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AN EXPERT SYSTEM FOR ESTIMATING SOIL THERMAL AND TRANSPORT PROPERTIES

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ABSTRACT

Prediction of soil thermal conductivity k is particularly difficult at high temperatures T (50-90°C) and very low moisture content θ; the k value may increase with temperature by a factor of 3-5. This phenomenon is due to water vapor migration resulting in latent heat transfer, which is strongly dependent on soil water characteristics (SWC). In the past, the SWC influence on k prediction was never studied in great detail – mainly due to a lack of reliable SWC experimental data at low θ. Currently, hydraulic properties of soils can be evaluated from numerous predictive models correlated with experimental data. The paper objectives focus on: effects of SWC on k prediction; explanation of nonlinear variation of k at high T with θ ranging over the full degree of saturation; large k over-predictions at low θ and high T. Results obtained show very strong k dependence on the SWC function; therefore, accuracy of SWC estimates cannot be disregarded. The paper explains a nonlinear k behavior at high T as a combined effect of water vapor migration, SWC, and soil air relative humidity. To this end the paper provides also information about Soil Thermal and Transport Properties – Expert System (STTP-ES), collection of the notable predictive models for these properties, for both moist and frozen soils, which have been gleaned from the literature and integrated into one software package. The appendix provides a brief description and recent modifications made to the STTP-ES. Closing discussion concentrates on STTP-ES shortcomings, development of the Windows driven package, Expert System extension to other porous media and the database development.

INTRODUCTION

Thorough knowledge of soil thermal and transport characteristics is required in computer modeling of heat and moisture flow in engineering and science applications such as: underground high voltage power cables; district heating systems (underground pipes); high-level radioactive waste underground storage; heat pump ground heat exchangers; high temperature ground heat storage; designing roads, airfields, buildings, and gas/oil pipelines in sub-arctic regions; artificial ground freezing; air pre-conditioning for greenhouses, livestock shelters, mushroom plants; modeling of heat and water transport in bare/vegetated soil; evaluation of the heat flow and temperature variation near the ground surface; and thermal soil remediation. Reliable estimates of these properties, particularly thermal and hydraulic conductivity, are not easy to obtain, partly due to their high textural variability in the field, and partly because measuring procedures are time consuming, expensive and error prone; hence the available data is often fragmentary and dubious. Consequently, there is a growing demand for reliable physically based predictive models based on easily obtained and reliable input data. Unfortunately, it is unlikely that a single model exists which can produce good estimates for all soils encountered in the field. Prediction of soil thermal conductivity k is particularly difficult at high temperatures (50–90°C) and very low moisture content; its value may increase with temperature by a factor of 3-5. This phenomenon is due to water vapor migration resulting in latent heat transfer, which is strongly dependent on soil water characteristics (SWC). In the past, the SWC influence on k prediction was never studied in a great detail – mainly due to a lack of reliable SWC experimental data at low θ. Currently, hydraulic properties of soils can be evaluated from numerous predictive models correlated with experimental data. The paper objectives focus on the following: analysis of effects of SWC on the k prediction, explanation of nonlinear variation of k at high T with θ ranging over the full degree of saturation, and large k over-predictions at low θ and high T.

MATERIALS AND METHOD

Three soils of different texture (Royal, Palouse-A and Palouse-B) whose thermal conductivity data were published by Campbell et al. (1994) are used in this paper. Soil texture and mineralogical information is summarized in Table 1.

Thermal conductivity data includes variation of soil temperature ranging from 30 to 90°C. Thermal conductivity of soil has been evaluated using deV-2 model (Tarnawski et al., 2000) which is similar to the model proposed by de Vries (1963). In contrary to the de Vries model, the deV-2 model

Table 1 Summary of soil physical properties (porosity and mass fractions of various components)

Soil	Porosity	x_{clay}	x_{sand}	x_{quartz}	$x_{feldspar}$	$x_{calcite}$	$x_{clay\text{-}minerals}$	x_{mica}
Royal	0.49	0.145	0.536	0.425	0.313	0.016	0.190	0.056
Palouse-A	0.52	0.205	0.113	0.385	0.220	0.044	0.270	0.081
Palouse-B	0.57	0.468	0.093	0.350	0.164	0.021	0.380	0.085

assumes that water is a continuous medium over the full range of saturation. Evaluation of the shape value of air pockets follows an empirical power relation proposed by Neiss (1982). The deV-2 model is one of ten thermal conductivity models built in the Soil Thermal and Transport Properties – Expert System (STTP-ES). The following information is applied to all k models: (i) five standard minerals, plus organic matter; (ii) temperature-dependent thermal conductivity of the principal minerals are taken from Neiss (1982) and Landolt-Börnstein (1982). In soils encountered in the field, quartz may exist in various mineralogical forms (crystalline, amorphous, and etc.). Often the smaller quartz grains in soils will show less crystallinity than larger idiomorphic crystals. As the thermal conductivity of quartz decreases with lower crystallinity, the STTP-ES uses a reduced k value for quartz (5.65 – 6.25 W/(m·K) at 20°C) as compared to that encountered in literature (7.75 – 8.8 W/(m·K)), which normally refers to measurements on larger idiomorphic minerals. The STTP-ES has also an option, available to all models, to account for the contribution of latent heat transport due to water vapor diffusion in soils exposed to high temperature gradient. This option requires, however, a good knowledge of soil water characteristics (SWC). Soil water relations, i.e. soil moisture characteristics, are evaluated from any of ten SWC models (see Appendix). Verification results show that the deV-2 model predictions follow closely experimental data (±15%) of soils exposed to moderate temperatures and for moisture contents near field capacity (FC). At a very low moisture content and high temperatures, the deV-2 model was not tested against the accuracy of SWC predictions.

ENHANCED HEAT TRANSFER MODEL

De Vries model (1963) has been described in a number of publications (e.g. Hopmans and Dane, 1986, and Tarnawski et al., 2000). Therefore, it will not be repeated here. However, for the purpose of this study, the de Vries model for the enhanced heat transfer due to latent heat transport of water vapor diffusion is given as follows:

$$k_{app} = k_a + RH \cdot k_{vs} \qquad (1)$$

k_{vs} refers to the transport of latent heat when soil air is saturated with water vapor. It is calculated according to de Vries (1963):

$$k_{vs} = \frac{H_L\,D}{R_v T_K}\,\frac{p_b}{p_b - p_{vs}}\,\frac{dp_{vs}}{dT} \qquad (2)$$

Once the retention curve (i.e. SWC) for the soil is defined, the relative humidity, RH, is calculated from the following relation which assumes local thermodynamic equilibrium linking RH to the soil water pressure head h:

$$RH = \exp\left(-\frac{g\,h}{R_v T_K}\right) \qquad (3)$$

Table 2 Values and expressions for parameters used in calculating the equivalent thermal conductivity of transport of latent heat when soil air is saturated with water vapor (T in °C)

Parameter	Value/expression
k_a, W/(m·K)	$0.02454 + 0.0000727\,T$
H_L, J/kg	$2503000 - 2432.1\,T$
D, m²/s	$0.0000225\,[(T + 273.15)/273.15]^{1.72}$
R_v, J/(kg·K)	461.5
T_K, K	$T + 273.15$
p_b, Pa	101325 – barometric pressure
p_{vs}, Pa	$\exp\left(\sum_{i=-1}^{3} a_i T_K^i + a_4 \ln T_K\right)$ where: $a_{-1} = -5.8002206\times10^3$; $a_0 = 1.3914993$; $a_1 = -4.8640239\times10^{-2}$; $a_2 = 4.1764768\times10^{-5}$; $a_3 = -1.4452093\times10^{-8}$; $a_4 = 6.5459673$
$\frac{dp_{vs}}{dT}$, Pa/K	$p_{vs}\left(\sum_{i=-1}^{3} i\,a_i T_K^{i-1} + a_4 T_K^{-1}\right)$
g, m/s²	9.81

Value and expressions used for all parameters are presented in Table 2. The soil water pressure head h is defined by a SWC model.

Two extreme SWC models are used to study the effect of SWC on predicting soil thermal conductivity k. The following SWC models are tested with respect to k prediction by the deV-2 model:

1. SWC Model I: Wösten et al. (1995)
2. SWC Model II: Brooks and Corey (1964)/Campbell (1974)

This investigation is applied to three different soils, namely: Royal (coarse soil), Palouse-A (medium soil), and Palouse-B (fine soil).

MODEL PREDICTIONS

Verification of SWC models

Figs. 1a, 1b and 1c show comparison of both SWC models with experimental data by Campbell and Shiozawa (1989) as a function of volumetric water content θ. For a very fine soil as Palouse-B, the SWC Model I shows very good predictions of the soil pressure head – particularly in a range of low moisture content. For medium and coarse soils (Palouse-A and Royal, respectively) the experimental data are between both model predictions. As the plots of SWC are in logarithmic scale, a highly nonlinear variation of soil pressure head can be observed at low water content range.

Soil Air Relative Humidity

Eq. (3) is used to calculate the soil air relative humidity. It is an exponential function of soil pressure head; therefore, the soil air relative humidity is a nonlinear parameter, especially at low water content where soil pressure head varies rapidly. For all soils under investigation, Figs. 2a, 2b, and 2c show evaluation of soil air relative humidity vs. volumetric water content at a temperature of 30°C. With other parameters held unchanged, the only variable in Eq. (3) is the pressure head. Hence, similar outcomes as the pressure head are expected, i.e., very good

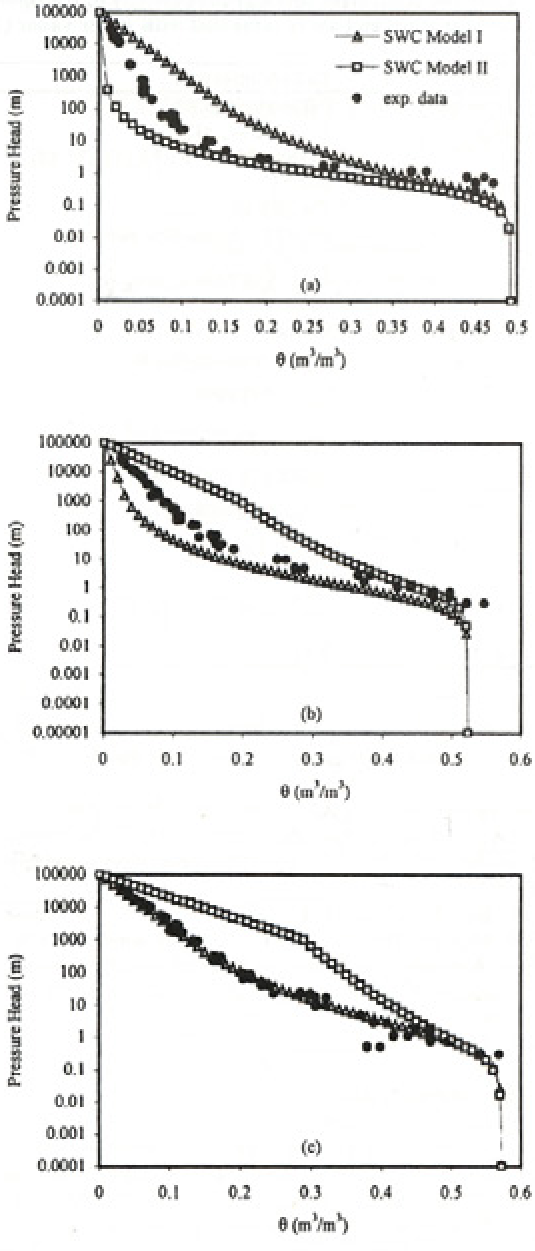

Fig. 1 Soil water characteristics models and experimental data of (a) Royal, (b) Palouse-A and (c) Palouse-B as a function of volumetric water content

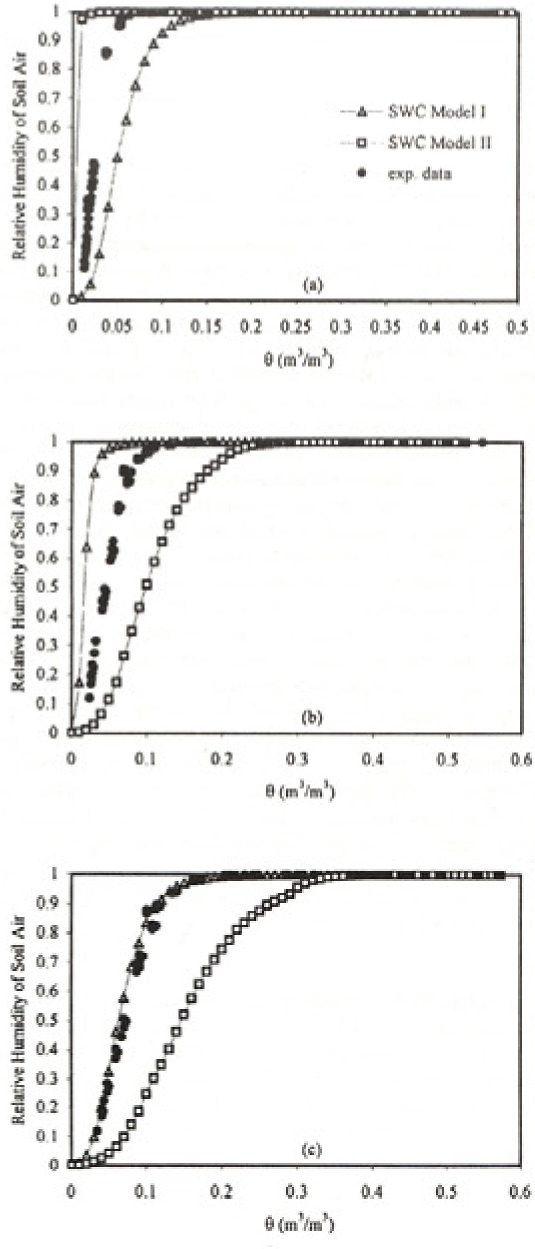

Fig. 2 Calculated relative humidity of soil air due to the SWC models and experimental data of (a) Royal, (b) Palouse-A and (c) Palouse-B as a function of volumetric water content

predictions of the soil air relative humidity for the fine soil (Palouse-B), while for medium and coarse soils (Palouse-A and Royal, respectively), the experimental data are between both model predictions.

Thermal Conductivity

Figs. 3a, 3b and 3c show comparison of experimental data at 30°C with predictive k influenced by two different SWC models. The results show that SWC has a definite effect on the prediction of soil thermal conductivity. Generally, the SWC Model II provides better predictive k than the SWC Model I, especially for Royal and Palouse-A at very low water content. Although the SWC Model I is a better model for Palouse-B, in terms of soil pressure head and relative humidity, it does not warrant a better prediction of k than the SWC Model II at low water content range. The deV-2 model over-predicts the thermal conductivity of all three soils. It appears that the enhanced heat transfer model due to water vapor migration by de Vries (1963), as given in Eq. (1), over-estimates the effects of heat and mass transfer at low water content.

As the temperature increases, the effect of SWC on the k predictions becomes more apparent. Figs. 4a, 4b and 4c show

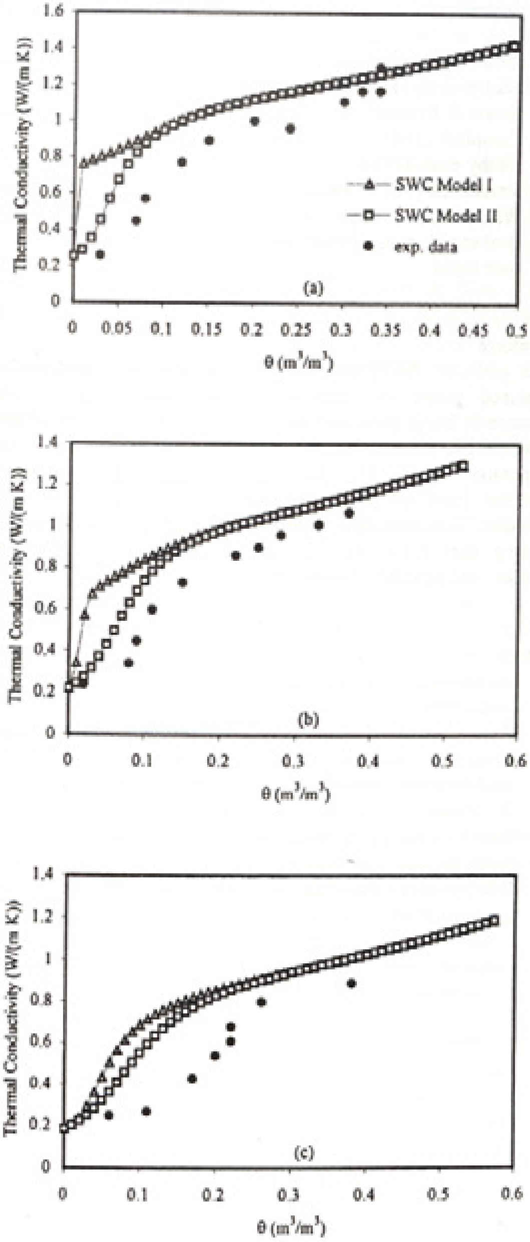

Fig. 3 Calculated thermal conductivity of soils due to the SWC models and experimental data at 30°C of (a) Royal, (b) Palouse-A and (c) Palouse-B as a function of volumetric water content

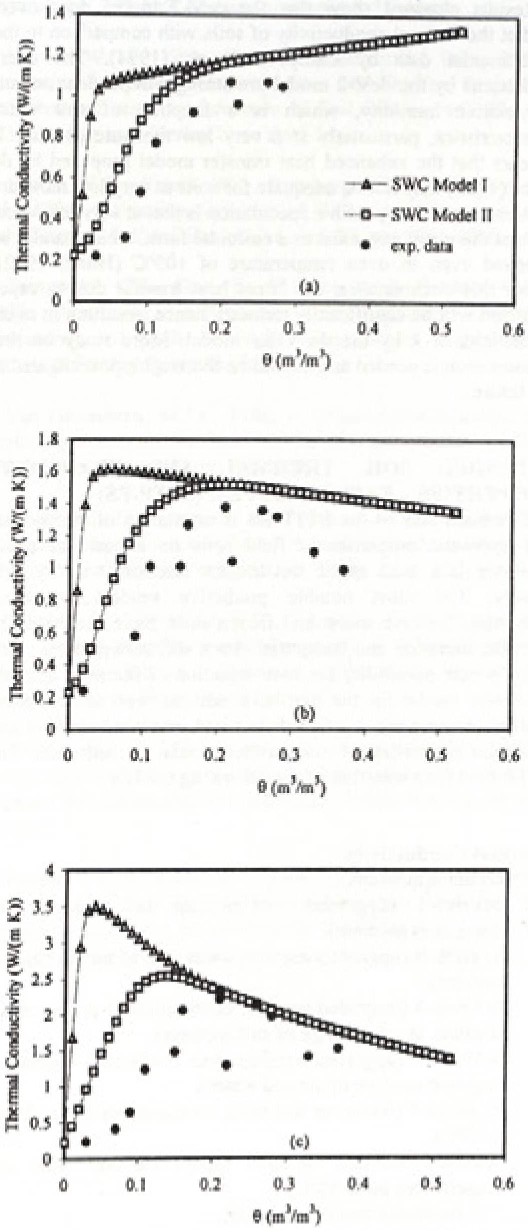

Fig. 4 Calculated thermal conductivity of soils due to the SWC models and experimental data of Palouse-A at (a) 50°C, (b) 70°C and (c) 90°C as a function of volumetric water content

the predictive k of Palouse-A at 50, 70 and 90°C, respectively. Similar trend is also observed for Royal and Palouse-B. At very low water content, the predictive k with the SWC Model I increases more than the one with the SWC Model II, hence, greater error as compared to the experimental data. At temperature of 90°C, the deV-2 model using the SWC Model I and II is able to produce a maximum k at about $\theta = 0.05$ and 0.15, respectively, as observed in the experimental data with a maximum k at about $\theta = 0.20$. The nonlinear variation of the thermal conductivity at a high temperature with θ ranging from dryness to saturation can be physically captured by the deV-2 model. However, it seems that, with such a large k over-predictions at low θ and high T, a better SWC model and apparent thermal conductivity model of soil air (k_{app}) are required in order to predict the thermal conductivity of soils at low water content range. As shown in Fig. 4c, the deV-2 model demonstrates a nonlinear behavior of the predictive k as a result of the combined effect of SWC function, soil air relative humidity and latent heat transport due to a high temperature gradient.

COMMENTS AND CONCLUSIONS

Results obtained show that the deV-2 model does over-predict the thermal conductivity of soils with comparison to the experimental data by Campbell et al. (1994). The over-predictions by the deV-2 model are strongly dependent on soil air relative humidity, which is a function of soil water characteristics, particularly at a very low moisture content. It appears that the enhanced heat transfer model proposed by de Vries (1963) may not be adequate for soils at very low moisture content range. One possible speculation is that at very low water content the water may exist as a colloidal form, which cannot be removed even in oven temperature of 105°C (Hillel, 1982). Under this circumstance, the latent heat transfer due to vapor diffusion will be significantly reduced, hence, resulting in over-predictions of k by the de Vries model. More study on this phenomenon is needed and should be thoroughly investigated in the future.

APPENDIX: SOIL THERMAL AND TRANSPORT PROPERTIES – EXPERT SYSTEM (STTP-ES)

The main task of the STTP-ES is estimation of the thermal and hydraulic properties of field soils on a basis of easily available data, such as the soil textural fractions and dry bulk density. The most notable predictive models for these properties, for both moist and frozen soils, have been gleaned from the literature and integrated into a software package. This offers a new possibility for easy selection of the most suitable predictive model for the particular soil, as well as an instant evaluation/comparison of predicted and measured thermal and hydraulic properties of soils either frozen or unfrozen. The STTP-ES offers selection of the following models:

Thermal Conductivity

1. Kersten Equations,
2. DeVries–1 (upgraded version: air or water as the continuous medium),
3. DeVries–2 (upgraded version: water only as the continuous medium),
4. DeVries–3 (upgraded version: continuous air pocket shape function, in a full range of soil wetness),
5. DeVries–4 (upgraded version: one continuous medium – weighted mixture of air and water),
6. Johansen–I (frozen or wet soils, temperatures from –20 up to 30°C),
7. Nonlinear Kersten function model for wet soils and temperatures up to 95°C,
8. Gori (unfrozen and frozen soils),
9. SCA+TCR Sundberg (unfrozen and frozen soils), and
10. Pande-Singh-Gori.

Transport Characteristics

Hydraulic conductivity, water retention and soil water diffusivity:

1. Model of Rawls (1991),
2. Model of Wösten et al. (1995),
3. Model of Wösten et al. (1998),
4. Model by Brooks and Corey (1964)/Campbell (1974),
5. Brooks-Corey model for aggregated soils (Wagner et al., 1996),
6. Model of Van Genuchten (1980),
7. Van Genuchten model with Vereecken regression equations for main parameters,
8. Gregson-Hector-McGowan model (paired measurements needed),
9. Van Genuchten model using RETC-program, and
10. Selection from a database

The saturated hydraulic conductivity of moist soils:

1. Saxton et al. (1986),
2. Rawls & Brakensiek (1989),
3. Campbell (1985),
4. Cosby et al. (1984),
5. Vereecken et al. (1990),
6. Wösten et al. (1995),
7. Brakensiek et al. (1984), and
8. user input.

Database

In addition, STTP-ES will have access to a database of measured properties extracted from various sources. The database is being generated according to the soil type (textural fractions and organic matter content), moisture content, and temperature range. The thermal conductivity data are being collected from the published/unpublished experimental data available. The hydraulic conductivity data will be based on existing data from Rawls, van Genuchten, Swedish Soils, German, and possibly Australian soils.

Future

1. Incorporation of new soil thermal and hydraulic models (pedo-transfer functions),
2. Development of a unified database – upgrade, model sensitivity analysis, comprehensive testing, STTP-ES modifications, statistical analysis, and graphical display,
3. Development of a complete Expert System,
4. Development of the Windows driven package,
5. Extension of the existing Soil Expert System to other heterogeneous materials of engineering and the physical sciences interest, such as granular back-filling materials, sandstones, building materials – including multifunctional concrete, timber/wood, foods, ceramics, fiber reinforced materials and composites, etc.,
6. k-modeling approaches to the above heterogeneous materials,
7. Development of the Windows/Web-based computer platform, with event driven package promoting modularity, and
8. Development of the STTP-ES server mode for heat and moisture flow in porous media applications, linked to the server providing the Internet user with required thermal and transport properties.

REFERENCES

Brakensiek, D.L., Rawls, W.J. & Stephenson, G.R., 1984, Modifying SCS Hydrologic Soil Groups and Curve Numbers for Rangeland Soils, ASAE Paper No. PNR-84-203, St. Joseph, Mich.

Brooks, R.H. & Corey, A.T., 1964, Hydraulic Properties of Porous Media, Hydrol. Paper 3.

Campbell, G.S., 1974, A Simple Model for Determining Unsaturated Conductivity from Moisture Retention Data, *Soil Science*, vol. 117, pp. 311-314.

Campbell, G.S., 1985, *Soil Physics with Basic*, Elsevier, New York.

Campbell, G.S. & Shiozawa, S., 1989, Prediction of Hydraulic Properties of Soils using Particle Size Distribution and Bulk Density Data, *Proc. Int. Workshop on 'Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils'*, Riverside, California, October 11-13, Eds. M.Th. vanGenuchten, F.J. Leij, and L.J. Lund.

Campbell, G.S., Jungbauer, J.D., Bidlake, W.R. & Hungerford, R.D., 1994, Predicting the Effect of Temperature on Soil Thermal Conductivity, *Soil Science*, vol. 158, no. 5, pp. 307-313.

Cosby, B.J., Hornberger, G.M., Clapp, R.B. & Ginn, T.R., 1984, A Statistical Exploration of the Relationship of Soil Moisture Characteristics to the Physical Properties of Soils, *Water Res. Research*, vol. 20, no. 6, pp. 682-690.

de Vries, D., 1963, Thermal Properties of Soils, in *Physics of the Plant Environment*, ed. W.R. Van Wijk, pp. 210-235, John Wiley & Sons, Inc., New York.

Hillel, D., 1982, *Introduction to Soil Physics*, Academic Press., Inc.

Hopmans, J.W. & Dane, J.H., 1986, Thermal Conductivity of Two Porous Media as a Function of Water Content, Temperature, and Density, *Soil Science*, vol. 142, no. 4, pp. 187-195.

Landolt & Börnstein, 1982, Numerical Data and Function of the Nature and Technology, in *Physical Properties of Rocks*, Part Ia, pp. 373, Springer.

Neiss, J., 1982, Numerical Simulation of Heat and Moisture Transport and Ice Formation in the Ground, *Fortschritt-Berichte der VDI-Zeitschriften*, Reihe 3, Nr. 73, pp. 293 (in German).

Rawls, W.J. & Brakensiek, D.L., 1989, Estimation of Soil Water Retention and Hydraulic Properties, in *Unsaturated Flow in Hydrologic Modeling – Theory and Practice*, ed. H.J. Morel-Seytoux, pp. 275-300, Kluwer Academic Publishers.

Rawls, W. J., Gish, T.J. & Brankensiek, D.L., 1991, Estimating Soil Water Retention from Soil Physical Properties and Characteristics, in *Advances in Soil Science*, vol. 16, pp. 213-234, Springer-Verlag New York Inc.

Saxton, K.E., Rawls, W.J., Romberger, J.S. & Papendick, R.I., 1986, Estimating Generalized Soil-water Characteristics from Texture, *Soil Sci. Soc. Am. J.*, vol. 50, pp. 1031-1036.

Tarnawski, V.R., Gori, F., Wagner, B. & Buchan, G.D., 2000, Modelling Approaches to Predicting Thermal conductivity of Soils at High Temperatures. International Journal of Energy Research (in print).

Van Genuchten, M.Th., 1980, A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils, *Soil Sci. Soc. Am. J.*, vol. 44, pp. 892-898.

Vereecken, H., Maes, J. & Feyen, J., 1990, Estimating Unsaturated Hydraulic Conductivity from Easily Measured Soil Properties, *Soil Science*, vol. 149, pp. 1-12.

Wagner, B., Tarnawski, V.R., Wessolek, G. & Plagge, R., 1996, Estimation of Hydraulic Properties of Aggregated Soils using a Two-Domain Approach, *Canadian Agricultural Engineering*, vol. 38, no. 4, pp. 241-247.

Wösten, J.H.M., Finke, P.A. & Jansen, M.J.W., 1995, Comparison of Class and Continuous Pedotransfer Functions to Generate Soil Hydraulic Characteristics, *Geoderma*, vol. 66, pp. 227-237.

Wösten, J.H.M., Lilly, A., Nemes, A. & Le Bas, C., 1998, Using Existing Soil Data to Derive Hydraulic Prameters for Simulation Models in Environmental Studies and in Land Use Planning, Report 156, DLO-Staring Centre, Wageningen.