Isothermal Phase Change Model for Freezing and Thawing Soils II: Model

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ABSTRACT

A FORTRAN computer program is available which accommodates two-dimensional heat and soil-water flow models as coupled by an isothermal phase change model. The program can be used to analyze two-dimensional freezing/thawing problems which have sufficient known information to supply the necessary modeling parameters, boundary conditions, and initial conditions. Because of the sophistication of the two-dimensional phase change model and the data requirements needed to properly represent inhomogeneity of the system, boundary conditions, and other complexities, a special data input program is developed in order to aid the model user. This general purpose data preparation program, PROTOØ, develops the data input file to be used directly by the two-dimensional phase change program.

INTRODUCTION

A FORTRAN computer program is available which accommodates two-dimensional heat and soil-water flow models as coupled by an isothermal phase change model. The program can be used to analyze two-dimensional freezing/thawing problems which have sufficient known information to supply the necessary modeling parameters, boundary conditions, and initial conditions.

Because of the sophistication of the two-dimensional phase change model and the data requirements needed to properly represent inhomogeneity of the system, boundary conditions, and other complexities, a special data input program is developed in order to aid the model user. This general purpose data preparation program, PROTOØ, develops the data input file to be used directly by the two-dimensional phase change program.

In this paper, the PROTOØ program will be reviewed in detail. The actual CRT screen pages will be displayed which show the data entry prompts in their respective order of appearance. Also shown on the provided CRT screen pages are the computer program variable names associated to each prompt in order to aid in understanding the FORTRAN code.

MODELING APPROACH

Heat and Soil-Water Flow

Hromadka (1977, 1980) provides the details of the mathematical models used to approximate the thermal and soil-water effects in two-dimensional problems. The analyst initially discretizes the problem geometry (two-dimensional domain) into a collection of triangle finite elements (Fig. 1). The computer model further subdivides these triangles into nodal domains such as shown in Fig. 2. The collection of nodal domains forms a control volume for each nodal point (Fig. 3). The computer model then balances the heat and soil-water flow over each nodal control volume using straight-line interpolation of temperature and soil-water energy head to compute the corresponding rates of flow. This straight-line interpolation function is shown graphically in Fig. 4.

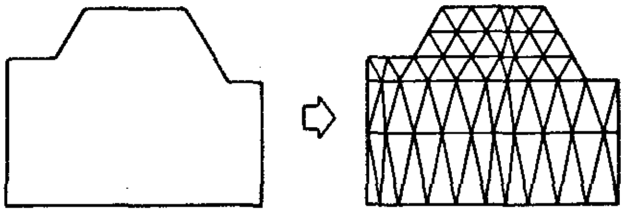

Fig. 1. Discretizing the Domain Ω into Finite Elements

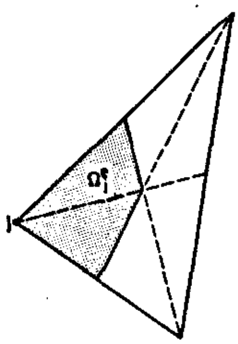

Fig. 2. Nodal Domain of Triangle Element Assigned to Node j

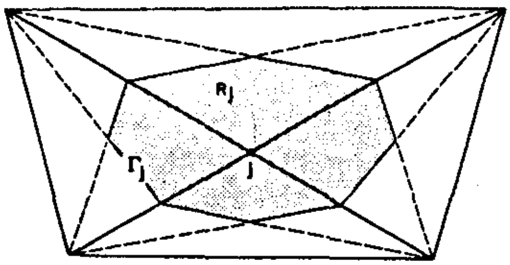

Fig. 3. The Area of Flow-balance for Node j (for heat and soil-water flow)

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Paper received on May 15, 1986. Referee: Dr. Paolo Zannetti

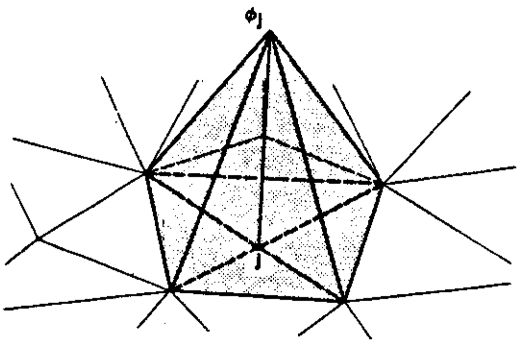


Fig. 4. Linear Distribution of State Variable ϕ_j (e.g. Temperature) from Node j Value

Phase Change

Hromadka (1980) describes the isothermal phase change algorithm used to approxiamte the freezing and thawing of soil-water. This algorithm is based upon the "lumped-mass" control volume shown in Fig. 5 (which conforms geometrically to the control volume used to balance heat and soil-water flow). Figure 6 illustrates the budget used for each nodal control volume which accounts for the residual water content (unavailable for freezing), the remaining water content available for freezing, and the ice content. During phase change, the nodal temperature is defined to equal the freezing point depression (usually 0°C).

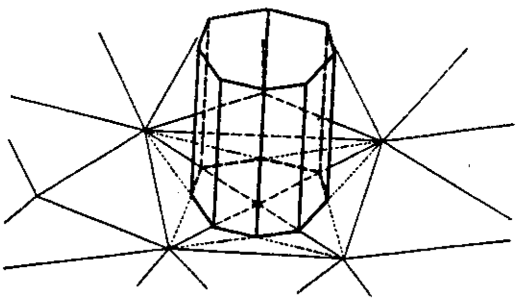


Fig. 5. Lumped Mass Control Volume (Used for ice content balance)

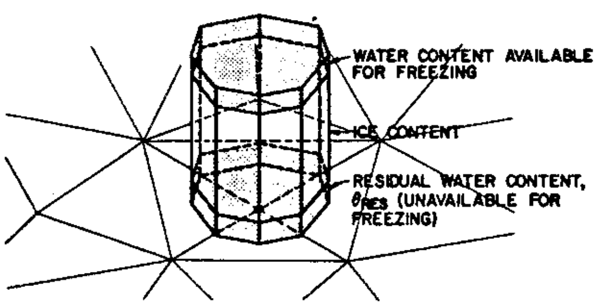


Fig. 6. Water Content Budget for Node j

MODELING PARAMETERS

The parameters needed for the computer model fall into three categories:

(i) heat flow parameters
(ii) soil-water flow parameters
(iii) phase change parameters

Heat Flow Parameters

Thermal conductivities and heat capacities are required to model heat flow. These parameters can be usually developed from published formulas, or obtained from charts and tables.

Soil-Water Flow Parameters

The soil-water flow model requires information regarding the coefficient and exponent used in the Gardner's function relationships for hydraulic conductivity and water content as related to pore pressure.

Phase Change Parameters

The volumetric latent heat of fusion and freezing point depression are defiend by the program user.

Parameter Groups

Rather than enter the several parameters for each finite element, parameter groupings are used to combine similar properties. Two types of groupings are used; namely, element parameter groups and nodal parameter groups.

- Element parameter groups include the conduction parameter data. This enables a better description of conduction values used to compute flow rates across control volume boundaries.
- Nodal parameter groups include the capacitance parameter data. This enables the program user to best define those parameters which are averaged over the control volume area (e.g., heat capacity).

Figure 7 demonstrates the flow balance models used, and where the conduction and capacitance parameters are assumed to apply.

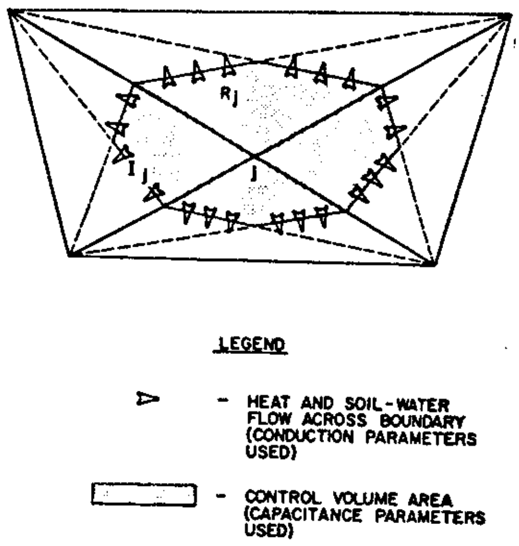


Fig. 7. Flow Balance Model and Parameter Usage

MODELING RESULTS

Nodal Values

The computed results provide nodal point values of temperatures, volumetric water content, and volumetric ice content produced at time intervals specified by the program user. A special feature afforded by the program is the ability to also print the previous timestep computed results (along with the current modeling results) in order to compare the change in nodal values of several variables during the recent timestep advancement.

Freezing Front Interpretation

Because the ice content values are specified at nodal points, and due to the mass-lumping budget used for the phase change algorithm (see Fig. 6), interpretation of the nodal ice content values are required in order to locate the freezing front (i.e., the line separating the frozen soil from the unfrozen soil). Similarly, the temperature values requrie interpretation in order to locate the 0°C isotherm (freezing front) at the boundary between the frozen and unfrozen soil regions. The interpretation effort required is directly related to the size of the finite elements used. Large triangular elements necessarily result in large control volume dimensions associated to each nodal point (see Figs. 2 and 3).

The usual interpretation procedure is to simply assume that the volume of ice estimated to exist in a nodal control volume exists as a single piece, and is located to the side of the control volume which has frozen.

This interpretation can be illustrated in terms of a one-dimensional problem involving rectangular-shaped finite elements. Figure 8a shows a nodal point control volume which is initiating freezing of available soil-water. The most recent timestep only evolved enough heat to freeze 10-percent of the soil-water available for phase change. Due to the lumped-mass model, the entire nodal control volume is associated with the nodal point value; hence, the nodal values of temperature and ice content indicate the freezing point depression and 10-percent frozen soil-water, respectively. Thus this information must be interpreted to indicate that the 10-percent frozen available soil-water is in one-piece and located as shown in Fig. 8a. Figure 8b illustrates the same control volume with 60-percent of the available soil-water frozen. Figure 8c illustrates a two-dimensional control volume with 60-percent of the available soil-water frozen.

THE TWO-DIMENSIONAL, PHASE CHANGE PROGRAM SYSTEM

The two-dimensional, coupled heat and soil-water flow, with an isothermal phase change approximation computer model is available as the FROST2X series of program developed for the U.S. Army Corps of Engineers Cold Regions Research and Engineering Laboratory, Hanover, New Hampshire where currently four versions are available (Table 1).

Similarly, the PROTOØ program has been extended to serve special purpose problems where the problem geometry is of a typical character. For example, PROTO1 enables for a quick data file preparation for roadway embankment problems where the interior nodal points and finite elements are developed by the program based on the entry of a few critical geometric coordinates of the problem boundary and locations of regional homogeneity (i.e., identical parameters for heat and soil-water flow).

It is noted that by considering the data entry requirements used in PROTOØ, the engineer can prepare special purpose data file preparation codes which are compatible with the FROST2X series, significantly reducing the data entry requirements associated with the PROTOØ general purpose code.

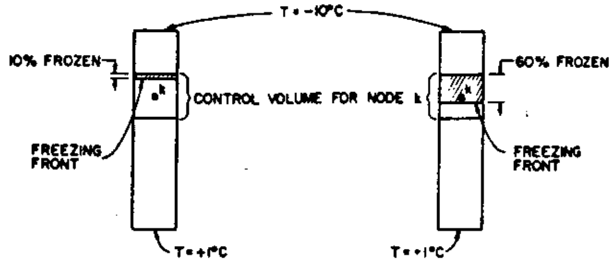


Fig. 8a. 10-percent frozen control volume

Fig. 8b. 60-percent frozen control volume

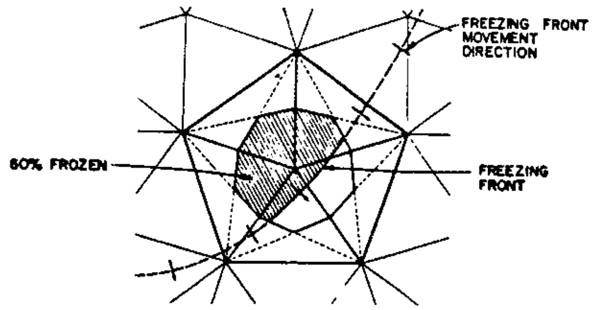


Fig. 8c. 60-percent frozen control volume (triangle elements)

TABLE 1. PROGRAM FROST2X DESCRIPTIONS

PROGRAM	DESCRIPTION
FROST2A	Base Development Version of FROST2X Series.
FROST2B	Two-Dimensional Heat and Soil-Water Flow Model With Isothermal Phase Change Model. Accommodates Heterogeneous But Isotropic Soil Systems. Includes an Apparent Heat Capacity During Phase Change Compatible With PROTOØ For Data File Preparation.
FROST2C	Extends FROST 2B To Include Anisotropic Soil-Water Flow.
FROST2D	Extends FROST2C To Include Vertical Frost Heave and Overburden Effects. Compatible With PROTO1 For Data File Preparation of Roadway Embankment Problems.

TABLE 2. SUBROUTINE TABULATION

PROGRAM	
FROST2B	Main, Indata, Bcsine, Trans, Phase, Output, Presol, Comb, Finsol.
FROST2D	Main, Indata, Bcsine, Trans, Phase, Output, Presol, Comb, Finsol, Over.

PROTOØ DATA REQUIREMENTS

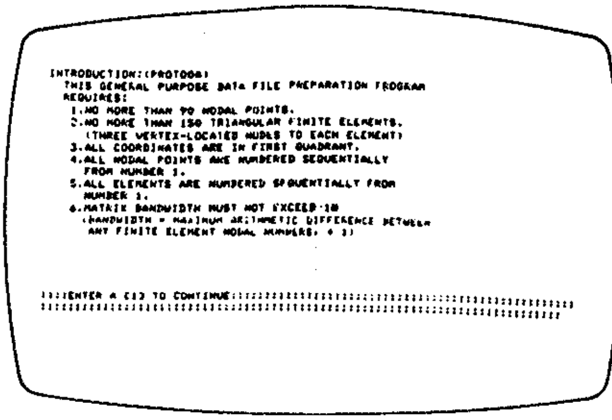
The data entry requirements associated with PROTOØ fall into four broad categories. These data groupings are illustrated in Fig. 9.

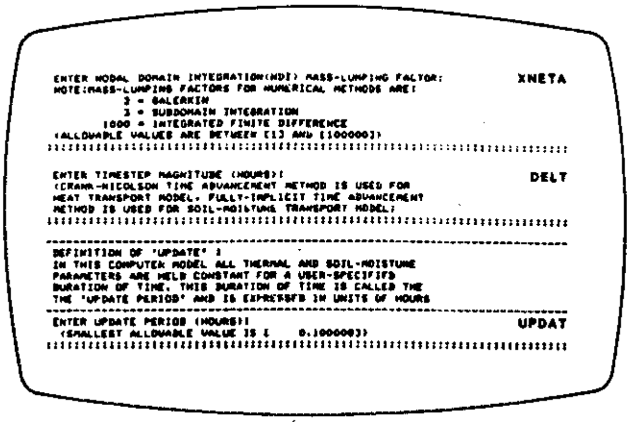
- MODEL CONTROL DATA
  - nodal domain integration mass lumping factor
  - timestep
  - time between global matrix regeneration
  - time of simulation
  - time between output of results
  - model selection:
    - heat and soil-water flow
    - heat flow
    - soil-water flow
    - include isothermal phase change
  - thermal parameters of water and ice
  - number of nodes
  - number of temperature boundary condition nodes
  - number of pore pressure boundary condition nodes
  - number of triangle finite elements
- FINITE ELEMENT PARAMETER GROUPS
  - thermal conductivity of soil
  - heat capacity of soil
  - saturated hydraulic conductivity of soil
  - exponent in Gardner's hydraulic conductivity
  - coefficient in Gardner's hydraulic conductivity
  - hydraulic conductivity ice content correction factor (exponent)
- NODAL POINT PARAMETER GROUPS
  - soil porosity
  - exponent in Gardner's water content
  - coefficient in Gardner's water content
  - frozen soil residual water content
  - heat capacity of control volume
- FINITE ELEMENT NODE NUMBER AND (x,y) COORDINATE DATA
- NODAL POINT INITIAL CONDITIONS
  - temperature
  - soil-water pore pressure head
  - ice content
- TEMPERATURE BOUNDARY CONDITIONS
  - node number
  - maximum temperature
  - minimum temperature
  - sine period
  - phase shift
- SOIL-WATER PORE PRESSURE BOUNDARY CONDITIONS
  - node number
  - maximum pore pressure head
  - minimum pore pressure head
  - sine period
  - phase shift

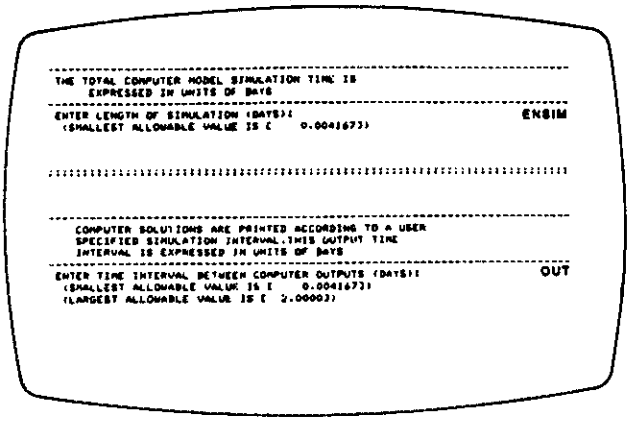
Fig. 9. PROGRAM FROST2B DATA REQUIREMENTS

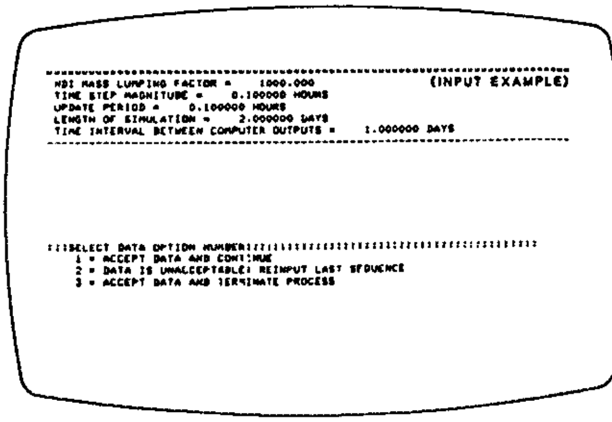
PROTOØ DATA ENTRY

Program PROTOØ prompts the model user for all data entries. In the following, a few of the data entry prompts are shown in their order of appearance. Included with the prompts are the associated PROTOØ variable names. It is noted that several of the prompts include suggested parameter values (for typical soil-water phase change problems), and the range of values allowed for use with program FROST2B.









APPLICATIONS

Three example problems are presented which illustrate the performance of the program FROST2B.

Heat Flow Application

A one-dimensional domain of unit length is discretized by 8 triangle finite elements as shown in Fig. 10a. At time t = 0, the temperature is given by T(x) = 1. Boundary conditions are given at x = 0 and x = 1 by T(x = 0) = T(x = 1) = 0. Using a normalized timestep of t = 0.01, the computed results from FROST2B and the exact solution (Myers, 1971) are shown in Fig. 10b. The data file prepared by PROTO0 is shown in Fig. 11.

Soil-Water Flow Application

A vertical homogeneous soil column is discretized by triangle finite elements as shown in Fig. 11a. A water table forms the base of a steady state 45-degree pore-pressure head profile through the vertical column. The column is insulated on both sides. The top of the column is suddenly flooded at a uniform depth of 2 cm. of water. The FROST2B modeling results are shown in Fig. 11b.

Phase Change Model Application

The vertical column of Fig. 11a is now considered with respect to soil-water freezing. Initially, the column is at a uniform temperature of +0.1°C. The top of the column is suddenly set at a constant temperature of -5°C. The FROST2B modeling results are shown in Fig. 12.

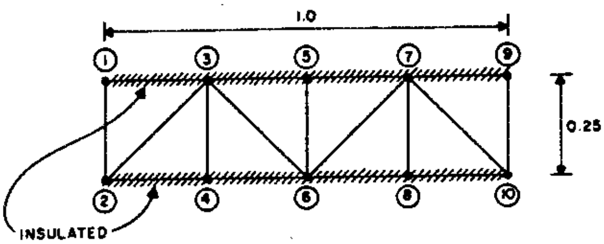


Fig. 10a. Heat Flow Example Problem

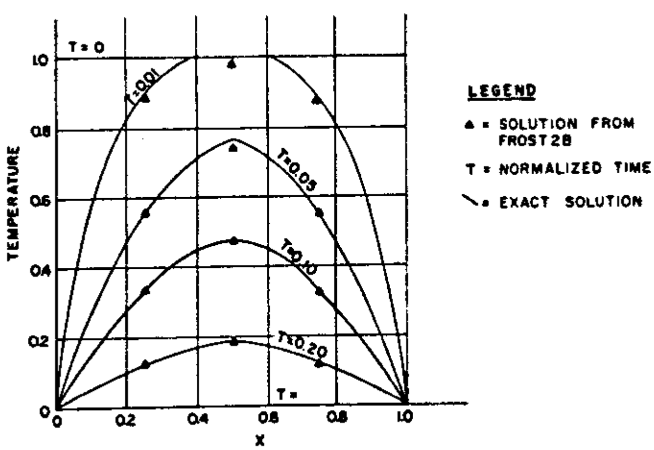


Fig. 10b. Heat Flow Example Problem Solution

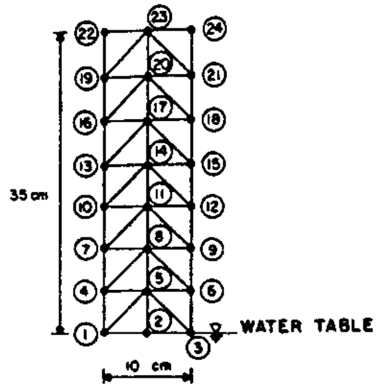


Fig. 11a. Soil-water Flow Example Problem

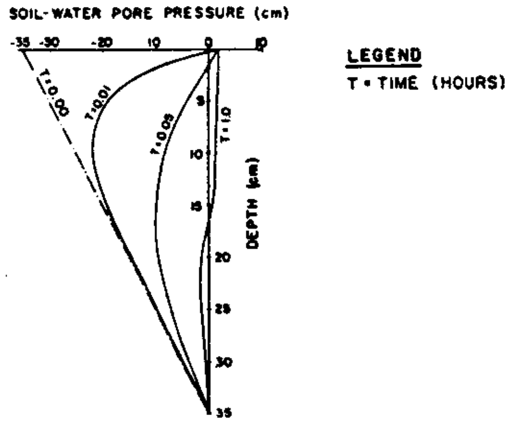


Fig. 11b. Soil-water Flow Example Problem Solution

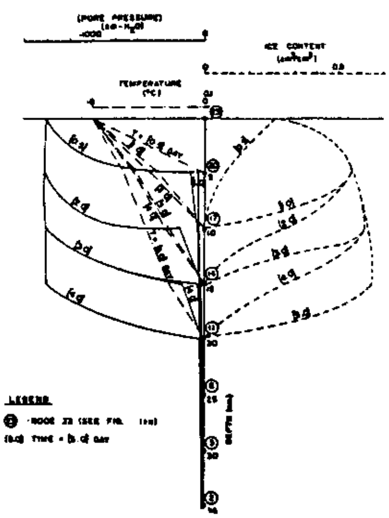


Fig. 12. Phase Change Problem Solution

REFERENCES

1. Hromadka II, T. V., "Finite Element Model of Transient Heat Conduction with Isothermal Phase Change," M.S. thesis, University of California, Irvine, Dept. of Civil Engineering, 1977.
2. Hromadka II, T. V., "Mathematical Model of Frost Heave in Freezing Soils," Ph.D. dissertation, University of California, Irvine, Dept. of Civil Engineering, 1980.
3. Myers, G. E., "Analytical Methods in Conduction Heat Transfer," McGraw-Hill, New York, 1971.