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Use of a General Partial Differential Equation Solver for Solution of Mass and Heat Transfer Problems in Geotechnical Engineering

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ABSTRACT: This paper illustrates the use of a general purpose partial differential equation (PDE) solver called FlexPDE for the solution of mass and heat transfer problems in saturated/unsaturated soils. FlexPDE uses the finite element method for the solution of boundary and initial value problems. A flexible input of the governing PDE's and of material properties functions allows the simulation of non-linear soil behaviour quickly and inexpensively. A two-dimensional problem, a cross section of a dam subjected to reservoir filling, was simulated. A three-dimensional simulation of the same dam is also included to show the three-dimensional capabilities of FlexPDE. Results compare well with those obtained in Seep/W. A problem in conductive heat transfer undergoing freezing and thawing of interest to the pipeline industry was also considered. The results compared well with those obtained from the finite element program Temp/W. The adaptability of the FlexPDE software for solving a variety of problem types was clearly demonstrated.

KEY WORDS: seepage, heat transfer, numerical solution

1 INTRODUCTION

The development of numerical techniques such as finite difference and finite element method has enabled engineers to solve extremely complex physical phenomena for a variety of boundary conditions and material properties.

In the 1990's, there appeared a greater acceptance and use of various pre-packaged finite element and finite difference codes. These codes could range from discipline specific products such as the Geo-Slope software to general partial differential equation solvers such as PDEase and FlexPDE. The advantage of the latter programs is the flexibility offered to researchers, allowing the modelling of a wide range of problems.

The objective of this paper is to introduce and verify the application of one of these general purpose solvers for geotechnical problems. FlexPDE was used to solve two and three dimensional transient seepage problems and two-dimensional heat transfer problems.

1.1 Solution of water movement (seepage)

Casagrande (1937) presented a complete discussion on the use of the flownet technique for predicting seepage through earth structures, originally developed by Forchheimer. Cassagrande (1937) divided the soil into two parts, the soil below the water table and the soil above the water. The assumption was made that water only flowed below the water table. The flownet method was used extensively in geotechnical practice.

Various investigators (Taylor and Brown, 1967; Freeze, 1971) developed finite element models for describing water flow and seepage in soils. Papagianakis and Fredlund (1984) and Lam et al. (1987) developed a finite element package for performing saturated/unsaturated seepage modelling. Nguyen (1999) showed that it is possible to use a general partial differential equation solver for modelling seepage in saturated/unsaturated soils. The finite element method has essentially replaced the flow net method for solving seepage problem, due to the robust nature of numerical modelling software.

1.2 Solution of heat transfer considering phase change

A large amount of research was conducted in the 1970's for development of numerical models for predicting heat flow in soils. This occurred in response to several proposals for construction of oil and gas pipelines in Northern Canada and Alaska. The models needed to account for the latent heat effects as the pore-water changes phases.

Ho et al. (1970), Nakamo and Brown (1971), and others developed finite difference models for heat flow in soils with phase change. Hwang et al. (1972) provided details on a finite element model for transient analysis of conduction in soils undergoing freezing and thawing. These models include instantaneous phase change of the pore-water from liquid to solid or vice versa.

Coutts and Konrad (1994) propose a model that makes use of the "node state" method. The nodes are assigned states on the basis of whether the water at the node is liquid, solid, or transitional and the latent heat effects are applied at the transitional nodes. The Temp/W finite element package (Geo-Slope, 1999) uses an average value for the latent heat between time steps. The time average solution is reasonable provided sufficient time steps are included in the model.

The numerical models developed for heat flow in soils undergoing freeze-thaw try to model an instantaneous phase change of the water. Various schemes are implemented to allow convergence of solution using this assumption. However, the pore-water does not freeze at a single temperature, but over a range of temperatures. Improved stability can be obtained in numerical solutions if latent heat effects are applied over a broader range of temperatures. Furthermore, the results obtained are more realistic.

2 SEEPAGE AND HEAT FLOW PDE'S

2.1 PDE for seepage

Seepage problems are among the most commonly analyzed problems in geotechnical engineering. Papagianakis and Fredlund (1984), Lam et al. (1987) and Nguyen (1999) among others provide details on the derivation of the partial differential equation for unsaturated seepage. Equation 1 presents the standard form of the equation in two-dimensions for transient seepage.

$$\frac{\partial}{\partial x}\left(k_x \frac{\partial h_w}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y \frac{\partial h_w}{\partial y}\right)=-m_2^w \gamma_w \frac{\partial h_w}{\partial t} \quad (1)$$

where: k_x and k_x are the coefficients of permeability in the x and y directions,

h_w is the hydraulic head ($h_w = u_w/\gamma_w + y$),

u_w is the pore-water pressure,

γ_w is the unit weight of water, and

m_2^w is the storage coefficient.

2.2 PDE for conductive heat flow

In geotechnical engineering, the heat flow component of greatest concern is the conductive heat flow. This is especially of concern in the design of structures that will affect the thermal regime of the soil. That includes warm foundations, hockey rinks, refrigerated storage, pipelines, etc. The general partial differential equation for conductive heat flow in a soil is given by Equation 2.

$$\frac{\partial}{\partial x}\left(\lambda_x \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_y \frac{\partial T}{\partial y}\right)=c\rho \frac{\partial T}{\partial t} \quad (2)$$

where: λ_x and λ_y are the thermal conductivity of the soil in x and y direction,

T is temperature,

c is the soil mass specific heat, and

ρ is the density of the soil.

The term $c\rho$ is referred to as the volumetric specific heat capacity of the soil.

Equation 2 generally applies for heat flow in soils. However, a modification must be made to the differential equation for cases where a change of phase is occurring in the soil (i.e., freezing/thawing). Accompanying this phase change is a large absorption or release of energy as the water changes from solid to liquid form, or vice versa.

One method for modifying Equation 2 uses an apparent specific heat term. The apparent specific heat includes the volumetric specific heat capacity and a term that accounts for the heat released or absorbed by phase change. So, equation 2 can be as follows:

$$\frac{\partial}{\partial x}\left(\lambda_x \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_y \frac{\partial T}{\partial y}\right)=\left(c\rho + L_f\theta \frac{\partial \theta_u}{\partial T}\right)\frac{\partial T}{\partial t} \quad (3)$$

where: L_f is the latent heat of fusion of water, 334 MJ/m³,

θ is the volumetric water content at the initiation of freezing, and

$\partial\theta_u/\partial T$ is the change in unfrozen water content of the soil with temperature.

The term $L_f\theta\,\partial\theta_u/\partial T$ represents the amount of heat released or absorbed as the temperature of the soil change by ∂T. A continuous function for $\partial\theta_u/\partial T$ was developed and implemented in the FlexPDE models in the current study.

Equation 3 reduces to 2 for cases where freezing or thawing are not occurring. The term $\partial\theta_u/\partial T$ has been referred to as m_2^i by Newman (1996) in analogy to the m_2^w term used in seepage analysis in unsaturated soils.

3 DESCRIPTION OF FlexPDE

Previous researchers (Nguyen, 1999; Vu, 1999) have used a general purpose solver called PDEase (Macsyma Inc., 1996) in conducting research into the behaviour of unsaturated soils. Consideration was given to the use of PDEase in the present research, but a decision was made to utilise a new software package, called FlexPDE (PDE Solutions Inc., 1999). FlexPDE is a program similar to PDEase, but with the advantage of three-dimensional capabilities. FlexPDE is a general partial differential equation solver that uses the finite element method for numerical solution of boundary value problems. Major features of FlexPDE include:

- Capable of solving non-linear partial differential equations of second order or less;
- Flexible and effective way to input non-linear functions for material properties, like unsaturated soil properties;
- Adaptive grid refinement, eliminating the need for manually determining an appropriate mesh;
- Adaptive time step definition, ensuring the user pre-determined accuracy and helping in achieving convergence.

Water flow and heat flow problems solutions obtained using FlexPDE were verified against the Geo-Slope (1999) software packages Seep/W and Temp/W results, respectively. Seep/W and Temp/W are finite element programs developed for solution of geotechnical problems. Seep/W is a saturated/unsaturated seepage package. Temp/W is a thermal modelling program for handling freezing and thawing of soils. The problems were solved on a Pentium III 450 MHz computer with 128 MB of RAM running under the Windows 98 operating system.

4 SEEPAGE VERIFICATION EXAMPLE

The verification of FlexPDE for seepage results in two dimensions is mostly a reanalysis of the research study conducted by Nguyen (1999). The purpose of this portion of the paper is to show that FlexPDE performs in a manner that is consistent with PDEase and Seep/W.

The seepage problem presented is the case of transient seepage through an earth fill dam, as the reservoir level is quickly raised. The permeability functions used are presented in Figure 1. Though an anisotropic permeability condition could be easily simulated, an isotropic condition was assumed for the sake of simplicity. A constant coefficient of volume change with respect to the water phase, m_2^w, of 0.003 kPa^{-1} was assumed for both materials. Figure 2 depicts the problem geometry, initial conditions, boundary conditions, and one of the meshes generated by FlexPDE.

The analysis of this problem follows two stages: first, establishing the initial steady state condition and second, solving for transient conditions. The initial steady state condition corresponds to a water level at 4 m above datum. In the downstream slope a review boundary condition was applied, where pore water pressures have to be equal or less than zero.

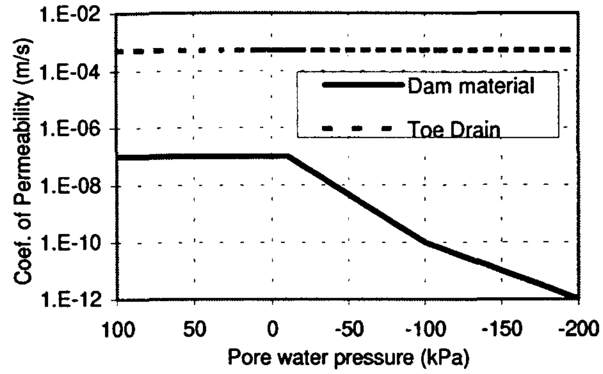

Figure 1 - Coefficient of permeability functions used in seepage problems.

The review boundary condition introduces an additional nonlinearity, besides the soil property nonlinearity, since the exit point is not known. FlexPDE handled successfully all these nonlinearities and convergence has generally been achieved.

Figure 3 presents a comparison of the heads computed by FlexPDE and Seep/W for the initial conditions. The smooth lines correspond to FlexPDE results and the rough lines to SEEP/W results. A good agreement can be observed.

The initial conditions established are used as input into the transient model. As FlexPDE uses adaptive grid refinement, multiple computation meshes can be developed over the course of the solution as the solution error dictates. In order to obtain an accurate solution in FlexPDE, it was necessary to place a line feature below the upstream surface, in order to force a denser mesh at the upstream face where the head is changing rapidly at early time steps. The addition of a feature below boundaries where large changes are occurring in the dependent variable often helps improve the reliability of the FlexPDE results.

Figures 4 and 5 present the heads computed by FlexPDE and Seep/W at times 15 and 16383 hr. Generally, good agreement is obtained between the solutions given by both softwares. Some differences appear, likely due to differences in temporal and spatial discretization between the two programs.

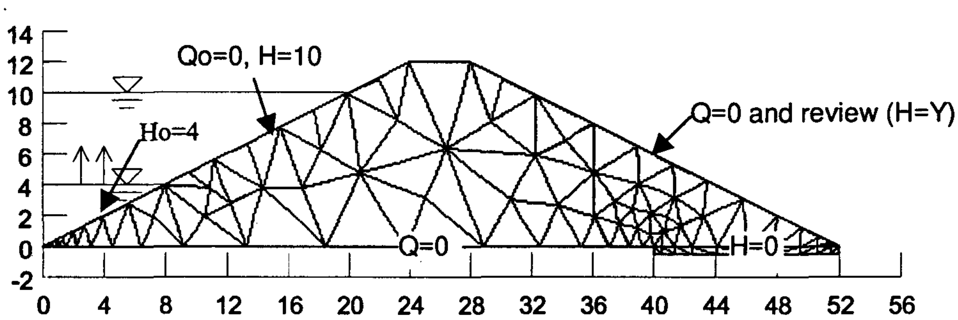

Figure 2 - Problem geometry, boundary and initial conditions, and one of the meshes used for two-dimensional seepage problem.

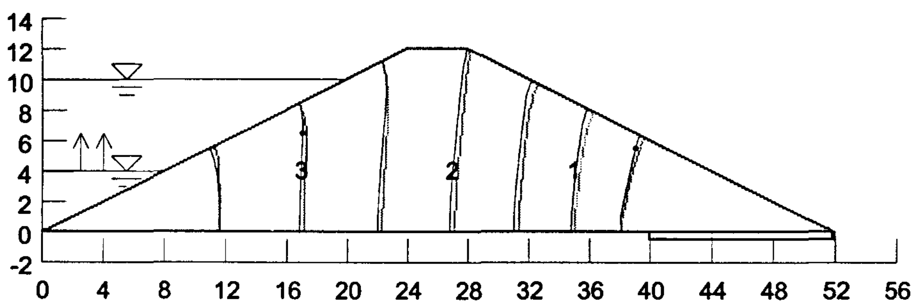

Figure 3 - Comparison of head (m) contours for two-dimensional seepage problem at initial conditions.

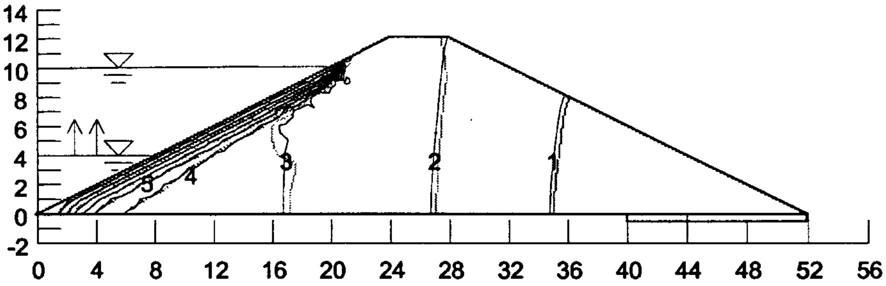

Figure 4 - Comparison of head (m) contours for two-dimensional seepage problem, time = 15 hr.

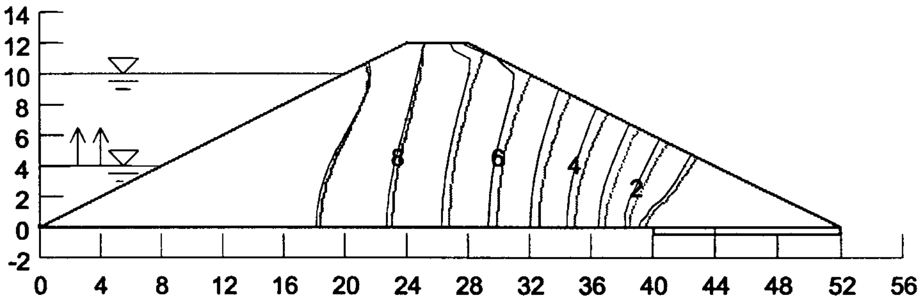

Figure 5 - Comparison of head (m) contours for two-dimensional seepage problem, time = 16383hr.

5 THREE DIMENSIONAL SEEPAGE

The capability of FlexPDE for solving three-dimensional problems was investigated in the course of this study. The three-dimensional seepage verification problem considered here is that of steady state seepage through an earth fill dam. The material properties are the same as those used in the two-dimensional seepage problem discussed in the previous section. The permeability functions can be found in Figure 1. The basic problem geometry is similar to what has been considered in the two-dimensional seepage problem. The dam is 12 m high, with a crest 4 m wide, and 2:1 side slopes, resulting in a total width of 52 m. The abutment is assumed to also be at a 2:1 slope as well. Figure 6 illustrates 3 three-dimensional views of the dam taken from the FlexPDE grid used to solve the problem.

One section of the dam was considered in detail, and the results compared with two-dimensional analysis done in Seep/W. The location of the sections analysed is shown on Figure 6. Results form section A-A' was expected to produce results that are essentially the same as the two-dimensional case.

Figure 7 show the head contours computed by FlexPDE (smooth lines) and Seep/W (rough lines) at section A-A'.

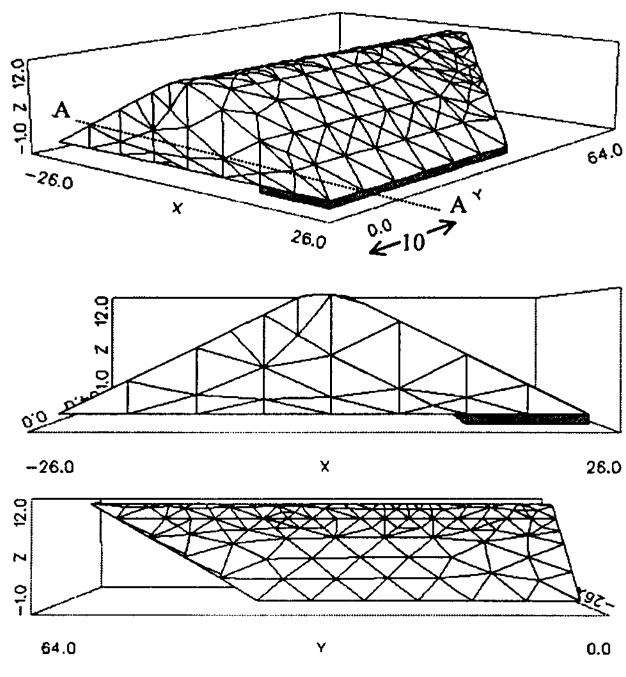

Figure 6 - Three views of the three-dimensional grid generated by FlexPDE for the three-dimensional seepage problem.

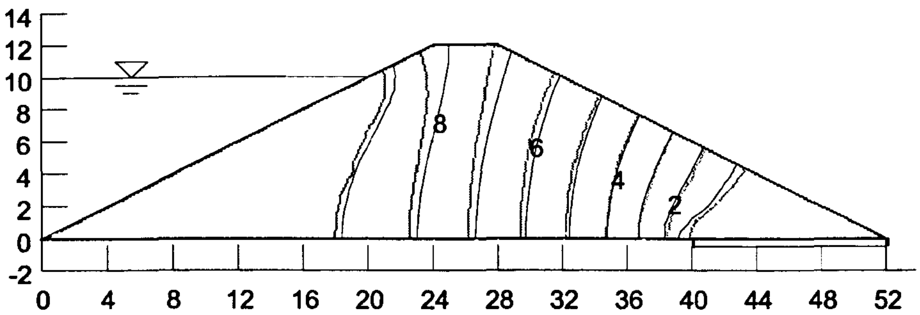

Figure 7 - Comparison of computed heads (m) for the three-dimensional seepage problem at section A-A'.

The results compare quite favourably. This is expected because near the centre of the dam, end effects are expected to be minimal and the flow regime is expect to be essentially two-dimensional. Differences between the two sets of results are likely due to lack of discretization in FlexPDE in the three-dimensional problem; fewer nodes are used in any one y-plane than would be in a two-dimensional analysis.

6 HEAT TRANSFER PROBLEM

The two-dimensional heat transfer example here presented considers a classic problem that is of interest to the pipeline industry. One option for shipping oil and gas in Canada, from northern fields to the south, is to chill the product and thus avoid thawing of permafrost terrain. The problem arises, though, in discontinuous permafrost, when the pipeline traverses non-frozen terrain. It would be expected that freezing of the soil would be initiated. This example was considered by Coutts and Konrad (1994).

A pipeline with an outside temperature of –2 °C is embedded in soil initially at a temperature of 3 °C. The soil has the soil-freezing curve, and thermal properties as shown in Figure 8. θ is assumed equal to 0.377 and cρ constant and equal to 0.157 for this problem. A constant surface temperature (upper boundary) of 3 °C is assumed. Figure 9 presents the geometry of the problem, boundary and initial conditions, and one of the meshes that were generated by FlexPDE for this problem.

Figures 10 and 11 show the isotherms around the pipeline for two time steps. Smooth lines are the FlexPDE results and rough lines are the Temp/W obtained results. As expected, the results between the two programs differ significantly at early time steps due to the differences in interpretation of the m_2^i function. Temp/W estimates m_2^i at each time step based on the estimated temperature at that time step and the temperature calculated at the previous time step. In the FlexPDE model that was implemented, m_2^i is implemented as a continuous function of temperature. As the solutions approaches the steady state condition the differences become smaller, since the effect of differing m_2^i decreases. At steady state conditions (i.e. time step 730 days), the results are identical. This is to be expected, as at steady state, $\partial T / \partial t$ goes to 0 and m_2^i has no effect on the solution.

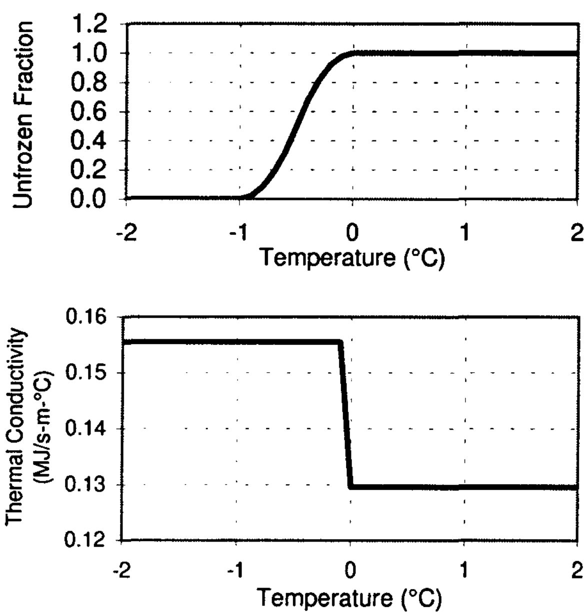

Figure 8 - Material properties specified for heat transfer problem.

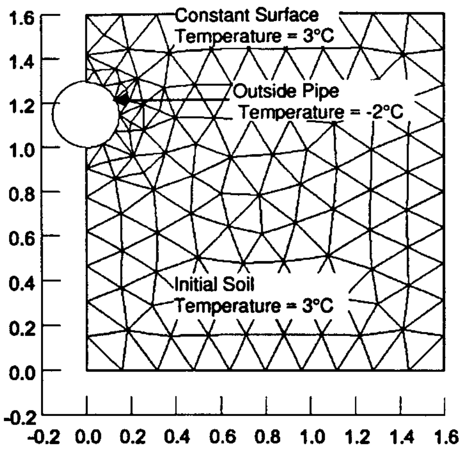

Figure 9 - Problem geometry, initial and boundary conditions, and computation grid used by FlexPDE for the heat transfer problem.

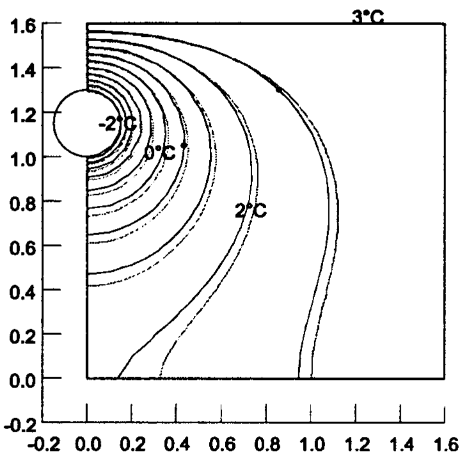

Figure 10 - Comparison of temperature contours (°C) for the heat transfer problem, time = 7 days.

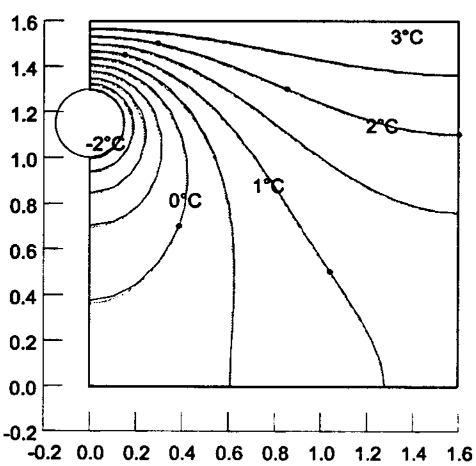

Figure 11 - Comparison of temperature contours (°C) for the heat transfer problem, time = 730 days.

7 DISCUSSION

The seepage modelling performed in this study verified that solutions of partial differential equations obtained using FlexPDE are comparable to established solutions. The results provided sufficient confidence in the accuracy of FlexPDE for seepage problems. The results also show that FlexPDE works in fundamentally the same manner as PDEase2D, which Nguyen (1999) used for modelling two-dimensional seepage problems. These results provided confidence to proceed with FlexPDE modelling of other geotechnical problems.

Three-dimensional modelling of steady state seepage through an earth fill dam showed that for problems demanding three-dimensional modelling FlexPDE is a suitable modelling package. Although FlexPDE appears to have promise for use in performing three-dimensional analysis of geotechnical problems, solution times and memory requirements for three-dimensional problems are quite excessive. The three-dimensional seepage problem that was considered was a simple steady state problem with simple boundaries, and isotropic material properties. Increasing the complexity of the problems considered lead to a corresponding increase in solution time and computer resources.

Regarding the heat transfer problem, FlexPDE uses a continuously defined function of m_2^i that is the slope or derivative of the soil-freezing curve. This representation of the soil-freezing curve realistically models the behaviour of soils. The Temp/W interpretation of the soil-freezing curve results in the necessity of having to incorporate small time steps in the solution to get correct results. Comparison between Temp/W and FlexPDE solutions showed that by defining m_2^i as a continuous function of temperature accurate results can be obtained without considering effects of temporal discretization on the solution.

The effect of the differences between solutions decreases as the problems approach steady state conditions. The Temp/W and FlexPDE results compare better at later time steps, as the effect of m_2^i on the solution decreases.

Modelling of heat flow processes involving phase change showed that the ability to use a variety of functions for describing material properties can be advantageous over traditional finite element solution for problems which rigidly enforce the definition of material properties. FlexPDE allows definition of thermal conductivity and volumetric specific heat capacity for any soil water content, ice content, or air content. Temp/W only allows definition of these properties as functions of temperature, resulting in the exclusion of the effects of partial saturation on thermal properties in analyses.

8 CONCLUSIONS

1. The PDE solver FlexPDE has been verified against well-established numerical solutions for problems of seepage. Comparison against Seep/W shows close agreement. These results show also that FlexPDE behaves functionally the same as PDEase2D.
2. Three-dimensional models run in FlexPDE appear to provide correct results. Comparison was made with two-dimensional sections. Three-dimensional behaviour was observed in the three-dimensional structure considered, but no comparison was made with other softwares.
3. The FlexPDE solution of transient heat flow in soil undergoing freezing-thawing agreed with the Temp/W results, provided the interpretation of the soil-freezing curve was the same in the two models. Continuous definition of the m_2^i function in FlexPDE was successful, assuring an accurate representation of the soil behaviour.
4. A variety of problems in geotechnical engineering can be solved using general finite element software.

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