Methane From Destabilized Permafrost in a Warmer World

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Acknowledgements

In putting my acknowledgements together I figured I had two options. I could thank everyone from my thesis advisor to the bus drivers who drove me to work while I was being environmentally pure my first year of grad school, or I could thank only those people who had been specifically helpful in this project. I'm not too happy with either but I'm going to go with the latter of the two (for the most part anyway).

Thanks to all my family and friends.

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Special thanks go out to Rei for doing all of the experimental work that this thesis presents and uses and to Keith Kvenvolden and Thomas Lorenson for discussion.

It has become something of a cliche for students to gush about their thesis advisors. Most of the time, these students are lying. Even though I fear that people will think that I am being mercenary, I will proceed since no one who has worked with Aslam will question my veracity. I can't imagine being in a better situation than I am working with Aslam. He is a most unlikely mixture of raw brilliance and humanity. He has been extremely kind to me, giving me many opportunities both directly and indirectly related to research. I could go on and on but I still have a dissertation to write, but this work would never have been completed without his constant help.

Dedication

to Amanda and the Animals

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List of Symbols

A	Temperature Dependant Water Content
B	Exponential Water Content Parameter
B_m	Amount of Gas Per Meter of Soil
C	Temperature Independent Water Content
C_a	Volumetric Heat Capacity of air
C_l	Volumetric Heat Capacity of liquid water
C_m	Volumetric Heat Capacity of minerals
C_o	Volumetric Heat Capacity of organic material
C_s	Volumetric Heat Capacity of solid water
C_{soil}	Volumetric Heat Capacity of soil
D	Gas diffusion constant in soil
D_0	Molecular diffusion constant of gas into air
K	Thermal Conductivity
K_a	Thermal conductivity of air
K_l	Thermal conductivity of liquid water
K_m	Thermal conductivity of minerals
K_o	Thermal conductivity of organic material
K_s	Thermal conductivity of solid water
K_{soil}	Thermal conductivity of soil
L	Model soil depth
L_f	Latent heat of fusion of water
$[O_2]_n$	Normalized Oxygen Concentration relative to atmospheric Concentration
S	Fraction of soil this is pore space
T	Temperature (measured in °C)
T_{ss}	Steady-state temperature distribution
T_t	Time-dependant temperature distribution
f_{pf}	Fraction of the earth's surface with a given permafrost
l_e	Effective path length through a soil element of length l
r_i	Yearly trend of the ith model day
s	Soil mass without water
t	Time
t_{pf}	Fraction of land underlain by permafrost
w	Soil water mass
x_a	Volumetric soil air content
x_l	Volumetric soil liquid water content
x_m	Volumetric soil mineral content

x_o	Volumetric soil organic material content
x_s	Volumetric soil solid water content
x_w	Volumetric soil water content
z	Soil Depth
γ	Neumann problem constant
κ	Thermal Diffusivity
η	Methane lifetime due to oxidation
η_{ox}	Methane lifetime due to oxidation with adequate oxygen
ρ	Density
ρ_{soil}	Soil density
ρ_w	Water density
θ	Percentage of soil water to other soil constituents

Abstract

A large amount of CH_4 is sequestered in the upper layers of permafrost soils. This CH_4 is likely to be released if the soil thaws due to increased surface air temperatures as predicted by most climate models. This thesis describes the process of quantifying the CH_4 release using available data from Alaskan soil cores, climate models, and a heat and gas transfer model. Based on this work, I conclude that permafrost will likely be a small though not negligible CH_4 source in the future.

Chapter 1

Introduction

Although it is well known that increasing concentrations of CO_2 and other trace gases should lead to a warming of the earth's atmosphere, the magnitude of the effect is still largely dependent on the feedbacks and buffers of the earth's climate system. Some of these processes are well understood, such as the ocean thermal inertia that delays and moderates global warming. Other processes, however, such as those involving clouds, are not well understood. Traditionally it has been these kinds of physical climate feedbacks that have been studied by climate researchers, but it is becoming clear that chemical and biospheric feedbacks may be of equal or even more importance.

One such feedback is related to the melting of permafrost. This question was first raised in the early 1980s when methane trapped in hydrate form in deep permafrost residing 250 or more meters under the surface was considered as a potential feedback factor on the global climate (Bell, 1982). Bell only considered the effect of the oxidized CH_4 in the form of CO_2 and thus greatly underestimated the potential of this source for perturbing the climate system (Khalil & Rasmussen, 1989), but his basic conclusion that at that depth it would take roughly 1000 years for an increased surface temperature to begin melting the ice lattice structure of the methane hydrate has gone unchanged (Kvenvolden, 1988). There has been speculation, starting with Bell, however, that permafrost in the shallow Arctic Ocean, although being small in areal extent, would release methane and cause a noticeable positive feedback to greenhouse warming due to the nearness of permafrost to the soil surface. This speculation too may be dismissed because of the massive oceanic thermal inertial which would insulate the soil surface from atmospheric temperature changes.

Data collected approximately two years ago by R.A. Rasmussen and M.A.K. Khalil at OGI suggested that permafrost may be a large reservoir of methane near

the surface. Because this permafrost reservoir is near the soil surface it was considered likely to be released quickly with an increase in the surface temperature. Because of this idea, permafrost was once again thought to be a potentially important climate feedback which could increase any global warming that would otherwise occur and might also be an important methane sources in the future.

Starting some nine months ago, I began to test these hypotheses. I began by analyzing the permafrost methane concentrations for the soil cores. These concentrations turned out to average 2.3 $\mu g CH_4$ g^{-1}soil with a range from 0.2 to 11.1 $\mu g CH_4$ g^{-1}soil, values that are high for soil concentrations. These results said nothing about the global store of methane, however, so a permafrost distribution was developed based upon literature data. With this I determined that for every meter depth of permafrost melted, approximately 60 Tg of CH_4 would be released. This amount is relatively small compared with the 500 Tg of methane that is released yearly from all sources. At this point it was clear that permafrost could not be a very large source of methane in the future but it could still be important. I had little quantitative idea what affect a warmer world would have on the permafrost soil structure and thus had little idea how quickly the methane would be released. As a result, I began work on the Permafrost Heat Transfer model (PHEAT) to allow me to answer this question. PHEAT was used with the results from two GCM double CO_2 experiments -- the UKMO and OSU models. A linear temperature increase over 100 years was assumed for the increase of temperature from current levels to the (model predicted) warmer levels. Using the Rasmussen and Khalil data, I calculated a maximum methane emission of 8 Tg yr^{-1} based on the first climate change scenario and 5 Tg yr^{-1} for the second.

This thesis considers each of the phases of the work outlined above in detail including all of the data from the permafrost cores. Chapter 2 discusses the soil CH_4 data in detail and also presents data for CO_2, H_2, CO, and N_2O. In chapter 3, the details of the permafrost distribution and the global extrapolations are given. The heat and gas portions of the model are detailed in chapters 4 and 5 with the model tests presented in chapter 6. Chapter 7 contains the results of the model runs, and conclusions are presented in chapter 8.

Chapter 2

Data and Data Analysis

Permafrost is generally defined as soil that remains below zero Celsius for more than two consecutive years. This definition of permafrost is modified however to better suit the type of study we were trying to execute. Our group wanted to know the concentration of methane in the upper levels of permafrost, and they were not able to study a particular site over an extended period of time. Thus, Dr. Rasmussen decided to drill soil core samples in August, the month when the active layer is at maximum depth. By sampling in this manner, we have implicitly assumed a definition of permafrost, namely, that it is soil that is frozen in August. In general, this definition will result in soils being classified the same way as they would be with the traditional definition. It is important to understand, however, that this similarity in classification will not always be the case. For the purpose of this study, however, our definition is equally good. We would prefer to have a number of years of climatic conditions indicative of the current climate and *then* do our sampling. This situation is of course impossible, and thus the data gathered has a potential error due to the fact that we may have cores of seasonally frozen soil. This possibility does not appear to be the case however, given the high methane concentrations found. Methane in soil which is unfrozen even a small fraction of the year would either diffuse to the atmosphere or be oxidized by aerobic processes; gas adsorption is generally only able to sequester three to five orders of magnitude lower concentrations than the concentrations we find (Philp and Crisp, 1982). In either case, the methane would not stay sequestered in the soil.

2.1: Experimental Procedure

Core samples were taken from Kuparik to Dead Horse along the northern coast of Alaska near Prudhoe Bay and then inland along the Haul Road approximately 150 km to Atigun.

Each core sample was analyzed by cutting a section of soil and adding it to a water filled syringe. The soil samples were roughly 25 grams in mass added to roughly 50 ml of water. The syringe was then warmed to room temperature to allow

Table 2.1: Permafrost Methane data.

Core Number	Soil Type	Mass (g)	He (ml)	CH_4 (ppmv)	CH_4 ($\mu g\ g^{-1}$)	Average CH_4
1	Silt	29.1	25	11,132	6.89	3.91
1	Silt	22.4	24	1,173	0.90	
1	Silt	22.8	25	4,470	3.53	
1	Silt	25.3	22	6,888	4.31	
3	Peat	20.5	15	3,971	2.09	2.69
3	Peat	25.3	20	5,765	3.28	
4	Peat	20.6	20	5,338	3.73	3.73
5	Ice	23.2	20	1,992	1.24	3.23
5	Peat	29.4	24	9,394	5.75	
5	Peat	21.0	25	6,064	5.20	
5	Peat	26.0	25	8,215	5.69	
5	Ice	17.0	22	2,444	2.28	
5	Ice	16.0	18	201	0.16	
5	Silt	34.1	20	5,420	2.29	
6	Silt	25.1	25	2,779	1.99	1.99
11	Peat	21.0	25	6,954	5.96	5.34
11	Peat	25.0	27	6,059	4.71	
12	Ice	28.1	28	10,522	7.55	4.48
12	Silt	32.4	30	5,717	3.81	
12	Peat	28.2	25	3,240	2.07	
14	Silt	23.4	23	4,109	2.91	4.50
14	Silt	27.1	25	5,295	3.52	
14	Silt	31.0	28	5,805	3.78	
14	Silt	23.9	20	12,968	7.81	
15	Peat	25.7	22	6,527	4.02	8.70
15	Silt/Peat	32.7	28	17,808	10.98	
15	Silt	32.6	28	17,937	11.09	
16	Silt	20.0	20	4,118	2.96	3.01
16	Silt	25.3	18	7,170	3.67	
16	Peat/Sand	21.1	16	4,216	2.30	
16	Peat/Sand	30.7	20	956	0.51	
17	Silt	25.2	24	1,108	0.76	0.53
17	Silt	32.2	25	813	0.45	
17	Silt	29.1	20	782	0.39	
17	Silt	27.2	20	956	0.51	
18	Silt	34.4	25	464	0.24	0.42
18	Silt	38.8	30	1,055	0.59	
20	Silt	37.3	25	2,503	1.21	1.13
20	Peat	18.2	15	880	0.52	
20	Peat	24.8	20	2,858	1.66	
21	Silt	25.8	25	1,248	0.87	1.26
21	Silt	31.7	25	3,010	1.71	
21	Silt	31.2	25	2,084	1.20	
22	Silt	37.3	25	2,503	1.21	1.02
22	Silt	30.1	20	1,727	0.83	

the soil to melt and mix with the water. At this point roughly 20 ml of *He* was drawn into the syringe and vigorously mixed with the soil-water mixture before being extracted and

measured for CH_4 and other gases. This procedure was generally repeated until the CH_4 measured was negligible, usually after three or four extractions. In the cases where the final measured value was not negligible compared to the blank, a decaying exponential was fit to the available data points and integrated. Dr. Rasmussen extracted and measured the methane concentrations in the samples using gas chromatography with flame ionization detector (GC/FID).

The data consist of the volumes of the He used as the head space for the accumulation of CH_4 and the CH_4 concentration from each extraction given in ppmv. This value is converted to micro-grams CH_4 per gram of soil by the following formula:

$$[CH_4](Vol\ He\ m^3)\left(\frac{45\ mole\ He}{m^3}\right)\left(\frac{16\ g}{mole}\right)\left(\frac{1}{soil\ mass}\right). \qquad (2.1)$$

The data and the derived soil methane concentrations are summarized in Table 2.2.

The final column in Table 2.1 is the average methane concentration for each core. This average is used because there are two ways to consider the data. The first is to assume that all of the core samples are independent and to average them. There is some support for this contention, specifically because there is considerable heterogeneity in the cores. This heterogeneity is particularly true of core number 5 which has peat, silt, and ice elements in it. In addition to this, two of the cores have only one sample taken from them, and the samples could therefore be unrepresentative of the core as a whole. On a more qualitative level, however, the ice and silt soil types are over-represented in the distribution of core samples, and the two single sample cores have little effect on the output because they average roughly the average of all the cores. The samples are used for the results in this thesis primarily because there are many more observations and so the distribution is more reliable. Regardless, the method used does not significantly affect the conclusions presented in this work as can be seen in Table 2.2.

Table 2.2: Soil Methane Concentrations ($\mu g\ g^{-1}$).

Method	Median	Upper Limit	Lower Limit
Sample	2.3	0.5	6.9
Core	3.0	0.5	5.3

As can be seen from Figure 2.1, the data do not conform to any well-studied distribution. Because of this fact, the median is used, and the 90% confidence limits are taken directly from the data as plotted in Figure 2.2.

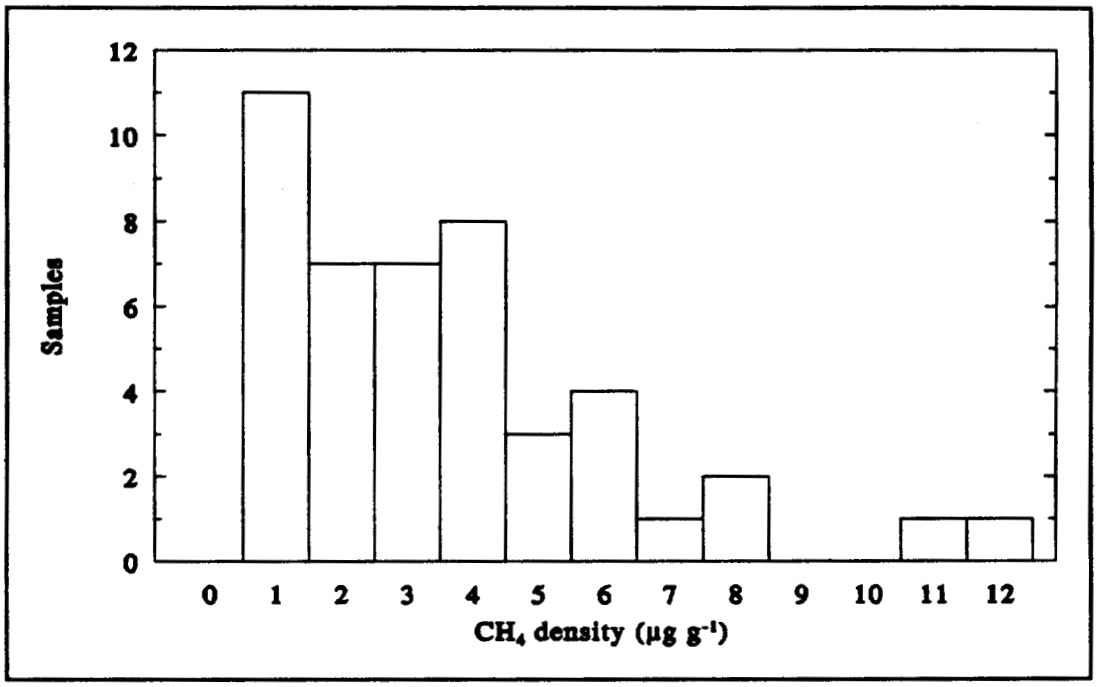

Figure 2.1: Distribution of soil methane concentrations.

2.2: Other Soil Gases

In addition to the methane, CO_2, H_2, CO, and N_2O were measured in the cores. Values for these gases are summarized in Table 2.3. They will be considered on a global scale with CH_4 in the next chapter.

Table 2.3: Concentrations of other trace gases measured in the permafrost cores.

Gas	Median	Lower Limit	Upper Limit
CO_2 (μg/g)	28.1	7.7	53.2
H_2 (ng/g)	21.1	3.6	35.5
CO (ng/g)	6.6	2.3	11.9
N_2O (ng/g)	2.4	1.4	2.8

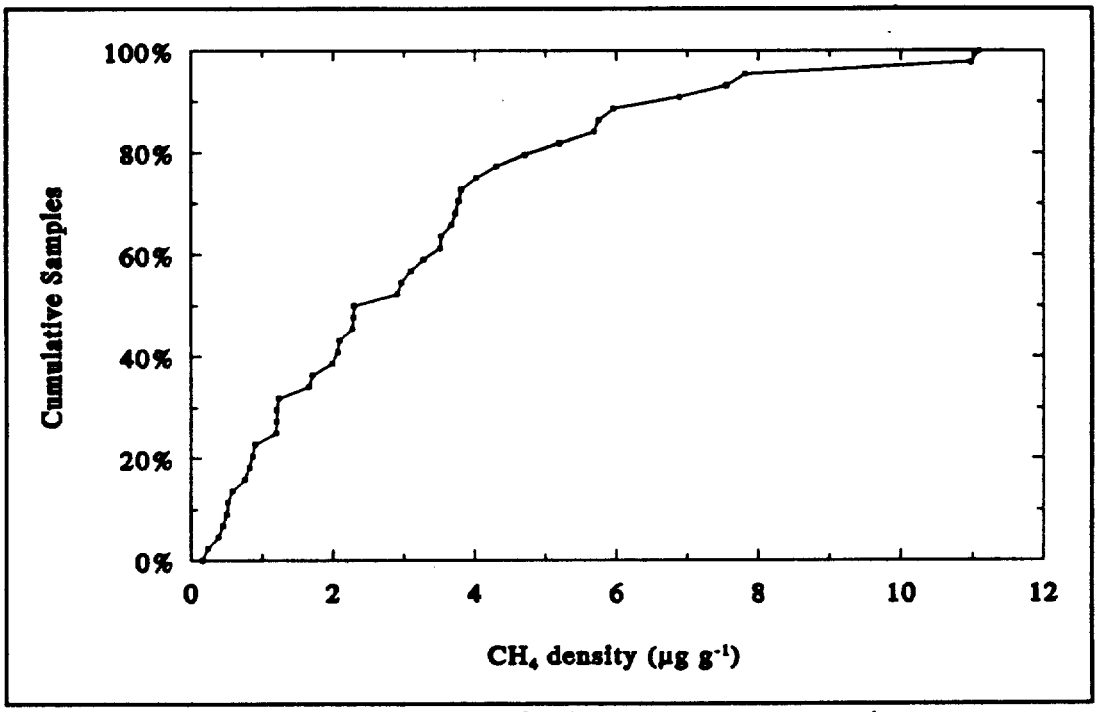

Figure 2.2: Cumulative distribution of soil methane concentrations.

Chapter 3

Permafrost Distribution

In the northern hemisphere almost all land areas above 60 degrees latitude are underlain by permafrost of one form or another. In addition a sizable portion of lower latitude locations, mostly alpine, have appreciable amounts of permafrost. The total land area containing some permafrost beneath, amounts to roughly three percent of the earth's surface area.

Cold regions are described as being underlain by either continuous, discontinuous, and sporadic permafrost. These categories are defined by the percentage of an area that has permafrost beneath it as shown in Table 3.1. The *assumed* column is the value used in determining the total permafrost amount. The discontinuous and sporadic values are simply the average of the range but for the continuous permafrost 100% was chosen because it more accurately reflects the nature of the high northern latitude permafrost which is highly resistant to climatic and topographical anomalies.

Table 3.1: Permafrost Types.

Type	Range	Assumed
Continuous	(80,100]%	100%
Discontinuous	(30,80)%	55%
Sporadic	(0,30)%	15%

Harris (1986) constructed detailed permafrost maps of North America and Asia and a less detailed map of the northern hemisphere based upon the current literature. These maps were subdivided into ten degree latitude by ten degree longitude grid boxes. For each box the percentage of the total area underlain by each of the three permafrost types were approximated. These values were multiplied by the area of each box and then divided by the total area of the earth to get the percentages in Table 3.2 which therefore represent the fraction of the earth's surface with the three permafrost types. Note two things however. First the values given

have already been multiplied by the values given in Table 3.1 in order to get actual amount of permafrost in a latitudinal band. And second, permafrost beneath glaciers were excluded.

Table 3.2: Permafrost Area in 10° latitudinal bands.

Northern Latitude	Permafrost Type			
	Continuous	Discontinuous	Sporadic	Total
5	0.00	0.00	0.00	0.00
15	0.00	0.00	0.00	0.00
25	0.00	0.00	0.00	0.00
35	0.17	0.00	0.04	0.21
45	0.07	0.05	0.06	0.18
55	0.24	0.42	0.11	0.77
65	1.39	0.35	0.05	1.79
75	0.37	0.00	0.00	0.37
85	0.05	0.00	0.00	0.05
Total	2.29	0.82	0.26	3.37

By using the data in Table 3.2 I find the total amount of gas present per meter depth of soil using the following equation

$$B_m = f_{pf}(5.1 \cdot 10^{14}\ m^2)\left(\frac{1{,}600{,}000\ g\ soil}{m^3}\right)\rho_{gas} \qquad (3.1)$$

where ρ_{gas} is the density of the gas of interest in the soil and f_{pf} is the fraction of the earth's surface area with the given permafrost type as taken from Table 3.2. Table 3.3 lists the amounts for each gas.

Table 3.3: Globally extrapolated trace gas budgets for all permafrost regions per meter thickness of soil.

Gas	Continuous	Discontinuous	Sporadic	Total
CH_4 (Tg m^{-1})	40	20	5	65
CO_2 (Tg m^{-1})	400	200	50	650
H_2 (Gg m^{-1})	300	100	30	430
CO (Gg m^{-1})	100	40	10	150
N_2O (Gg m^{-1})	40	20	5	65

In order to get a quantitative feel for the amount of each of the gases sequestered in the permafrost, Figure 3.1 displays the amount of each gas per meter depth of all permafrost regions as a percentage of the gas's current yearly source due

to all the processes that create the gas[1]. Clearly CH_4 is the only gas for which permafrost might have a significant impact.

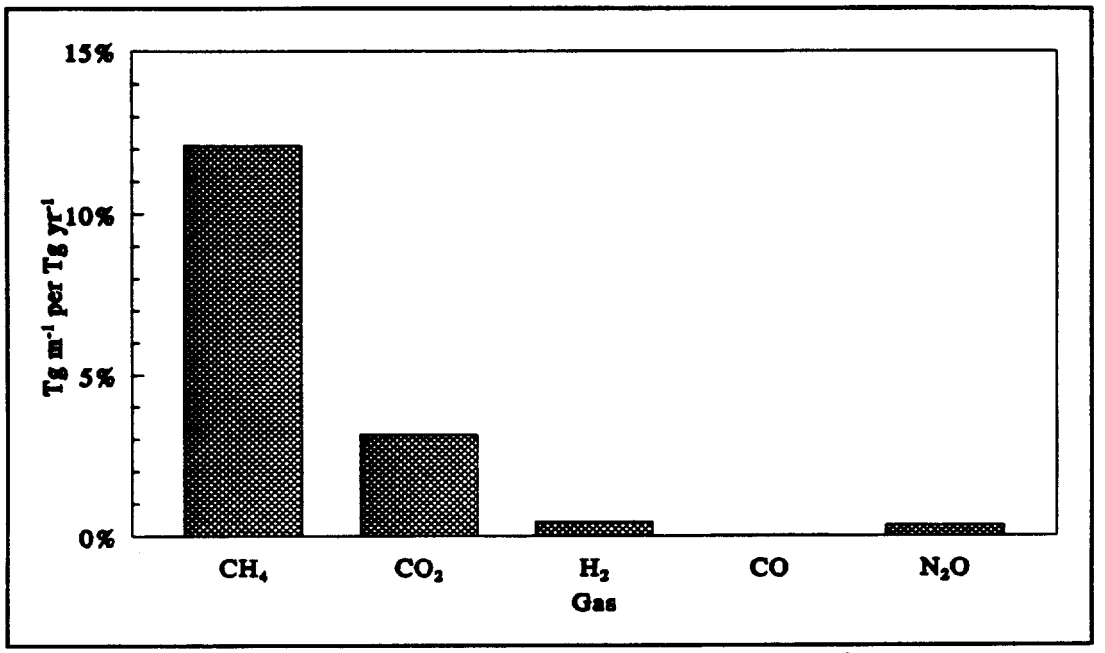

Figure 3.1: Budget of soil gases relative to their yearly global sources

[1] The sources are taken to be 520 Tg for CH_4 (Khalil and Rasmussen, 1990a), 20,000 Tg for CO_2 (Warneck, 1990), 180 Tg for H_2 (Khalil and Rasmussen, 1990b), 2,500 Tg for CO (Seiler and Conrad, 1987), and 20 Tg for N_2O (Khalil and Rasmussen, 1992a).

Chapter 4

Permafrost Soil Model: Heat

There are two distinct parts to the soil model, the first involving the movement of heat and the second the movement of gas. The aspects relating to the transfer of heat are discussed in this chapter and those relating to the movement of gas in the next chapter.

There are three mechanisms by which heat may move through a system: radiation, convection, and conduction. In general, energy movement due to radiation is negligible because of the opaqueness of soil, the small pore volumes, and the short distances between radiating objects. Convection is mainly manifested in soil systems by water movement and in frozen soils mainly by capillarity. Taylor & Luthin (1978) showed that for frozen soils the mass heat transfer due to the flow of water was at most 1% of that due to conduction (and generally much less). Thus heat transfer by water flow can be ignored. Heat transfer due to capillarity is more important. In fact, for soils very near the freezing temperature (within a few tenths of a °C), it can dominate conduction. However, this temperature range is very small for almost all soil types. In addition, heat conduction due to capillarity is always less than 10% below -0.25 °C and it is completely absent for soils above 0 °C. For this reason I neglect capillarity without compromising the validity of the model results. This procedure is helpful since the hydraulic conductivity is not a simple function of temperature like the thermal conductivity and heat capacity discussed later in this chapter (eg. Burt & Williams, 1976). Conduction is the process by which heat is exchanged between objects due to the differences in their temperatures. It is the dominate heat transfer mechanism for soils.

4.1 Heat Conduction

The fundamental equation governing the movement of heat in a medium due

to conduction in one-dimension is given by

$$C_{soil}\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[K_{soil}\frac{\partial T}{\partial z}\right]. \tag{4.1}$$

were C is the volumetric heat capacity and K is the thermal conductivity (Carslaw and Jaeger, 1959). For soils, C and K are generally functions of time, space, and temperature. This complication not only makes for a difficult equation to solve, but it also requires a detailed knowledge of the soil structure. Clearly it is not possible to provide this information when one wishes to do a global extrapolation given the spacial heterogeneity of soil structure. Fortunately it is not terribly important to take this heterogeneity into account because it is primarily the water content of the soil that defines its thermal characteristics. The water contents of the soils of interest do not vary greatly. In this work, I therefore assume an homogeneous soil structure both in space and time. The temperature dependence of heat movement cannot be ignored, however. As will be discussed later in this chapter, the speed with which heat flows is highly dependent upon the temperature of the soil, due primarily to the acquisition of latent heat over a range of negative temperatures.

4.2 Soil Composition

Due to the lack of soil parameter data specific to our soil samples, I assume that the soil is composed of approximately 20 percent air, 20 to 40 percent water, depending upon the soil type, and the remaining volume mineral and organic material with the latter being 10 percent of the total of the two (Brady, 1974). These data are summarized in Table 4.1.

Table 4.1: Soil Composition

Soil Constituent	Volumetric Fraction
water	x_w
mineral	$0.9(0.8-x_w)$
organic material	$0.1(0.8-x_w)$
air	0.2

4.3 Liquid Water Content

Thermally, water defines a soil system, especially for soils near the freezing

point of water. The thermal diffusivity of liquid water is approximately 10 times smaller than that of the other soil constituents (except for organic matter which is a small part of most soils). In addition to these factors the release of latent heat completely dominates the heat budget near zero Celsius.

Water does not freeze at a single temperature in soil. This freezing phenomenon is primarily due to two processes known as capillarity and adsorption. For both these processes, the water in contact with other particles (eg. a pore wall), is less able to form the crystalline structure necessary for ice. Capillarity is the dominant process whereby water in a pore (or capillary) forms a meniscus of greater and greater height with smaller and smaller pore radius. As some ice in a pore forms it causes the pore radius to diminish due to the smaller density of ice compared to water. This smaller pore radius then causes a higher percentage of water molecules to be affected by the pore walls (or other particles) and so the freezing temperature of the remaining liquid water is lowered (Williams and Smith, 1989).

In the field of frozen soil science convention is generally to present data for the liquid water content of soils as water percentage of dry soil weight. These units are not useful for modeling soil so I convert it into percentage of total volume:

$$\theta = \frac{w}{s}100 \tag{4.2}$$

where w is the mass of water in the soil, s is the mass of everything else, and θ is the water percent of dry soil weight. The volumetric water content is then

$$x_w = \frac{w}{s(1 + \theta)}\frac{\rho_{soil}}{\rho_w}100 = \frac{\theta}{1 + \theta}\frac{\rho_{soil}}{\rho_w}100. \tag{4.3}$$

where x_w is the volumetric water content as a percentage of the total soil volume, ρ_w is density of water, and ρ_{soil} is the density of the entire soil[2].

From Figure 4.1, derived from Williams and Smith (1989), it is clear that soil liquid water content can be approximated as an exponential function of temperature. Given this assumption I assume:

---

[2] Taking the density difference of water and ice into account greatly complicates matters and so the densities of the two are assumed to be the same ($\rho_{ice} = \rho_{water} = 1\ g\ cm^{-1}$).

$$x_l = \begin{cases} Ae^{BT} + C & T \le 0 \\ A + C & T \ge 0 \end{cases} \tag{4.4}$$

where x_l is the volumetric liquid water content and T is measured in °C.

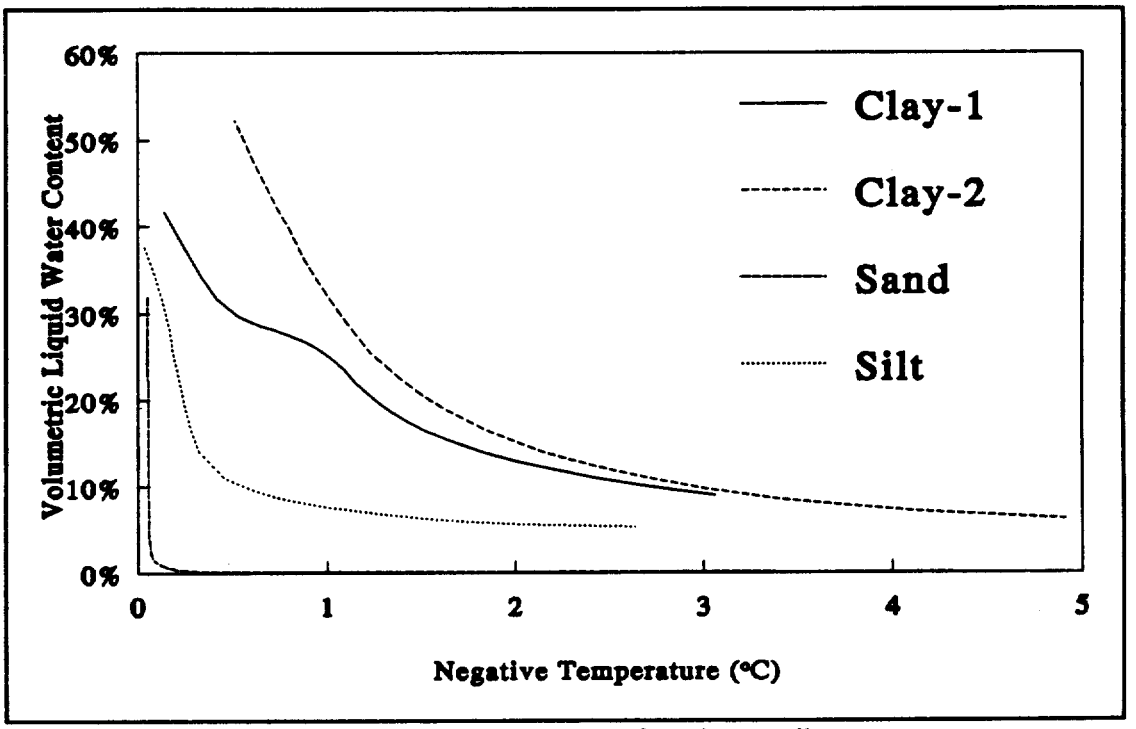

Figure 4.1: Volumetric liquid water content of various soils

For each curve in Figure 4.1 a simple grid search to an accuracy of 0.01 for A and B and 0.1 for C was performed (Bevington, 1969). The results are summarized in Table 4.2. A quick perusal of the data will show that an exponential function does *not* fit the data for sandy soils. In fact, an unconstrained parameter search for sandy soils requires a water content of more than 100%! The fits for the other data

Table 4.2: Liquid Water Content Parameters

Soil Type	A	B	C
Clay One	39.67	0.74	4.6
Clay Two	83.44	1.18	6.8
Sand	100.00	33.51	0.0
Silt	39.16	4.04	6.0

are quite acceptable however, and because our data are from mostly silty soils this formalism is used throughout.

4.4 Soil Thermal Parameters

There are two fundamental non-constant parameters that govern the flow of heat in soil: the thermal conductivity and the volumetric heat capacity. Both of these are discussed separately.

4.4.1 Thermal Conductivity

The thermal conductivity is a measure of the amount of heat that will flow through a substance per unit time per unit temperature gradient. This parameter thus has units of $Js^{-1}m^{-2}(Km^{-1})^{-1}$ or $Wm^{-1}K^{-1}$. The thermal conductivity of a soil may be expressed by the sum of the thermal conductivities of its parts. Thus:

$$K_{soil} = x_l K_l + x_s K_s + x_o K_o + x_m K_m + x_a K_a \qquad (4.5)$$

where K represents the thermal conductivity of a constituent, x represents the volumetric fraction of a constituent, and l, s, o, m and a represent the constituents liquid water, solid water, organic matter, mineral, and air respectively. Table 4.3, taken from Monteith (1973), lists average values for the thermal conductivities of these constituents.

Table 4.3: Thermal Properties of Soil Constituents.

Constituent	Thermal Conductivity ($Wm^{-1}K^{-1}$)	Heat Capacity ($MJm^{-3}K^{-1}$)
Liquid Water	0.56	4.18
Solid Water	2.24	1.93
Organic Matter	0.25	2.50
Minerals	2.92	2.38
Air	0.025	0.0012

Given the data from Table 4.3, the thermal conductivity of the soil is

$$K_{soil} = x_l(0.56) + x_s(2.24) + (0.8 - x_w)(2.65) + 0.005. \qquad (4.6)$$

Substituting equation (4.4) into (4.6) yields

$$K_{soil} = \begin{cases} (Ae^{BT}+C)(0.56)+(1-Ae^{BT}-C)(2.24)+ \\ \quad (0.8-A-C)(2.65)+0.005 & T\leq 0 \\ (A \quad +C)(0.56)+(1-A \quad -C)(2.24)+ \\ \quad (0.8-A-C)(2.65)+0.005 & T\geq 0 \end{cases} \tag{4.7}$$

4.4.2 Volumetric Heat Capacity

The amount of heat required to change the temperature of a unit volume of soil by one unit is the volumetric heat capacity. It is therefore a measure of a substance's resistance to changing temperature and has units of $Jm^{-3}K^{-1}$. Like the thermal conductivity, the volumetric heat capacity can be expressed by a sum of the heat capacities of it parts, but unlike the thermal conductivity, an extra term must be added for the latent heat of formation for ice. Thus:

$$C_{soil} = x_l C_l + x_s C_s + x_o C_o + x_m C_m + x_a C_a + \rho_w L_f \frac{dx_l}{dT} \tag{4.8}$$

where C represents the volumetric heat capacity of the constituent and the other symbols are the same as for the thermal conductivity. Following in analogy to the calculations for the thermal conductivity, the volumetric heat capacity of a soil element is given by:

$$C_{soil} = \begin{cases} (Ae^{BT}+C)(4.18)+(1-Ae^{BT}-C)(1.93)+(0.8-A-C)(2.39)+ \\ \quad 0.0002+(335{,}000{,}000)(ABe^{BT}) & T\leq 0 \\ (A \quad +C)(4.18)+(1-A \quad -C)(1.93)+(0.8-A-C)(2.39)+ \\ \quad 0.0002 & T\geq 0 \end{cases} \tag{4.9}$$

Chapter 5

Permafrost Soil Model: Gas

5.1 Introduction

There are two parts to the soil model relating to gas transport and release. The first is the movement of gases out of the soil by diffusion. The second is specific to methane, namely, its uptake by microbial oxidation.

The gas model consists of two steps: first the oxygen from the atmosphere is allowed to diffuse into the soil, and second the methane is allowed to diffuse out of the soil as given in the following equations.

$$\frac{\partial C_{O_2}}{\partial t} = D\frac{\partial^2 C_{O_2}}{\partial z^2} \tag{5.1}$$

$$\frac{\partial C_{CH_4}}{\partial t} = D\frac{\partial^2 C_{CH_4}}{\partial z^2} - \eta C_{CH_4} \tag{5.2}$$

In these equations, D is the gas diffusion coefficient in soil (discussed in the next section) and η is the inverse lifetime of methane due to oxidation. The oxygen concentration is needed to determine the amount of oxidation that will take place but it is not used in the calculations done in this thesis.

There are several mechanisms other than diffusion by which air is moved in soil: for example, the effects of temperature, pressure, wind action, and rainfall. All of these processes appear to contribute very little to the net movement of gases amounting to less than 1/200, 1/100, 1/1000, and 1/12 of the total movement, respectively (Baver et al., 1972). Diffusion is thus used as the sole mechanism for the transport of gases out of the soil.

5.2 Gas Diffusion

Two constant diffusion coefficients are used, one for frozen and one for unfrozen soil. Specifically:

$$D = \begin{cases} D_0 S \frac{l}{l_e} & T>0 \\ 0 & T\leq 0 \end{cases} \qquad (5.3)$$

where D_0 is the molecular diffusion constant for the gas into air, S is the fraction of the soil that is pore space, and l_e is the effective path length through a soil element of length l.[3] The values used for each of the diffusional constants are given in Table 5.1.

Table 5.1: Diffusion constant parameters

Parameter	Value
D_0	$1.5\ 10^{-5}$
S	0.34
l/l_e	0.4

Two gases are diffusing in the model at all times: the methane diffusing out of the soil and oxygen diffusing into the soil. The soil oxygen concentrations are used in the oxidation model discussed next.

5.3 Oxidation

In general, dry soils are a sink of methane and wet soils are a source. Soils are believed to account for up to 10% of the total methane source every year (Warneck, 1988)[4]. In any soil, microbial activity will both produce and destroy methane. It has been shown that soil microbes can respond to increases in methane

[3] The term l/l_e is also known as the tortuosity.

[4] Other estimates are much lower, however.

without lag (Whalen & Reeburgh, 1990), and so it is likely that at least some of the sequestered methane will be consumed before being diffused to the atmosphere.

Oxygen is assumed to be the limiting element in the oxidation process and so the lifetime of methane due to oxidation in the soil is

$$\eta = \eta_{ox}[O_2]_n \tag{5.4}$$

where η_{ox} is the lifetime of methane when there is adequate oxygen and $[O_2]_n$ is the normalized oxygen concentration (relative to atmospheric concentration).

Chapter 6

Model Testing

The model was solved numerically because there are no general analytic solutions to the diffusion equation with non-constant coefficients. Two analytic solutions are readily available for testing purposes, however. The first is with fixed end temperatures and constant coefficients which test the general model structure and its reproduction of linear diffusional processes. The second is the Neumann problem which tests how the model handles latent heat.

6.1 Fixed End Temperatures

With constant coefficients, equation (4.1) takes on the much simpler form of

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial z^2} \tag{6.1}$$

where κ is the thermal diffusivity or K/C. I then use the following boundary and initial values:

$$\begin{aligned} T(0,t) &= T_0 \\ T(L,t) &= T_L \\ T(x,0) &= 0 \end{aligned} \tag{6.2}$$

where L is the total length of the soil column. The steady state solution follows quickly from separation of variables

$$T_{ss} = T_0 + (T_L - T_0)\frac{x}{L}, \tag{6.3}$$

and the time dependent solution follows from the product rule (Powers, 1987)

$$T_t = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) \exp\left[-\frac{(n\pi x)^2}{L^2}\kappa t\right] \tag{6.4}$$

where

$$b_n = \frac{-2}{n\pi}\left[T_0 - T_L(-1)^n\right] \tag{6.5}$$

The model was run with a soil without water (therefore bypassing the model's latent heat and temperature dependant heat transfer parameter calculations). The results are shown in Figure 6.1. The maximum error for any grid point is 0.002 °C for a 3.2 year simulation. For the analytic solution only the first four terms of the (infinite) series were used, but since they are $O(10^{-1})$, $O(10^{-4})$, $O(10^{-10})$, $O(10^{-20})$ they are clearly sufficient.

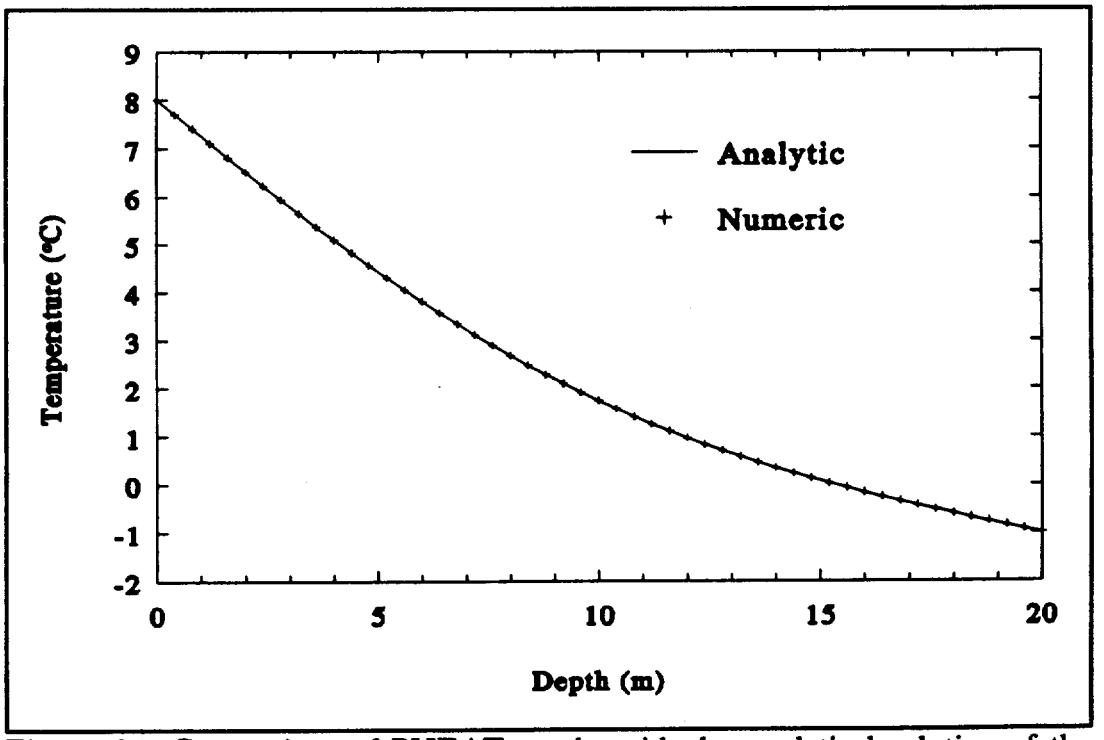

Figure 6.1: Comparison of PHEAT results with the analytical solution of the heat equation with constant coefficients.

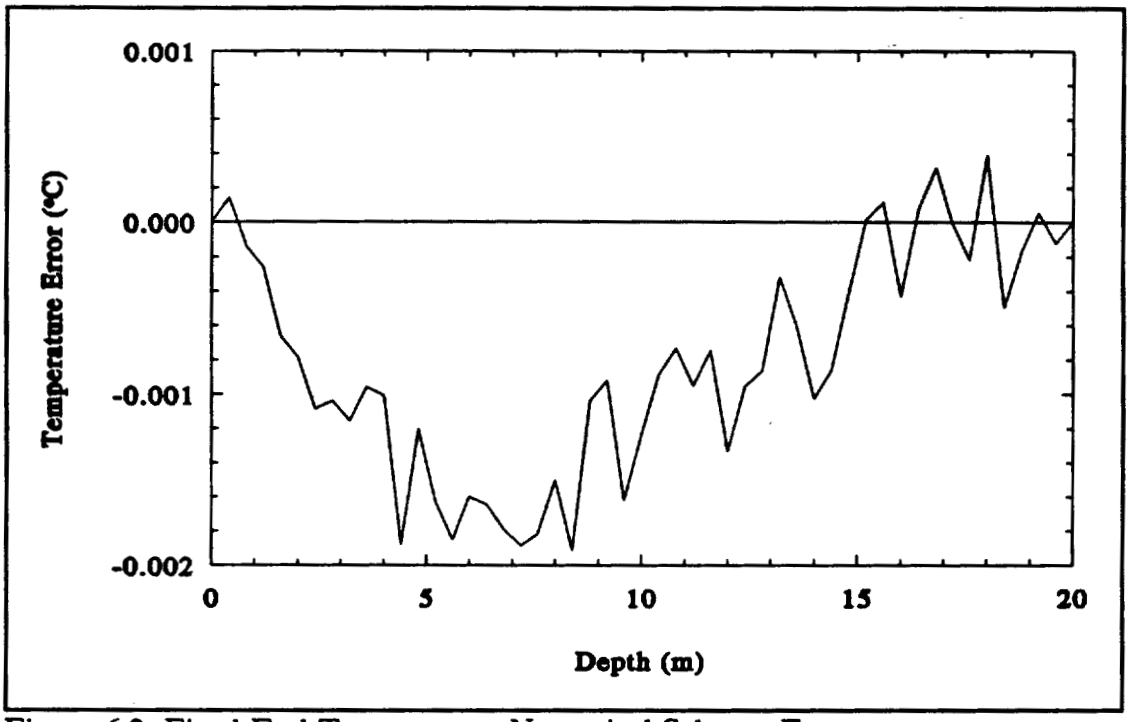

Figure 6.2: Fixed End Temperature Numerical Scheme Errors.

6.2 The Neumann Problem

The Neumann Problem is the classic problem of heat conduction with phase change. A semi-infinite region starts with a constant *liquid* temperature, T_0. The surface temperature is dropped to some temperature below the freezing temperature (T_f) which is taken to be T_s. Because I am working with water (in terms of phase change) and I am using the Celsius temperature scale, $T_f=0$. With these conditions, Lunardini (1981) shows that the temperatures are given by:

$$T_{solid} = T_s\left(1 - erf\frac{\frac{x}{2\sqrt{\kappa_{solid}t}}}{erf\gamma}\right) \tag{6.6}$$

and

$$T_{liquid} = T_0\left(1 - \frac{erfc\dfrac{x}{2\sqrt{\kappa_{liquid}t}}}{erfc\gamma\sqrt{\kappa_{solid}/\kappa_{liquid}}}\right) \tag{6.7}$$

where γ is a constant which depends upon T_s and T_0 and is tabulated for water in Carslaw and Jaeger (1959).

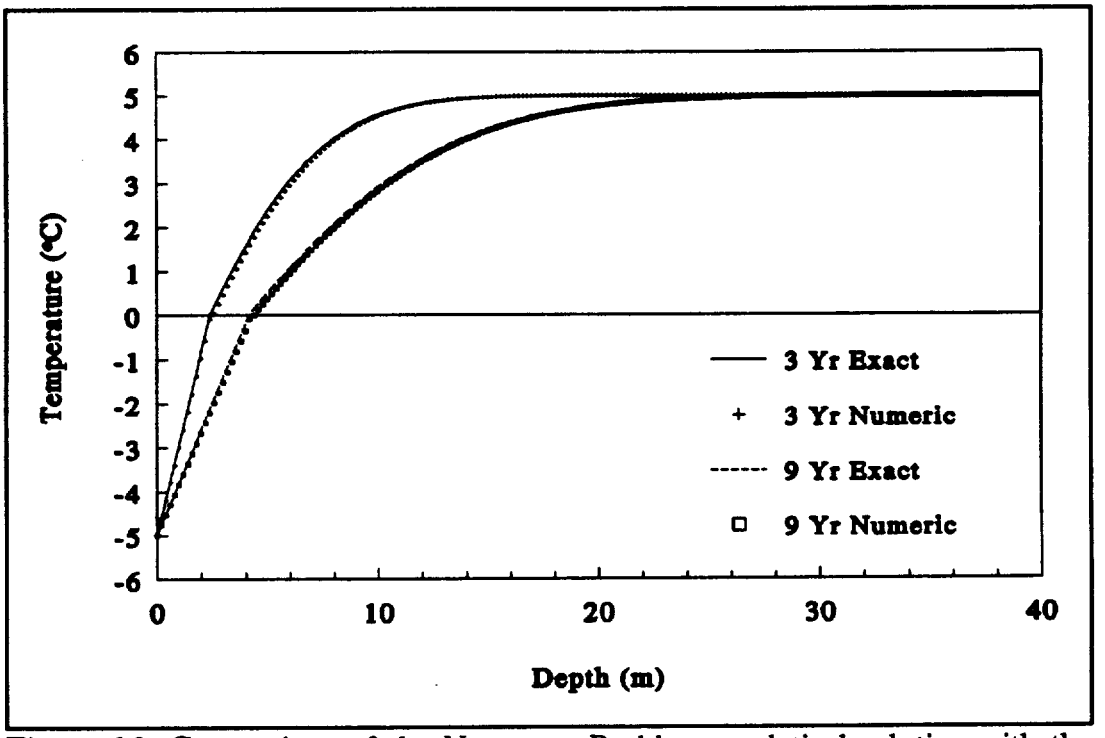

Figure 6.3: Comparison of the Neumann Problem analytical solution with the numerical model.

The results of 3 and 9 year simulations with a starting temperature of 5 °C and surface boundary condition of -5 °C and with the soil comprised completely of water are presented in Figure 6.2. In Figure 6.3 the absolute error is plotted for each of the runs. The errors are relatively small, especially considering the analytic and numerical solutions assume different liquid water content temperature dependance. The Neumann problem assumes that the phase change takes place at a single temperature (T_f), whereas the numerical scheme assumes an exponential temperature dependance as discussed in Chapter 4. In order to get as close a fit as possible, however, a value of B=8 was used for the exponential factor which approximates a

step function well. It is possible, of course, to alter the numerical scheme to match the Neumann problem more closely, but this alteration would not be testing the present model which is a more accurate model of soil than the Neumann model.

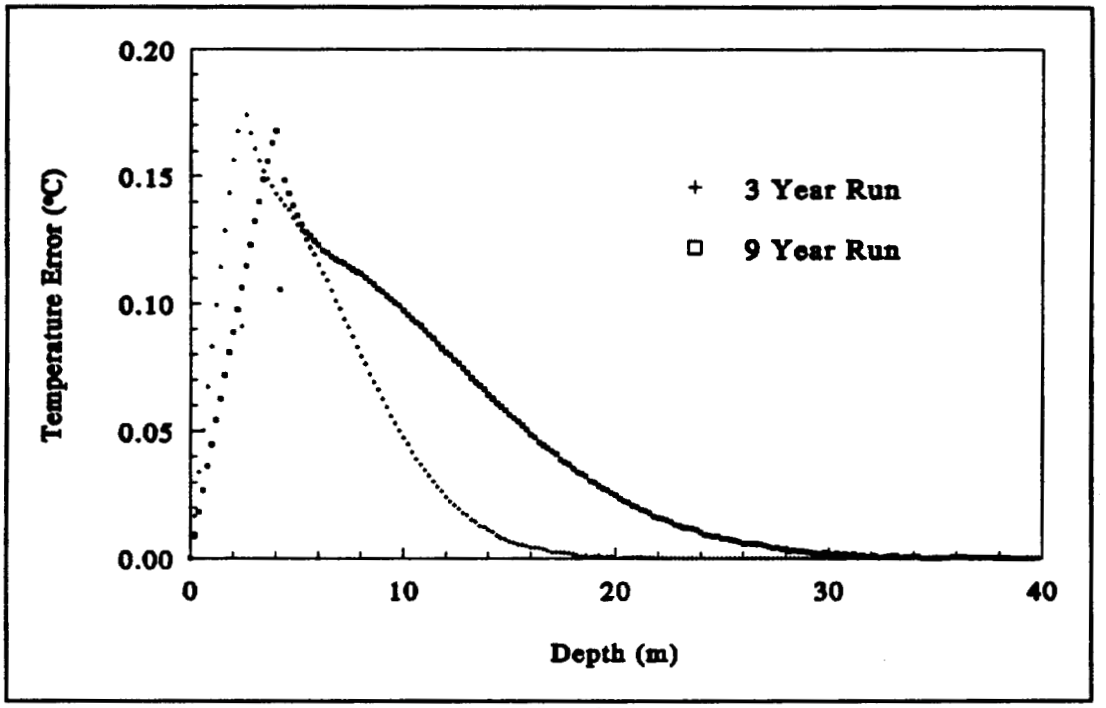

Figure 6.4: Neumann Problem Numerical Scheme Errors

Chapter 7

Model Results

7.1 Input Parameters

Current temperature data were taken from the "NCAR Global Temperature Climatology" database. This data set was given in monthly averages which were converted to daily averages using a parabolic interpolation scheme (Press et al. 1988).

Two climate change scenarios were used, both based upon double CO_2 experiment GCM results. The first was the UKMO model (Wilson and Mitchell, 1987) and the second was the OSU model (Schlesinger and Zhao, 1989). The temperature increases from these models were assumed to take place over a 100 year period. Unfortunately, both papers presented only steady-state results for summer and winter. In order to get temperature trends for each day the following approach was used. The daily temperature data were scaled to run from 0 to 1

$$T_i' = \frac{T_i - T_{min}}{T_{max} - T_{min}} \tag{7.1}$$

and then inverted with respect to 0.5

$$T_i'' = 1 - T_i'. \tag{7.2}$$

where T_{max} is the maximum temperature and T_{min} is the minimum temperature. These values were then multiplied by the winter to summer temperature change gradient (taken from the GCM results) and added to the summer temperature change.

$$T_i''' = T_i''(\Delta T_w - \Delta T_s) + \Delta T_s \quad (7.3)$$

where the *w* and *s* subscripts refer to winter and summer, respectively. Finally, this value was divided by 100 to get the yearly temperature trend

$$r_i = \frac{T_i'''}{100}. \quad (7.4)$$

The temperature increases for the two models are given in Table 7.1.

Table 7.1: Model Temperature Increases

Model	Summer	Winter
UKMO	7	10
OSU	3	7

The initial temperature distribution consisted of a 0 °C surface temperature and -8.8 °C temperature at 40 meters depth linearly interpolated (Molochuskin, 1973). The model was run initially for 100 years with no trend in order to stabilize the temperature. After this 100 years of surface warming is run, then finally another 100 years is run at the new elevated temperate.

7.2 Results

7.2.1 Yearly CH_4 Release

The two model results are shown in figures 7.1 and 7.2. The OSU model scenario yields an average CH_4 emission rate of roughly 2 $Tg\ yr^{-1}$ for the entire 200 years. The maximum emission rate is 5 $Tg\ yr^{-1}$. The UKMO results are somewhat higher, 4 $Tg\ yr^{-1}$ for the 200 year interval and a maximum emission rate of 8 $Tg\ yr^{-1}$.

The upper and lower limits in Figures 7.1 and 7.2 indicate the variability of the data. Maximum emission rates range from roughly 1 to 23 Tg yr^{-1}. Whereas this range might be considered large it is actually rather constrained relative to other sources of CH_4. For example the current range of CH_4 emissions from termites (a source of similar size to this permafrost source) is only slightly smaller than this range, and termites have been very well studied. With more measurements this budget could be much more tightly constrained.

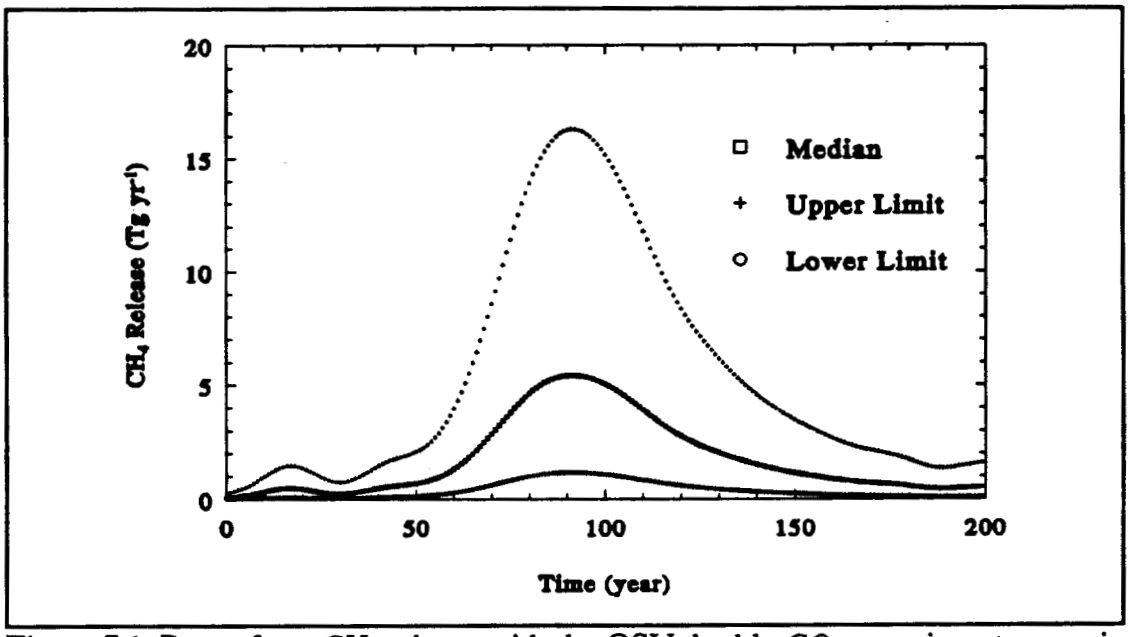

Figure 7.1: Permafrost CH_4 release with the OSU double CO_2 experiment scenario

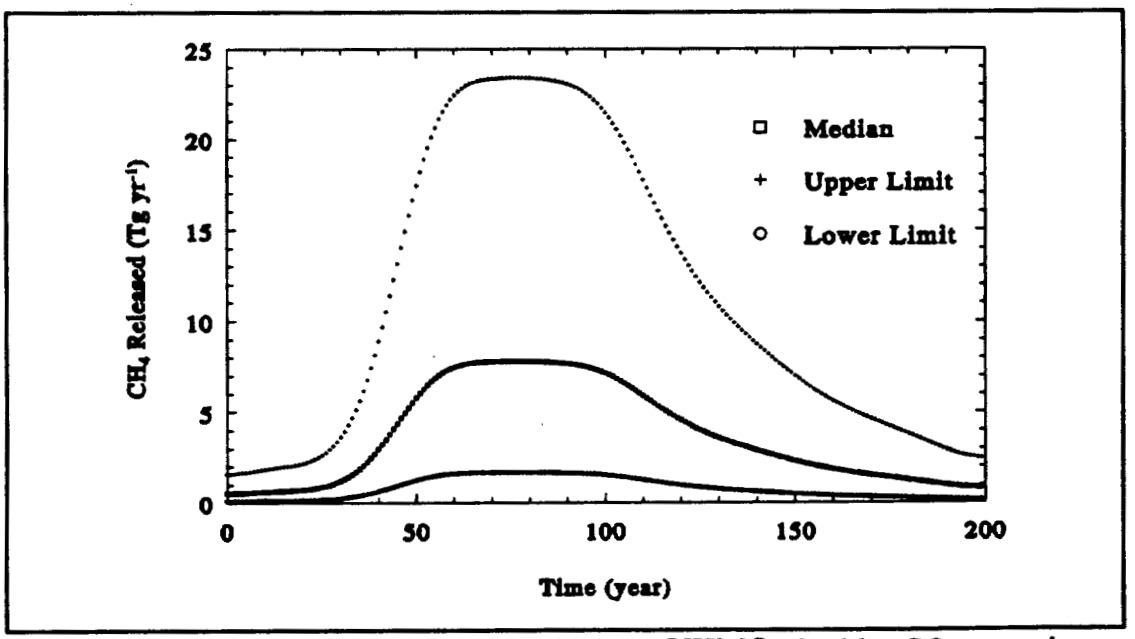

Figure 7.2: Permafrost CH_4 release with the UKMO double CO_2 experiment scenario

7.2.2 *Seasonal CH_4 Release*

The release of CH_4 from the soil is a seasonal phenomenon. Figure 7.3 represents the monthly release of CH_4 for the 100th year of the simulation for both climate scenarios.

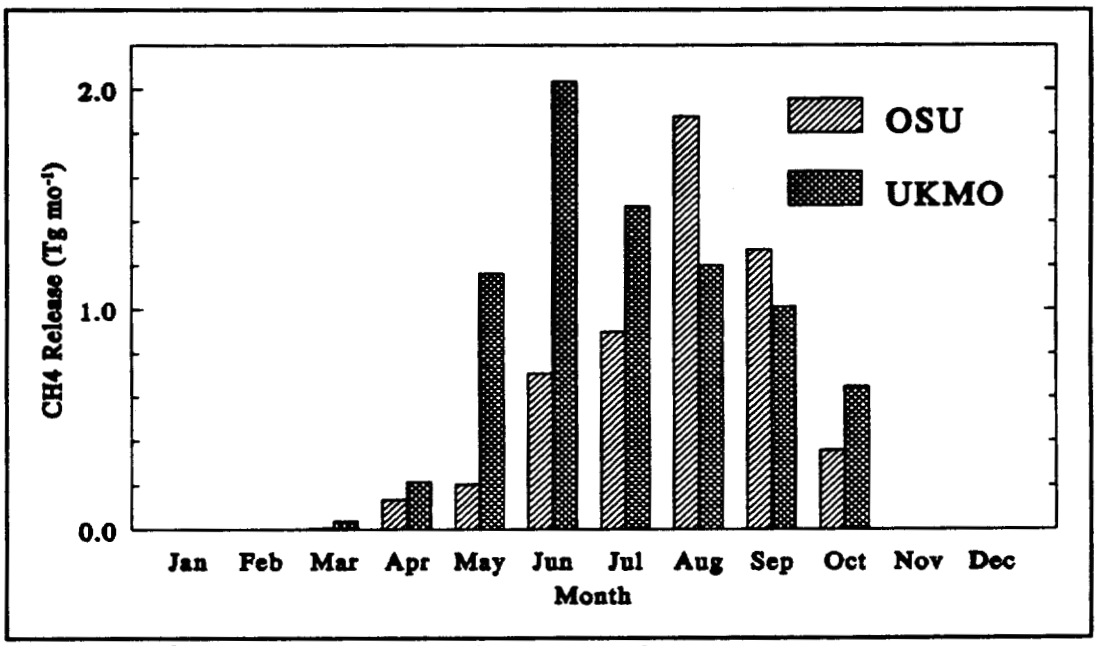

Figure 7.3: Seasonal CH_4 release from permafrost

Chapter 8

Conclusions

The total source of atmospheric methane is approximately 500 Tg/yr (Warneck, 1988). But CH_4, being primarily a biologically produced gas, has many sources as shown in figure 8.1. A few sources, such as ruminants and wetlands make up the majority of the budget each putting 20 to 200 Tg of CH_4 into the atmosphere every year. Approximately 20% of the budget is made up of medium sized sources between 5 to 20 Tg/yr. Although these sources are relatively small, they account for such a large percentage of the budget that they cannot be reasonably ignored (Khalil et al., in press).

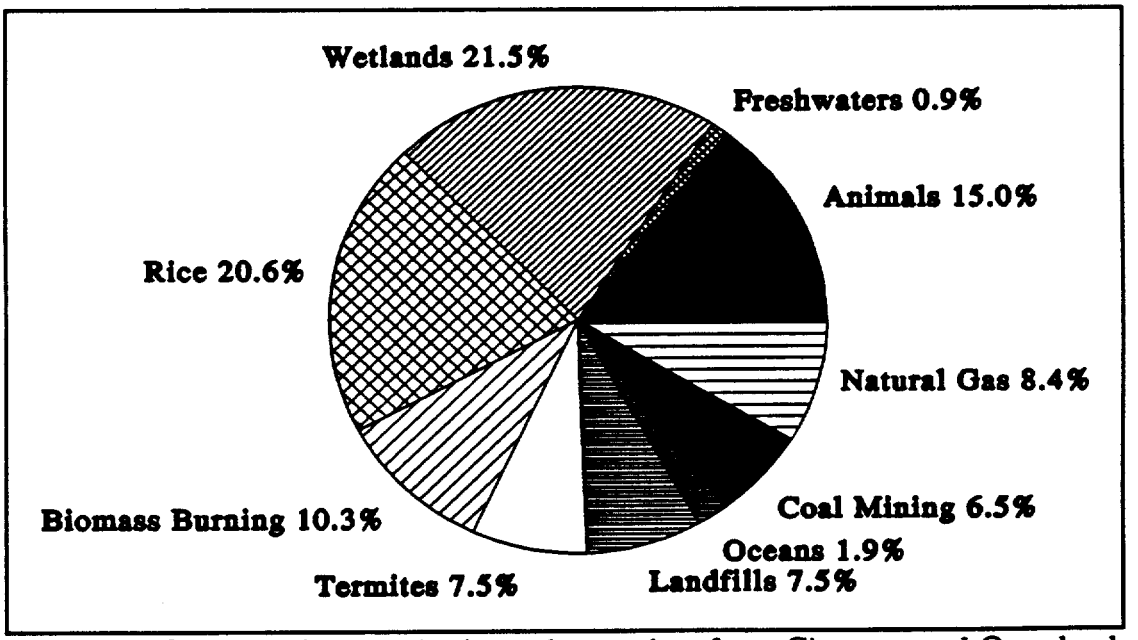

Figure 8.1: Sources of atmospheric methane taken from Cicerone and Oremland, 1988

This work studied the possible effects of the permafrost store of CH_4 on atmospheric concentrations. In the beginning it was thought that these effects might

be very large but with the completion of this work I can say that even with large atmospheric temperature changes the amount of CH_4 released from permafrost regions would be small though not necessarily negligible. The total CH_4 released would be between 1 and 23 Tg yr^{-1} at its maximum.

The effect of this source on the methane cycle is not limited to the bulk CH_4 introduced into the atmosphere. CH_4 release from permafrost is a seasonal process, taking place in the summer months when the concentration is at its lowest. This variable release will tend to increase the importance of the permafrost source relative to its importance if it were emitted throughout the year because it affects the seasonal cycle of methane.

Other issues relating to the role of permafrost areas on global climate have not been addressed here. In particular, a warmer climate would probably completely change the ecosystems of these regions. A great increase in bacterial methane production is likely to occur especially in water saturated areas which will likely become wetland ecosystems. Finally land cover, such as snow, have not been considered here. The net result of these factors will tend to decrease the amount of sequestered methane released into the atmosphere and so the results presented here should be considered as upper limits.

Appendix 1

PHEAT Source Code

```
/*
 * PROGRAM: PHEAT (Permafrost HEAt Transfer model)
 *
 * Copyright 1992    F. Moraes and M.A.K. Khalil
 *                   Global Change Research Center
 *                   Dept. of Environmental Science and Engineering
 *                   Oregon Graduate Institute
 *                   Beaverton, OR 97006
 *
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 * documentation. No representation is made about the suitability of this
 * software for any purpose.  It is provided "as is" without express or
 * implied warranty.
 *
 * Author: Francis Moraes
 *
 * Version 1.0 Created: 2 April 1992
 *
 * SYNOPSIS: This program simulates the release of methane from permafrost
 * soils due to climate change. The program inputs soil parameters (water
 * content, heat capacity, and others), starting temperature and methane
 * concentration distribution in the soil, and the boundary conditions for
 * the top and bottom layers of the soil as well as the yearly trend for
```

```
* the top soil layer.
*
* IMPLEMENTATION: For each time step the diffusion equation is solved for
* the soil temperature. For this the latent heat capacity and the thermal
* conductivity are assumed exponential functions of temperature. Within
* every time step the gas diffusion is calculated. Due to the generally
* much larger value of the diffusion coefficient for gas transport than for
* heat it is necessary to use smaller time steps for numerical stability.
* Two diffusion equations are solved. The first is for oxygen diffusing
* down into the soil from the atmosphere and the second is for the methane
* diffusing out the soil. The oxygen content in any soil element is taken
* to be limited by oxygen content of that element in a linear way. The only
* tricky part of this process is dealing with the interface between the
* frozen and unfrozen soil sections. This is done by assuming the pore space
* of frozen soil is an exponential function of negative temperature.
*
* The program begins by iterating a (user defined) number of years with
* no temperature change. It then iterates the same number of years with
* the top soil level trend applied and finally iterates that number of
* years again at the final climate change ending temperature.
*
* VARIABLES:
*
* t: temperature array
* o2: oxygen concentration (normalized) array
* ch4: methane concentration array
* trend: trend array, one trend for every "month"
* yr: the current year counter
* iterate: the number of "years" to iterate through (actually there are
*          three times this many iterations, see implementation above)
* mo: the sub-year counter (not necessarily a month)
* rep: the number of "months" to iterate through
* soildata: soil data, where
*      K are the thermal diffusivities
*      C are the volumetric heat capacities
```

```
*       water is the water content of the soil
*       B is the exponential factor the thermal calculations
* latent: the latent heat capacity of water
* tbctop: Temperature Boundary Conditions at the soil TOP
* tbcbot: Temperature Boundary Conditions at the soil BOTtom
* tempchange: the difference between the starting top temperature and
*             the current top temperature
* deltat: the time step
* deltaz: the spacial step
* deltaz2: the spacial step squared
* gasinc: parameter controlling volume change of water as a function of
*         temperature
*
* max: array of maximum temperatures reached by each soil element
* etat: diffusion constant for gases in soil
* etao2: oxidation constant for methane with adequate oxygen
* subrep: the number of gas diffusion time steps per heat diffusion step
* section: the counter for the part of the model we are on, 0 for no
*          temperature change and no trend, 1 for just trend, and 2 for
*          just temperature change
* depth: the number of soil elements
*
* RETURNS:
*
* 0: successful completion
* 1: error
*/

#include <malloc.h>
#include <stdio.h>
#include <math.h>

#define RHO 1000.0

float deltat, deltaz, latent, deltaz2;
```

```
float tempchange;
float *tbctop, *tbcbot;

float gasinc;

struct soildata
{
  float Kl, Ks, Ko;
  float Cl, Cs, Co;
  float A, B, C;
};

struct frozen
{
  int box, bmax;
  float max, cur;
};

int get_new_temp(int, float *, int, struct soildata);

void get_new_o2(float *, float *, float, int);

float get_new_ch4(float *, float *, float *, float, float, int);
char *allocate_array(int);
void msgexit(char *);
float findzero(float *, int, float);
float avg2(float,float);
void tridiag(float *, float *, float *, float *, float *, int);

void solvemat();

main(int argc, char *argv[])
{
  float *max;
  float *t, *o2, *ch4, *ch4i, *trend;
```

```
float ch4air;
float etat, etao2;
float stability;

int yr, mo;
int i;
int output, iterate;
int rep, subrep;
int section;
int depth;
int dir = 0;

struct soildata soil;
struct frozen fr = { 0, 0, 0.0, 0.0 };

FILE *fpin, *fpout, *fptime;

extern float deltat, deltaz, latent;
extern float *tbctop, *tbcbot;
extern float deltaz2;

/* make sure that the program was called correctly */

if (argc != 4)
   msgexit("Usage: heat input output timeseries");

/* input all of the parameters, first the single values */

if ( (fpin=fopen(argv[1],"r")) == NULL )
{
   perror(argv[1]);
   exit(1);
}

fscanf(fpin,"%d", &output);
```

```
fscanf(fpin,"%d", &iterate);
fscanf(fpin,"%d", &(depth));

fscanf(fpin,"%f %f", &deltat, &deltaz);
fscanf(fpin,"%f", &latent);
fscanf(fpin,"%f %f %f", &(soil.Kl), &(soil.Ks), &(soil.Ko));
fscanf(fpin,"%f %f %f", &(soil.Cl), &(soil.Cs), &(soil.Co));
fscanf(fpin,"%f %f %f", &(soil.A), &(soil.B), &soil.C);
fscanf(fpin,"%f %f", &etat, &etao2);
fscanf(fpin,"%d", &rep);
fscanf(fpin,"%d", &subrep);

stability = soil.Kl*soil.C + soil.Ks*soil.A + soil.Ko*(1.0-soil.A-soil.C);
stability *= (deltat/(deltaz*deltaz));
stability /=  (soil.Cl*soil.C+soil.Cs*soil.A+soil.Co*(1.0-soil.A-soil.C));

fprintf(stderr,"Stability: %f\n", stability);

/* allocate arrays for initial value input */

t = (float *) allocate_array(depth*sizeof(float));
o2 = (float *) allocate_array(depth*sizeof(float));
ch4 = (float *) allocate_array(depth*sizeof(float));
ch4i = (float *) allocate_array(depth*sizeof(float));
max = (float *) allocate_array(depth*sizeof(float));

for (i=0;i<(depth);i++)
{
  fscanf(fpin,"%f %f %f", t+i, o2+i, ch4+i);
  ch4i[i] = ch4[i];
}

/* allocate arrays for time series input */

tbctop = (float *) allocate_array(rep*sizeof(float));
```

```
tbcbot = (float *) allocate_array(rep*sizeof(float));
trend = (float *) allocate_array(rep*sizeof(float));

for (i=0;i<rep;i++)
  if ( fscanf(fpin,"%f %f %f", tbcbot+i, tbctop+i, trend+i) == EOF)
     msgexit("Error in input file");

fclose(fpin);

/* initialize variables */

for (i=0;i<depth;i++)
  max[i] = -1000.0;

deltaz2 = pow(deltaz,2.0);

etat = etat * (deltat/subrep) / deltaz2;
etao2 = etao2 * (deltat/subrep) / deltaz2;

/* Output the time series information as we go along */

if ( (fptime=fopen(argv[3],"w")) == NULL )
{
  perror(argv[1]);
  exit(1);
}

fprintf(fptime,"# transport time: %f\n", etat);
fprintf(fptime,"# oxidation time: %f\n", etao2);
fprintf(fptime,"# water content: %f\n", soil.A+soil.C);

/* enter main loop: section, yr, mo, gas diffusion */

fr.max = 0;
for (section=0;section<3;section++)
```

```
{
  for (yr=0;yr<iterate;yr++)
  {
    /* ch4air is the amount of ch4 released to the atmosphere this yr. */

    ch4air = 0;

    for (mo=0;mo<rep;mo++)
    {
      /* determine the proper atmospheric temperature depending upon
       * the section of the model currently being run. In section 0
       * there is no temperature change, in section 1 there is a
       * temperature change depending upon the year, and in section
       * 2 the temperature is completed and so the temperature is
       * constant (from year to year) although at a higher level.
       */

      switch (section)
      {
        case 0:
          tempchange = 0;
          break;
        case 1:
          tempchange = trend[mo] * yr * (section);
          break;
        case 2:
          tempchange = trend[mo] * iterate;
          break;
        default:
           msgexit("Critical Error");
           break;
      }

      fr.box = get_new_temp(mo,t,depth,soil);
```

```
/* The initial iterations (section = 0) are only to meant
 * to bring the temperature distribution to pseudo
 * equilibrium.  For this reason the gas diffusion code
 * is only used for the temperature change sections with
 * the exception of the last initial iteration which is
 * used for the initial values.
 */

if (section > 0 || yr > iterate-3)
{
  /* determine the new thaw level */

  fr.cur = findzero(t,fr.box,tbctop[mo]+tempchange);

  /* fr.max holds the maximum thaw level thus far (the active
   * layer level).  If the new thaw level is great than this
   * then new ch4 is input into the active layer.  This new
   * ch4 is injected directly into the thawed level _above_
   * the partially frozen level for computational convenience.
   */

  if (fr.cur > fr.max)
  {
     if (ch4[fr.box] > ch4i[fr.box]*(fr.cur-fr.max))
    {
      ch4[fr.box-1] += ch4i[fr.box]*(fr.cur-fr.max);
      ch4[fr.box] -= ch4i[fr.box]*(fr.cur-fr.max);
    }
    else
    {
      ch4[fr.box-1] += ch4[fr.box];
      ch4[fr.box] = 0;
    }
  }
```

```
            get_new_o2(o2,t,etat,depth);
            ch4air += get_new_ch4(ch4,t,o2,etao2,etat,depth);

            /* This code keeps track of the maximum temperature reached
             * of every soil element. The maximum temperatures are
             * output at the end of the program to avoid outputting
             * seasonal (usually mid-winter) data which provides less
             * information to the user.
             */

            for (i=0;i<depth;i++)
              if (t[i] > max[i])
                max[i] = t[i];
          }                          /* end gas diffusion code */
        }                            /* end monthly iteration code */

        if (section > 0)
        {
          fprintf(fptime,"%5d %15.7f %15.7f\n",
                  yr+iterate*(section-1), deltaz*ch4air, fr.max);
          fflush(fptime);
        }
      }                              /* end yearly iteration code */
    }                                /* end section iteration code */

    fclose(fptime);

    /* output the final temperature and maximum methane depth distributions */

    if ( (fpout=fopen(argv[2],"w")) == NULL )
    {
      perror(argv[1]);
      exit(1);
    }
```

```
  fprintf(fpout,"# transport time: %f\n", etat);
  fprintf(fpout,"# oxidation time: %f\n", etao2);
  fprintf(fpout,"# water content: %f\n", soil.A+soil.C);
  fprintf(fpout,"#%7s %10s %10s %10s\n", "Depth","Temp","CH4", "O2");
  fprintf(fpout,"#==========================================\n");

  for (i=0;i<(depth);i++)
    fprintf(fpout,"%8.2f %10.3f %10.3f %10.3f\n",
                deltaz*(i+1), max[i], ch4[i],o2[i]);
  fclose(fpout);

  return 0;
}                                   /* end main() */


/*
 * FUNCTION: get_new_temp
 *
 * SYNOPSIS: Get_new_temp determines the new temperature distribution for
 * a one-dimensional soil column given the previous temperatures and top
 * and bottom boundary conditions.
 *
 * IMPLEMENTATION: Euler's method is used to solve the diffusion equation
 * for each soil element.  First, the diffusion "constant" eta is determined
 * which is defined as the dt*K/(C*dz^2) where dt is the time step, K is
 * the thermal conductivity, C is the volumetric heat capacity, and dz is
 * the spacial step. K and C are given as follows:
 *
 *      K = (1-x)*K-other + x*alpha*K-water + x*(1-alpha)*K-ice
 *      C = (1-x)*C-other + x*alpha*C-water + x*(1-alpha)*C-ice +
 *          latent*rho*x*alpha'
 *
 * Next, the diffusion equation is used to solved for each soil element
 * using the eta's found previously.
 *
```

```
 * VARIABLES:
 *
 * mo: the month of the year, used for determining the air temperature
 * t: the temperatures
 * depth: the number of soil elements
 * soil: a structure containing soil parameters
 *
 * RETURNS: the thaw depth in number of soil elements.
 */

int get_new_temp(int mo, float *t, int depth, struct soildata soil)
{
  float eBt, *t1;
  float *a, *b, *c;
  int i, *indx;
  float lat;
  float *Ca, *Ka;
  float Katop, Kabot;

  extern float deltat, deltaz, deltaz2, tempchange, latent;
  extern float *tbctop, *tbcbot;

  Ca = (float *) allocate_array(depth*sizeof(float));
  Ka = (float *) allocate_array(depth*sizeof(float));
  t1 = (float *) allocate_array(depth*sizeof(float));
  indx = (int *) allocate_array(depth*sizeof(int));

  a = (float *) allocate_array(depth*sizeof(float));
  b = (float *) allocate_array(depth*sizeof(float));
  c = (float *) allocate_array(depth*sizeof(float));

  for (i=0;i<(depth);i++)
  {
    if (t[i] < 0)
    {
```

```
        eBt = (soil.A*exp(soil.B*t[i]) + soil.C);
        lat = latent*RHO*soil.A*soil.B*exp(soil.B*t[i]);

        Ca[i] = (1-soil.A-soil.C)*soil.Co + eBt*soil.Cl +
            (soil.A+soil.C-eBt)*soil.Cs + lat;
        Ka[i] = (1-soil.A-soil.C)*soil.Ko + eBt*soil.Kl +
            (soil.A+soil.C-eBt)*soil.Ks;
    }
    else
    {
        eBt = (soil.A+soil.C);

        Ka[i] = (1-soil.A-soil.C)*soil.Ko + (soil.A+soil.C)*soil.Kl;
        Ca[i] = (1-soil.A-soil.C)*soil.Co + (soil.A+soil.C)*soil.Cl;
    }
}

if (tbctop[mo]+tempchange < 0)
{
    eBt = (soil.A*exp(soil.B*(tbctop[mo]+tempchange)) + soil.C);
    lat = latent*RHO*soil.A*soil.B*exp(soil.B*(tbctop[mo]+tempchange));

    Katop = (1-soil.A-soil.C)*soil.Ko + eBt*soil.Kl +
        (soil.A+soil.C-eBt)*soil.Ks;
}
else
{
        eBt = (soil.A+soil.C);

        Katop = (1-soil.A-soil.C)*soil.Ko + (soil.A+soil.C)*soil.Kl;
}
if (tbcbot[mo] < 0)
{
    eBt = (soil.A*exp(soil.B*tbcbot[mo]) + soil.C);
    lat = latent*RHO*soil.A*soil.B*exp(soil.B*tbcbot[mo]);
```

```
  Kabot = (1-soil.A-soil.C)*soil.Ko + eBt*soil.Kl +
      (soil.A+soil.C-eBt)*soil.Ks;
}
else
{
      eBt = (soil.A+soil.C);

      Kabot = (1-soil.A-soil.C)*soil.Ko + (soil.A+soil.C)*soil.Kl;
}

t1[0] = deltat/(deltaz2*Ca[0])*(avg2(Ka[1],Ka[0])*(t[1]-t[0]) -
      avg2(Katop,Ka[0])*(t[0]-tbctop[mo]-tempchange)) + t[0];

for (i=1;i<depth-1;i++)
  t1[i] = deltat/(deltaz2*Ca[i])*(avg2(Ka[i+1],Ka[i])*(t[i+1]-t[i]) -
                                  avg2(Ka[i],Ka[i-1])*(t[i]-t[i-1])) +
                                  t[i];

t1[i] = deltat/(deltaz2*Ca[i])*(avg2(Kabot,Ka[i])*(tbcbot[mo]-t[i]) -
                                avg2(Ka[i],Ka[i-1])*(t[i]-t[i-1])) + t[i];

for (i=0;i<depth;i++)
  t[i] = t1[i];

free(indx);
free(t1);
free(a);
free(b);
free(c);
free(Ka);
free(Ca);

for (i=0;t[i]>0.0 && i<depth;i++)
  ;
return i;
```

```
}


/*
 * FUNCTION: get_new_o2
 *
 * SYNOPSIS: Get_new_o2 determines the new oxygen concentration distribution
 * for a one-dimensional soil column given the previous concentrations and top
 * boundary condition which is assumed to be unity.
 *
 * IMPLEMENTATION: Euler's method is used to solve the diffusion equation with
 * constant coefficients. There are two transport times, one for unfrozen
 * soil (etat) and the other for frozen soil which is zero. Thus for any
 * soil element which is unfrozen gas diffuses into and out from each of its
 * neighboring elements if they are unfrozen. The bottom boundary is a no-
 * flow boundary which oxygen neither diffuses in or out of.
 *
 * VARIABLES:
 *
 * o2: the normalized oxygen concentrations
 * t: the temperature array
 * etat: the diffusion parameter for oxygen in soil
 * depth: the number of soil elements from the soil top to the frozen bottom
 */

void get_new_o2(float *o2, float *t, float etat, int depth)
{
  float *a, *b, *c;
  float *o21;
  int i;


  a = (float *) allocate_array(depth*sizeof(float));
  b = (float *) allocate_array(depth*sizeof(float));
  c = (float *) allocate_array(depth*sizeof(float));
```

```
o21 = (float *) allocate_array(depth*sizeof(float));

for (i=0;i<depth;i++)
{
  if (t[i] > 0.0)
  {
    if (t[i-1] > 0.0)
       a[i] = -etat;
    else
       a[i] = 0;

    if (t[i+1] > 0.0)
       c[i] = -etat;
    else
       c[i] = 0;

    b[i] = 1.0 - a[i] - c[i];
  }
  else
  {
     b[i] = 1.0;
     a[i] = c[i] = 0.0;
  }

  o21[i] = o2[i];
}
a[0] = c[depth-1] = 0;

o21[0] = o2[0] + etat;
o21[depth-1] = o2[depth-1];
tridiag(a,b,c,o21,o2,depth);

free(a);
free(b);
free(c);
```

```
  free(o21);
}


/*
 * FUNCTION: get_new_ch4
 *
 * SYNOPSIS: Get_new_ch4 determines the new ch4 concentration distribution
 * for a one-dimensional soil column given the previous concentrations and top
 * boundary condition which is assumed to be zero.
 *
 * IMPLEMENTATION: Euler's method is used to solve the diffusion equation with
 * constant coefficients.  There are two transport times, one for unfrozen
 * soil (etat) and the other for frozen soil which is zero.  Thus for any
 * soil element which is unfrozen gas diffuses into and out from each of its
 * neighboring elements if they are unfrozen.
 *
 * VARIABLES:
 *
 * ch4: the methane concentrations for each soil element
 * t: the temperature of each soil element
 * o2: the normalized oxygen concentration for each soil element
 * etao2: the methane lifetime due to oxidation
 * etat: the gas transport coefficient in unfrozen soil
 * depth: the number of soil elements
 *
 * RETURNS: the amount of ch4 diffused into the atmosphere
 */

float get_new_ch4(float *ch4,float *t,float *o2,
                  float etao2,float etat,int depth)
{
  int i;
  float newch4;
  float *a, *b, *c, *ch41;
```

```
a = (float *) allocate_array(depth*sizeof(float));
b = (float *) allocate_array(depth*sizeof(float));
c = (float *) allocate_array(depth*sizeof(float));
ch41 = (float *) allocate_array(depth*sizeof(float));

for (i=0;i<depth;i++)
{
  if (t[i] > 0.0)
  {
     if (t[i-1] > 0.0)
       a[i] = -etat;
     else
       a[i] = 0.0;

     if (t[i+1] > 0.0)
       c[i] = -etat;
     else
       c[i] = 0.0;

     b[i] = 1.0 - etao2*o2[i] - a[i] - c[i];
  }
  else
  {
     b[i] = 1.0;
     a[i] = c[i] = 0.0;
  }

  ch41[i] = ch4[i];
}
a[0] = c[depth-1] = 0.0;

tridiag(a,b,c,ch41,ch4,depth);

if (t[0] > 0.0)
  newch4 = etat*ch41[0];
```

```
  else
    newch4 = 0;

  free(a);
  free(b);
  free(c);
  free(ch41);

  return newch4;
}


/*
 * FUNCTION: findzero
 *
 * SYNOPSIS: Findzero determines the current thaw level in factional soil
 * elements; this is necessary in order for the model output to be
 * continuous rather than discrete.
 *
 * IMPLEMENTATION: A parabola is fit to the two points above and below
 * as well as the point itself that is the highest frozen soil element.
 *
 * VARIABLES:
 *
 * t: the temperatures of each soil element
 * n: the number of the highest frozen soil element
 * bc: the air temperature
 *
 * RETURNS: the current thaw level
 */

float findzero(float *t, int n, float bc)
{
  float a, b, c;
  float ans;
```

```
  float yx2, yx, y;

  if (n > 0)
  {
    yx2 = t[n-1] + t[n+1];
    yx = -t[n-1] + t[n+1];
    y = t[n-1] + t[n] + t[n+1];

    a = 1.5 * yx2 - y;
    b = 0.5 * yx;
    c = -yx2 + y;

    ans = (-b + sqrt(pow(b,2.0)-4.0*a*c))/(2.0*a);
    if (ans > 0 || ans < -1)
      ans = (-b - sqrt(pow(b,2.0)-4.0*a*c))/(2.0*a);
    if (ans > 0 || ans < -1)
       ans = -1;
  }
  else if (n == 0)
  {
    ans = 0;
  }

  return ((float) n + ans + 1.0) /* deltaz */;
}


/*
 * UTILITY FUNCTIONS:
 *
 * allocate_array: allocates array and exits with error message if it fails.
 * msgexit: exits program with error message.
 * avg2: averages two floating point numbers.
 */
```

```
char *allocate_array(int n)
{
  char *dum;
  if ( (dum = malloc(n)) == NULL)
    msgexit("Error allocating array");

  return dum;
}

void msgexit(char *str)
{
  fprintf(stderr,"%s\n", str);
  exit(1);
}

float avg2(float t1, float t2)
{
  return (t1+t2)/2.0;
}
```

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