_n = 0.15, θ_s = 0.45, and C = 1.5. A time interval Δt = 0.05 d was used with grid spacings of Δz = 2.5 m, 1.25 m, and 0.3125 m. 31 data points representing relative hydraulic conductivity versus saturation and capillary pressure versus saturation were obtained from Equations 3 and 9, respectively, and provided as input to NUFT. Figure 2 shows a plot of pressure head versus z distance for the analytical solution and the three Δz values. As Δz decreases, the curves match more closely, showing convergence of the NUFT solution to the analytical solution.

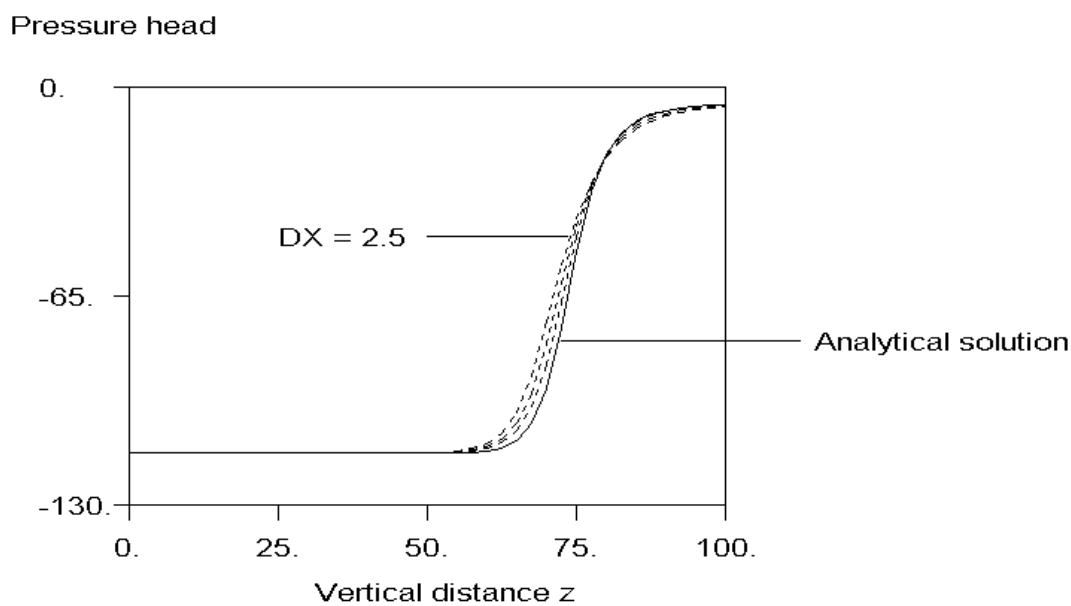

Figure 2. Comparison of results

TWO-PHASE FLOW

Unsaturated flow is really two-phase flow with the gas phase at atmospheric pressure. Here, the problem of flow of oil and water is considered. There are even fewer analytical solutions of two-phase flow. However, an exact integral 1-D solution (McWhorter and Sunada 1990) where the sum of oil and water velocities equals zero has been derived. This author has derived an analytical solution for steady-state two-phase flow that can be either 2-D or 3-D with the restriction of total flow equal zero removed, so this will be the solution used.

GOVERNING EQUATIONS

Steady-state two-phase flow with constant density and dynamic viscosity is modeled by

$$\begin{aligned} &\nabla\cdot(k_w\nabla h_w)+\frac{\partial k_w}{\partial z}=0 \\ &\frac{\rho_w}{\rho_o}\nabla\cdot(k_o\nabla h_o)+\frac{\partial k_o}{\partial z}=0 \end{aligned} \tag{13}$$

where k_w is the hydraulic conductivity of water, k_o is the hydraulic conductivity of oil, h_w is the pressure head of water, h_o is the pressure head of oil, and

$$k_w = k_{wr}k_{ws} \qquad k_o = k_{or}k_{os} \tag{14}$$

where the subscript r represents relative, and the subscript s denotes saturated. Also,

$$h_w = \frac{p_w}{\rho_w g} \qquad h_o = \frac{p_o}{\rho_w g} \tag{15}$$

where p_w is the pressure due to water, p_o is the pressure due to oil, ρ_w is the density of water, ρ_o is the density of oil, and g is the acceleration due to gravity.

DESCRIPTION OF PROBLEM

The problem consists of applying water at the top to a rectangular region of dimension a x L of mostly oil to get the oil to come out as shown in Figure 3. Thus, k_{wr} = 1 and p_{o34}

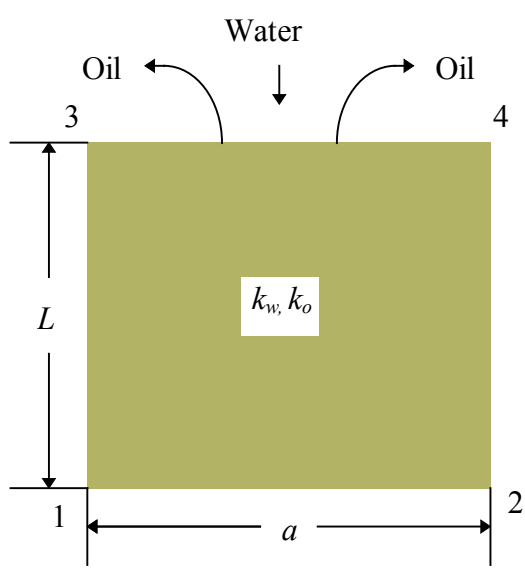

Figure 3. Two-phase flow example

= 1 bar (near atmospheric pressure) along 3-4. For a porosity n and parameter α, relative hydraulic conductivity and moisture content vary as

$$k_{wr} = \frac{\theta_w - \theta_n}{\theta_s - \theta_n} \qquad k_{or} = 1 - k_{wr}$$
$$\theta_w = \left(\theta_s - \theta_n\right) e^{\alpha\left(h_w - h_o\right)} + \theta_n \qquad \theta_o = n - \theta_w \tag{16}$$

ANALYTICAL SOLUTION

First, let $\rho_w \approx \rho_o = \rho_{av}$. Then define ϕ_i for the four corner points of the region as

$$\phi_i = 1 - (1 - k_{wri})^2 \tag{17}$$

Then compute

$$\phi = \left(1 - \frac{x}{a}\right)\left(1 - \frac{y}{L}\right)\phi_1 + \left(\frac{x}{a}\right)\left(1 - \frac{y}{L}\right)\phi_2 + \left(\frac{x}{a}\right)\left(\frac{y}{L}\right)\phi_3 + \left(1 - \frac{x}{a}\right)\left(\frac{y}{L}\right)\phi_4$$
$$\bar{h} = 1 - \sqrt{1 - \phi} \tag{18}$$

The solution for pressure head is

$$h_o = \frac{1}{\alpha}\left(1 - \bar{h}\right) - y + L + \frac{10^5}{\rho_w g} \qquad h_w = \frac{1}{\alpha}\ln \bar{h} + h_o \tag{19}$$

NUFT SOLUTION

A NUFT data set was created with the following data: a = 20 m, L = 10 m, k_{ws} = 0.84672 m/d, k_{os} = 1.12896 m/d, θ_n = 0.1, $\theta_s = n$ = 0.4, α = 0.02, and ρ_{av} = 1000 kg/m^3. The steady-state solution was input as the initial conditions, and how much the solution changed was the error as in a calibration study. A grid spacing of Δx = 2 m and Δy = 1 m was used. Table 1 shows oil pressure values along the line y = 5 for the analytical solution and NUFT computation. The agreement is acceptable for the coarse grid.

Table 1. Two-phase flow oil pressure (bar) along y = 5 m

x (m)	Analytical	NUFT
0	4.61	4.61
4	4.54	4.44
8	4.47	4.34
12	4.41	4.27
16	4.33	4.23
20	4.26	4.26

APPROVAL

The Chief of Engineers has approved the publication of this paper.

REFERENCES

McWhorter, David B. and Sunada, Daniel K. "Exact Integral Solutions for Two-Phase Flow." (1990). *Water Resources Res.*, 26(3), 399-413.

Nitao, John J. (1995). "User's Manual for USNT Module of the NUFT Code, Version 1.0 (N-phase, N-Component, Thermal)." Lawrence Livermore National Laboratory, Livermore, CA.

Segol, Genevieve. (1993). *Classic Groundwater Simulations: Proving and Improving Numerical Models*., 316-323. Englewood Cliffs, New Jersey: PPR Prentice Hall.

Tracy, Fred T. (1995). "1-D, 2-D, and 3-D Analytical Solutions of Unsaturated Flow in Groundwater." *J. Hyd*., 170, 199-214.