A PRELIMINARY EVALUATION OF NUMERICAL MODELS SUITABLE
FOR THERMAL ANALYSIS OF ROADWAYS AND AIRSTRIPS

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A Preliminary Evaluation of Numerical Models Suitable
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SUMMARY

A literature search and brief evaluation of numerical models suited
to the analysis of the thermal regime of roadways and airstrips have been
made. Several of the more promising models have been inspected with respect to
1) whether they incorporate the physical processes and parameters associated
with heat conduction in freezing soils in a realistic manner, 2) the
expected computational efficiency of the computer program for the model, if
available and 3) whether purchase, license or other agreement scheme for
using the program could be implemented. Under these conditions, it appears
that three or possibly four existing models may be suitable for use by the
Alaska Department of Transportation and Public Facilities (ADOTPF) - the
model of Guymon and Hromadka (U.C.-Irvine) the Battelle (Columbus Laboratoriës)
model, the Exxon Production Research (EPR) model and possibly the R & M
Model (Irvine). It is recommended, as a second phase, that several analy-
tical models be solved for a realistic set of boundary conditions and the
above recommended numerical models be compared to the analytical ones.
This procedure would test the numerical models and help to further "weed out" errors in the physics or in the numerical computational schemes. The
remaining models should be applied to ADOTPF problems using a realistic set
of data for testing and comparison.
INTRODUCTION

With the explosive growth of the computational capacity of computers in the past decades and the increasing sophistication of numerical methods of analysis, thermal problems associated with geometries, thermal properties and boundary and initial conditions of increasingly greater complexity are now being attacked. The problem of a soil subjected to temperatures below freezing has received particular attention in recent years by researchers dealing with the thermal regime due to expanding resource development, specifically oil and gas, and the need for engineering structures, such as roads, in the Arctic.

Hot oil pipelines and roads can cause thermal degradation of the underlying permafrost with subsequent settlement and sometimes mechanical failure, whereas the cold gas pipeline may lead to frost heaving of the soil. It is precisely because of the great potential for structural damage and associated environmental concerns that most of the more sophisticated models of the freeze-thaw problem in soils have been developed in an attempt to predict the thermal regime, given a knowledge of the thermal properties of the soils and the initial and boundary conditions. Predictions provide a guide for selecting between different construction modes and for preventative measures to mitigate the most serious problems that may arise from thermal degradation and from frost-heaving relative to pipelines.

With respect to the existing road network in Alaska, it has been estimated (private communication, B. G. Connor, ADOTPF) that about a quarter (a few tens of millions of dollars) of the road maintenance budget of the ADOTPF is a direct result of road damage associated with the seasonal frost in the road bed and the transient thermal response of the underlying permafrost to the presence of the road. It is clear that lower '48
road-building technology does not suffice in the more severe climatic conditions of Alaska. New techniques for reducing the potential damage that might occur to roadways from seasonal freezing and thawing and from permafrost-degradation must be developed. Thus, as with pipelines, reasonably accurate thermal models are required to predict the thermal regime of roadbeds (and runways, as well). To this end, ADOTPF requested proposals to meet the need for an efficient, accurate, two-dimensional thermal model. However, due to the diversity of modelling techniques, applicability and other factors, it was agreed upon by the engineers-in-charge to first investigate the availability and suitability of existing numerical models. The present report addresses these concerns.

A literature search and brief evaluation of numerical models suitable for investigating the temperature in a roadway or airstrip embankment have been made and are reported here. The minimum features required of a thermal analysis model for an embankment structure are 1) that it be at least, two-dimensional, 2) that it must include coupled heat and moisture flux terms and allow for variable thermal properties, 3) that the effect of latent heat sources or sinks be included in a reasonably self-consistent manner, 4) that it be able to accept a variety of boundary and initial conditions, 5) that the model preferably use finite elements in numerical calculations, 6) that it be user oriented, that is, it be well-documented and easily implementable on existing Alaskan systems or accessible through a computer terminal network, and 7) that it be available for general and long-term use under purchase, license or other agreement between ADOTPF and the originator(s) of the computational scheme(s).
DESCRIPTION OF THE PROBLEM

The problem of freezing of a geotechnical material (rock, silt, peat, sand, gravel, etc.) is exceedingly complex. Some factors which influence freeze and thaw rates in natural systems include, snow cover, vegetative cover, soil type, soil moisture, soil thermal characteristics and initial temperature distribution of soil and snow cover as well as external atmospheric factors such as air temperature, pressure and net solar long-wave radiation. While it cannot be hoped to include every factor in a mathematical prediction of the evolution of the thermal regime in a soil, certain simplifying assumptions can be made which may allow reasonable estimates of temperature and depth to freeze/thaw front (the phase boundary) in a soil for given initial and boundary conditions.

The mathematical description of the thermal regime of a material such as a soil undergoing a phase change is complex. In fact, analytical solutions exist only for a few idealized geometries and simplistic boundary and initial conditions. With the addition of a convection term for fluid in the pore spaces of the material to the transient Fourier conduction equation, the heat flow equation may be written in cartesian coordinates

\[ \nabla \cdot (\tilde{k} \cdot \nabla T) - C_w (\mathbf{v} \cdot \nabla T) = \partial (CT)/\partial t \]  

(1)

where \( \tilde{k} \) is the thermal conductivity tensor, \( T \) the temperature, \( C_w \) the volumetric heat capacity of the fluid, \( \mathbf{v} \) is the convective velocity field of the fluid, \( C \) is the average volumetric heat capacity of the material including the fluid and \( t \) is time. This equation holds on either side of the phase boundary with suitable choice of the thermal properties of the material on either side of the boundary. Note, however, that \( \mathbf{v} = 0 \) where \( T \) is below the freezing temperature.
A layered material, which is approximately the case with soils, may be regarded as orthotropic (see Carslaw and Jaeger, 1959). For such materials, we may relate the release of latent energy at the freezing front to the incoming and outgoing heat flux as

\[ \kappa_f \cdot \nabla T_f - \kappa_u \cdot \nabla T_u = L \phi \frac{dR}{dt} \]  

(2)

where \( L \) is the latent heat of fusion per unit volume, \( \phi \) is the porosity, \( R \) is a radius vector from the origin to a point on the freezing front and \( f \) and \( u \) refer to the frozen and unfrozen materials, respectively. Note that \( dR/dt \) can be thought of as the velocity of the moving boundary and that in general \( dR/dt \) may not coincide with the normal to the freezing boundary.

F. Neumann, whose results were given in a series of lectures in the 1860's (see Tamura, 1905 and Riemann-Weber, 1912), appears to have been the first to study mathematically the transient heat problem in a phase-changing material. Stefan (1891) independently attacked the problem of the freezing of a still body of water, to which Neumann's more general solution is also applicable. The problem solved by Neumann was that of an initially isothermal, homogeneous material in a half-space whose boundary is suddenly subjected to a fixed temperature \( T_S \) below the initial temperature \( T_0 \) and the fusion temperature \( T_L \).

For the Neumann problem, ignoring fluid motion, equations (1) and (2) reduce to:

\[ \frac{a}{ax} (k_f \frac{aT_f}{ax}) = c_f \frac{aT_f}{at} \quad (0 < x < \epsilon) \]

\[ \frac{a}{ax} (k_u \frac{aT_u}{ax}) = c_u \frac{aT_u}{at} \quad (x > \epsilon) \]
\[ k_f \frac{\partial T_f}{\partial x} \bigg|_{\epsilon-\delta} - k_u \frac{\partial T_u}{\partial x} \bigg|_{\epsilon+\delta} = L \phi \left( \frac{de}{dt} \right) \]

where \( x = \epsilon \) is the depth to the freeze front. The initial conditions are \( T_f = T_u = T_0 \) and \( x = \epsilon = 0 \) at \( t = 0 \), whereas the boundary conditions are \( T_f = T_s \) for \( x = 0, t > 0 \), \( T_u + T_0 \) as \( x \to \infty, t > 0 \) and \( T_u = T_f = T_L \) at \( x = \epsilon \) and \( t > 0 \).

Neumann obtained solutions of the form \( T = \alpha_1 + \alpha_2 \text{erf} (\alpha_3 x t^{-1/2}) \) (where \( \text{erf} (\alpha_4 x t^{-1/2}) \) is the error function with the argument shown) in both the frozen and unfrozen materials and \( \epsilon = \alpha_4 t^{-1/2} \) for the depth of the frozen layer. The constants \( \alpha_1, \alpha_2, \alpha_3 \) and \( \alpha_4 \) depend on the initial, fusion and surface temperatures and the thermal properties of the material on both sides of the boundary.

The Neumann and Stefan solutions have been applied to freezing of soils containing significant moisture (see Berggren, 1943; Aldrich and Paynter, 1953, Aitken and Berg, 1968; Lunardini, 1980). However, predictions based on these solutions are not likely to be very accurate because several other important factors, such as heat transport by convective liquid motions, temperature-dependent thermal properties and heat flux originating from the interior of the earth, are not taken into account.

For extremely dry, unfrozen or frozen course-grained soils and unsaturated gravels such as in road beds, a significant quantity of heat may also be transported by the convection of water vapor, especially if there exists a large thermal gradient through the material. Equation (1) is therefore incomplete, because it does not contain heat source or sink terms representing sublimation and condensation of moisture.

An additional complication is that the thermal properties of real soils including the latent heat of sublimation are temperature dependent.
Thus, finding solutions of Equations (1) and (2) by numerical means can be exceedingly difficult even for the most simple of realistic systems.

Numerical solutions to the transient heat conduction problems with phase change under certain simplifying assumptions have been obtained using finite difference and finite element techniques or a combination of these for the time and spatial coordinates. The finite difference technique is best-suited for a regular spacing of grid points where temperature is evaluated numerically for a given number of time steps and thus has been applied extensively to the one-dimensional transient heat problem with phase change. For irregular-spacing and two or three-dimensional geometries, the finite element method is preferred, because the application of finite-differences to such geometries and spacings leads to restrictions on allowable time step sizes due to stability criteria, which may substantially increase computational time of the finite difference formulation over an equivalent finite element formulation.

The problem to be attacked by Equations (1) and (2) with suitable initial and boundary conditions is the freezing/thawing cycle of geotechnical materials in the form of an embankment. The boundary conditions at the surface of the material are extremely important to the results of the modelling. Temperature boundary conditions are normally used, but since the surface temperature is the result of energy flux, at the surface, flux boundary conditions may give better accuracy. Although inherently three-dimensional, the embankment problem may be treated to first approximation as two-dimensional. In the next section several existing models for the freeze-thaw problem will be examined.
MODELS EXAMINED

We have examined the models listed below by name of authors and/or by industrial organization with affiliation and dates of publications noted.

1) Battelle*, Columbus, OH. Labs, (Contact: Dr. S. Pimputkar)
2) Bechtel Corp*, S.F., CA., (Contact: Dr. C. Arnold)
3) Berg*, Guymon and Johnson (1980), CRREL, NH and U.C. Irvine
4) Exxon Production Research (EPR)*, (Wheeler, 1973; Miller, 1979), Houston, TX, (Contact: Dr. C. C. Heuer)
5) Goodrich* (1978), Div. of Bldg. Res., NRC, Ottawa, Canada
6) Guymon* and Hromadka (1977), U.C.-Irvine, CA.
7) EBA Engineering Consultants, Ltd.*, (Hwang, 1977; Hwang, et al., 1980), (Contact: Dr. C. T. Hwang), Edmonton, Canada
9) Lunardini (1980), CRREL - N.H.
10) Outcalt, S.* (1980)?, U of Michigan
11) Taylor, George*, Ohio State University
12) R & M Consultants, Inc.*, Irvine, CA., (Contact: Dr. C. L. Vita)

The papers shown by author and date are listed in the references along with a few additional papers. The asterisk denotes firms or persons contacted personally via telephone.

The firms or organizations (Battelle, Bechtel, EPR, EBA and R & M) listed above have working two-dimensional computer-programmed models of the heat transport problem with phase change. Except for the R & M model, which is relatively recent, all the models have been applied, as a test of the models, to identical data sets supplied by the Alaskan Northwest Gas
Pipeline Company. Apparently, the thermal histories and structures predicted by each of the models, when compared with the actual in-soil data, were not so significantly different from each other that any one could be singled out as superior.

Neither the EBA nor the Bechtel models are available publicly according to C. T. Hwang of EBA and Charles Arnold of Bechtel. This effectively eliminates these models as candidates for ADOTPF use.

Of the remaining three models, proprietary to organizations, the R & M model is best-documented in terms of writing down the equations and for comparison with analytic and numerical (of the EPR model) solutions. Unfortunately, there are many errors of editorial nature in the version of the description of their thermal model denoted "Geotherm" which was sent to us (a later corrected version of a single section of the program description was received by a member of ADOTPF).

The numerical calculation scheme for R & M's Geotherm model is based on iso-parametric finite elements which allows for a more realistic simulation of natural boundaries. Moisture flow, unfortunately, is not coupled to the system, but must at present be specified externally. This lack of coupling may be a serious drawback in certain situations. Soil properties including moisture content vary nearly discretely above and below the freeze front, although some attempt is made to model the non-isothermal phase change in a realistic way. Surface energy balance has been included and this is a reasonably ambitious attempt to model the more important of the surface sources and sinks of energy flow.

All in all, the R & M computer model appears to take advantage of most of the methods to increase computer speed and to incorporate all important
physical processes that exist in and over a freezing soil. C. Vita of R & M has indicated in a telephone conversation that R & M has yet to license use of Geotherm by other organizations, however, he did not indicate this would not be possible.

On the other hand, EPR has had licensing or other agreements with other organizations. The exact nature and total number of the licensing agreements are unknown, but C. C. Heuer of EPR has indicated such a procedure would probably be possible with ADOTPF. Also, according to Heuer, licensing of the EPR program cost about $50K a few years ago and would be somewhat more expensive now.

The basic EPR program though older than the R & M model has been upgraded with the addition of a detailed surface heat balance option. It uses a finite element (though non-isoparametric) approach in the spatial domain, but a finite difference scheme for the time steps. It is unsatisfactory in its present form, for it does not allow for moisture transport in the soil, so that it does not entirely satisfy all the criteria initially set forth at the outset of this report. Nevertheless, this singular fault may be outweighed by several other characteristics of the program, e.g., the rather thorough and elegant surface heat balance simulation.

The EPR model is the best documented of the three from industry/organizations being considered here. The brief, thorough description of the program was received from Heuer along with three well-written papers of Wheeler and Miller.

Little documentation was received from S. M. Pimputkar of Battelle-Columbus Laboratories on the program which they call the "Battelle Thermal Soil Behavior Model". However, the short, accompanying, description of the model plus the cover letter suggest it is all-encompassing and that it
could be made available to the State of Alaska under contract by interactive access to the code stored at Battelle. Battelle is a non-profit organization and contractual agreements may be more easily consummated with them than the other organizations listed previously.

Battelle has a long history of dealing with agricultural soils and ground water hydrology especially with regard to radioactive wastes, although the inclusion of chemical sources, sinks and transport mechanism is probably not very important to the problem at hand.

Their modular-based program apparently has grown by adding subroutines to extend lower '48' conditions to the Arctic. The model is claimed to include a finite element technique, soil moisture convection (transport or conduction) as well as thermal conduction, and surface heat balance. These claims cannot be verified at this time without additional documentation, say, in the form of published papers by the originators of the Battelle model.

Finally, several university/government researchers were contacted. Most (Taylor, Outcalt, Berg and Goodrich) were frank in indicating their models were probably not adequate in meeting all the criteria we have listed for thermal studies of embankments. Some are now working on two-dimensional models, but had not progressed far enough to be considered here.

Goodrich of the Division of Building Research, N.R.C., Canada has a one-dimensional finite difference model and is now actively working on a two-dimensional model. Goodrich has kindly provided us with the coding for the 1-d model and this has been checked out on our computer. It should be noted that a one-dimensional model may often be sufficient for some engineering purposes and in general they may allow crude, but useful estimates and physical insight into the freezing of complicated soils and geometries.
It appears that Guymon and Hromadka of U.C.-Irvine are closest to producing a viable thermal model for cold regions of all the university personnel working on the problem. Dr. Guymon has provided us with the latest versions of their programs - NDIFH - a one-dimensional frost heave model and Frost 2A, a two-dimensional model for both heat and moisture transport in freezing/thawing soils. We are currently implementing the programs on the VAX computer to verify the coding. We hope to compare the Goodrich and Guymon/Hromadka models against some simple thermal soil problems with analytic solutions.

The Guymon/Hromadka model is relatively sophisticated having coupled heat and moisture transport. The numerical methods incorporated into the program are efficient and have been upgraded over the past years. However, it may not be possible for their annual frost heave model to predict long-term performance of roadbeds or, if it is possible, the computational scheme may not be efficient. Also there appears to be no surface heat balance subroutine to provide the soil/air (or snowpack) interface temperature from meteorological parameters, and thus the model is deficient on this point. Guymon has funding from CRREL for the next 2-3 years and could remedy the lack of a surface balance simulator in the future.

Collaborators, Lynch of Dartmouth and O'Neil of CRREL, have not been contacted directly but papers by them were provided by Berg of CRREL. Although, they have not yet published accounts of studies in more than one dimension, their studies are worth mentioning here because they have used a continuously deforming finite element system on the moving freeze front. This method may improve accuracy and speed of computing the thermal regimes of freezing soils.
RECOMMENDATIONS

Licensing or other contractual agreements are possible for the thermal models of EPR and Battelle. If Battelle's model performs as claimed, it would appear to be the superior model. R & M's model also appears to be nearly equivalent to the Battelle model, but we suspect licensing may be more difficult.

It is doubtful that licensing agreements would allow extensive modification of the coding of the programs which might be necessary, if it is found that they are needed to meet criteria unique to Alaska. However, the possibility of modification should be investigated with the Licensor.

Use of a model constructed through grants from the government should present fewer problems of access and refinement of the computer codes. Thus, the Guymon/Hromadka model, which is being continually upgraded with CRREL funding, is the most likely candidate for use in ADOTPF thermal analysis program.

In summary, we recommend in descending order (if Battelle's claim for their model is verified, but that the contractual agreement implies inflexibility in program modification) the

1) Guymon/Hromadka model
2) Battelle model
3) EPR model
4) R & M model

for use in the ADOTPF thermal analysis program. The Guymon/Hromadka model should be the least expensive to use as it has been programmed using government funds. Battelle's model may be less expensive to license than EPR's or R & M's since it is a non-profit organization.
A key point in model development and application is that the numerical models must agree with analytical models when applied to the same problem. Such comparisons provide a check on both the physics and the numerical computational schemes used. We recommend that 2 or 3 problems with realistic initial, conditions, boundary conditions and soil parameters be defined, analytical solutions obtained and that these solutions be compared to the results of 2 or 3 of the numerical models to check their performance at several time scales.

The following is a list of contacts (addresses and telephones) for the models:

1) Professor Gary Guymon, Department of Civil Engineering, U.C. - Irvine, Irvine, CA. 92717, (714) 833-6725

2) Dr. S. M. Pimputkar, Principal Research Scientist, Energy and Thermal Technology Section, Battelle-Columbus Laboratories, 505 King Ave. Columbus, OH 43101, (614) 424-6424

3) Dr. C. C. Heuer, Exxon Production Research Company, P.O. Box 2189, Houston, TX 77001, (713) 965-4390

4) Dr. C. L. Vita, R & M Consultants, Inc., 19700 Fairchild, Suite 180, Irvine, CA 92715, (714) 833-0843

We mention in passing that Professor Arvind Phukan, Civil Engineering, University of Alaska, has stated he should have a model comparable to the EPR or Battelle model in 2-3 months from the time of this writing (Feb. 82), but did not give specific details as to the source(s) of the model and other information.
REFERENCES


