**IMPROVED TEMPORAL RESOLUTION IN PROCESS-BASED MODELLING
OF AGRICULTURAL SOIL AMMONIA EMISSIONS**

A Thesis

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The Faculty of Graduate Studies

of

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by

JESSICA BEUNING

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ABSTRACT

IMPROVED TEMPORAL RESOLUTION IN PROCESS-BASED MODELLING OF AGRICULTURAL SOIL AMMONIA EMISSIONS

Jessica Beuning
University of Guelph, 2007

Advisor:
Dr. Bill Van Heyst

An emerging environmental issue in Canada is how to quantify the contribution of agricultural soil emissions of ammonia (NH_3) to environmental pollution. Due to the high spatial and temporal variability of NH_3 emissions, emission inventories based on measurements or emission factors are inadequate. Process-based models can account for the complex soil interactions, but current models lack temporal refinement and few consider both NH_3 emissions and the influence of microbial processes. This thesis presents the development of a one-dimensional, time dependent process-based model that predicts NH_3 emissions from a slurry applied to a bare soil. The model is tested with experimental data and an example application over the growing season is presented. Testing demonstrated the model's ability to predict the large NH_3 emissions immediately following application and subsequent emission trends associated with diurnal patterns. Results showed that model performance could benefit from an empirical or process model of surface pH.

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NOMENCLATURE

Note that the units stated are best suited for the application of each parameter.

a	volumetric soil air fraction (cm^3 air cm^{-3} soil) or the drag coefficient in neutral conditions (unitless)
a^I	curve-fitting parameter for anaerobic fraction (unitless)
a_{max}	maximum death rate for nitrifiers (h^{-1})
b	soil characteristic from soil water retention curve (unitless)
B_{denit}	denitrifier biomass (g C cm^{-3} soil)
B_{nit}	nitrifier biomass (g C cm^{-3} soil)
B_s	soil buffering power (mol kg^{-1} soil pH^{-1})
c	fractional cloud cover (unitless)
C	organic carbon concentration (g C cm^{-3} soil)
C_{air}	concentration of species in air (g m^{-3} air)
C_G	mass concentration in gas phase (g cm^{-3} air)
C_{hv}	volumetric heat capacity of vapour ($\text{J cm}^{-3} \text{K}^{-1}$)
C_L	mass concentration of a species in the liquid phase ($\text{g C cm}^{-3} \text{H}_2\text{O}$)
C_{pair}	volumetric specific heat of air ($\text{J cm}^{-3} \text{K}^{-1}$)
c_{pair}	heat capacity of air ($\text{J g}^{-1} \text{K}^{-1}$)
$C_{p,part}$	volumetric specific heat of soil particulates ($\text{J cm}^{-3} \text{K}^{-1}$)
C_{prod}	organic C production from potential decomposition of residue pool (g C cm^{-3} soil)
C_{ps}	volumetric specific heat of soil ($\text{J cm}^{-3} \text{K}^{-1}$)
C_{pw}	volumetric specific heat of water ($\text{J cm}^{-3} \text{K}^{-1}$)
C_s	mass concentration of a species sorped to the solid phase (g g^{-1} soil)

CN	C:N ratio ($\text{g C g}^{-1} \text{N}$)
D_{denit}	death rate of denitrifiers ($\text{g C cm}^{-3} \text{soil h}^{-1}$)
D_G	gaseous diffusion coefficient of a species in soil ($\text{cm}^2 \text{h}^{-1}$)
D_G^{air}	molecular diffusivity of the species in air ($\text{cm}^2 \text{h}^{-1}$)
D_L	aqueous diffusion coefficient in soil ($\text{cm}^2 \text{h}^{-1}$)
D_L^{water}	molecular diffusivity of the species in water ($\text{cm}^2 \text{h}^{-1}$)
D_{nit}	death rate of nitrifiers ($\text{g C cm}^{-3} \text{soil h}^{-1}$)
e	solar elevation angle or solar altitude
E	evaporative flux (cm h^{-1})
F_M	stability parameter for momentum flux (unitless)
F_H	stability parameter for heat flux (unitless)
F_{pH}	pH factor for denitrification (unitless)
$F_{T,denit}$	temperature factor for denitrification (unitless)
g	gravitational constant (9.8 m s^{-2})
G	soil heat flux (W m^{-2})
G_{denit}	growth rate of denitrifiers ($\text{g C cm}^{-3} \text{soil h}^{-1}$)
G_{nit}	growth rate of nitrifiers ($\text{g C cm}^{-3} \text{soil h}^{-1}$)
h	soil suction head (cm)
h_{dec}	rate of decomposition for resistant fraction (h^{-1})
H	sensible heat flux (W m^{-2})
H_0	surface potential temperature flux (m K s^{-1})
I_c	organic input ($\text{g C cm}^{-3} \text{soil}$)
J	Julian day

J_s	soil vertical flux of species ($\text{g cm}^{-2} \text{ h}^{-1}$)
J_w	vertical soil water flux, also denoted as q_L (cm h^{-1})
K_{air}	thermal conductivity of air ($\text{W m}^{-1} \text{ K}^{-1}$)
K_c	half-saturation value with respect to carbon ($\text{g cm}^{-3} \text{ H}_2\text{O}$)
K_d	liquid-solid partitioning coefficient ($\text{cm}^3 \text{ H}_2\text{O g}^{-1} \text{ soil}$)
K_D	ammonium dissociation constant (unitless)
K_H	parameter for calculation of bulk transfer coefficient for aerodynamic resistance to heat and solute surface flux (unitless)
K'_H	corrected parameter for calculation of bulk transfer coefficient for surface solute flux accounting for laminar surface layer resistance (unitless)
k_H	soil thermal conductivity ($\text{J h}^{-1} \text{ cm}^{-2}$)
K_h	Henry's Law constant (units vary)
k_{imm}	immobilization rate coefficient (h^{-1})
k_{dec}	rate of decomposition of labile fraction (h^{-1})
K_L	soil hydraulic conductivity (cm h^{-1})
k_{nit}	maximum nitrification rate (h^{-1})
K_{NOx}	half-saturation value with respect to N oxide ($\text{g cm}^{-3} \text{ H}_2\text{O}$)
K_s	saturated soil hydraulic conductivity (cm h^{-1})
L	Monin Obukhov length (m)
L_{hvo}	latent heat of vaporization (J cm^{-3}) at reference temperature T_0 (K)
LE	latent heat flux (W m^{-2})
m	curve-fitting parameter for van Genuchten functions (unitless)
M	molecular weight of water (18.0 g mol^{-1})
$M_{c,denit}$	maintenance coefficient for carbon ($\text{g C g}^{-1} \text{ biomass h}^{-1}$)

M_{NO_x}	maintenance coefficient with respect to N oxide ($\text{g NO}_x \text{ g}^{-1} \text{ biomass h}^{-1}$)
n	curve-fitting parameter for van Genuchten functions (unitless)
$N_{ass,denit}$	assimilated N during denitrification ($\text{g N cm}^{-3} \text{ soil}$)
N_{avail}	N available for potential decomposition of residue pool ($\text{g N cm}^{-3} \text{ soil}$)
N_{min}	net mineralization in each organic matter pool ($\text{g N cm}^{-3} \text{ soil}$)
P_f	parameter to calculate thermal conductivity ($\log_{10}(\text{cm})$)
Q_o	potential solar radiation (W m^{-2}) or solute flux ($\text{g m}^{-2} \text{ s}^{-1}$)
q_h	soil heat flux at each node (W m^{-2})
q_L	soil water flux at each node, also denoted as J_w (cm h^{-1})
P_x	partial pressure of species X (atm)
R	gas constant ($8.314\text{E}7 \text{ erg mol}^{-1} \text{ K}^{-1}$)
r_ψ	radius of typical air-filled pore at moisture tension ψ (m)
R_b	bulk Richardson number (unitless)
R_{hum}	relative humidity of soil surface (unitless)
R_{imm}	upper limit on rate of immobilization ($\text{g N cm}^{-3} \text{ soil h}^{-1}$)
R_n	net radiation (W m^{-2})
R_{nit}	rate of nitrification ($\text{g N cm}^{-3} \text{ soil h}^{-1}$)
$R_{NO,nit}$	rate of NO production from nitrification ($\text{g N cm}^{-3} \text{ soil h}^{-1}$)
$R_{N_2O,nit}$	rate of N ₂ O production from nitrification ($\text{g N cm}^{-3} \text{ soil h}^{-1}$)
R_{slurry,H^+}	rate of H ⁺ ion addition from slurry application ($\text{mol cm}^{-3} \text{ soil h}^{-1}$)
R_{vol}	rate of volatilization of a species ($\text{g cm}^{-3} \text{ soil h}^{-1}$)
S	source-sink term ($\text{g cm}^{-3} \text{ h}^{-1}$) or labile fraction of organic matter pool
S_e	reduced volumetric water content ($\text{cm}^3 \text{ cm}^{-3}$)

S_t	incoming solar radiation (W m^{-2})
t	time (h)
t_o	solar noon (1200 hr)
T	soil temperature (K)
T_a	air temperature (K)
T_0	reference temperature (273.16 K)
T_s	soil surface temperature (K)
T_t	transmission coefficient, ratio of potential to actual solar radiation (unitless)
u	horizontal wind speed (m s^{-1})
u^*	friction velocity (m s^{-1})
X_c	soil clay content (g g^{-1})
$[X]$	concentration of a species X in the soil (g cm^{-3} soil)
$[X]_g$	concentration of a species X in the gas phase (g cm^{-3} gas)
$[X]_l$	concentration of a species X in the soil solution (g cm^{-3} H_2O)
$[X]_s$	adsorbed concentration of a species X (g g^{-1} soil)
X_{rate}	rate of increase or decrease of species within soil profile ($\text{g cm}^{-3} \text{ cm}^{-1}$)
$Y_{c,denit}$	maximum growth yield for carbon ($\text{g biomass g}^{-1} \text{ C}$)
$Y_{NOx,max}$	maximum growth yield on N oxide ($\text{g biomass g}^{-1} \text{ NO}_x$)
z	depth below soil surface (cm)
z_0	surface roughness length (cm)
z_r	reference height for wind speed and air temperature measurements (m)
ZZ	thickness of soil layer (cm)

GREEK SYMBOLS

α	curve-fitting parameter for van Genuchten and anaerobic fraction functions
γ	curve-fitting parameter for anaerobic fraction function
β	curve-fitting parameter for anaerobic fraction function
δ	solar declination angle or curve-fitting parameter for anaerobic fraction function
α_s	surface albedo
ε_a	atmospheric emissivity under clear skies
ε_{ac}	atmospheric emissivity under cloudy skies
ε_s	soil emissivity
η	soil porosity
θ	volumetric soil water content ($\text{cm}^3 \text{ cm}^{-3}$)
θ_a	volumetric soil air content ($\text{cm}^3 \text{ air cm}^{-3} \text{ soil}$)
θ_r	residual volumetric soil water content ($\text{cm}^3 \text{ cm}^{-3}$)
θ_s	saturated volumetric soil water content ($\text{cm}^3 \text{ cm}^{-3}$)
θ_T	potential temperature (K)
θ_l	soil surface volumetric water content ($\text{cm}^3 \text{ cm}^{-3}$)
κ	von Karman constant (0.4)
μ_{air}	molecular viscosity of air ($\text{g s}^{-1} \text{ cm}^{-1}$)
μ_c	clay reduction factor for composition
μ_{CN}	N availability reduction factor
μ_{dec}	decomposition rate reduction factor

$\mu_{max,nit}$	maximum growth rate for nitrifiers (h^{-1})
μ_{NOx}	actual relative growth rate for N oxide (h^{-1})
$\mu_{NOx,max}$	maximum relative growth rate on N oxide (h^{-1})
μ_T	temperature reduction factor
$\mu_{total,denit}$	total relative growth rate for denitrifiers (h^{-1})
μ_W	moisture reduction factor
ρ_{air}	density of air (g cm^{-3})
ρ_b	soil bulk density (g cm^{-3})
ρ_{va}	atmospheric vapor density (g cm^{-3})
ρ_{vs}	soil surface vapor density (g cm^{-3})
ρ_{vss}	saturated soil surface vapor density (g cm^{-3})
ρ_w	density of water (1.0 g cm^{-3})
σ	Stephan-Boltzmann constant ($5.76\text{E-}8 \text{ J s}^{-1} \text{ m}^{-2} \text{ K}^{-4}$)
τ	tortuosity factor
ϕ	latitude
Φ	anaerobic soil fraction
χ	ratio between the oxygen diffusion coefficient in air and the oxygen diffusion coefficient in water
Ψ	pressure potential of water (cm)
ψ_s	saturation matric potential (cm)

1.0 INTRODUCTION

An emerging issue in Canada is how to better quantify agriculture's contribution to environmental pollution generated by ammonia (NH_3) emissions and other nitrogen trace gases. In 1995, the Canadian National Inventory of Ammonia Emissions estimated that agricultural NH_3 emissions represent 95% of all anthropogenic sources and 56% of total emissions (Agriculture and Agri-Food Canada, 2003). These emissions can have adverse environmental impacts including ecosystem acidification, eutrophication, and climate change. Ammonia also contributes to the formation of secondary particulates that are components of airborne fine particulate matter (known as $\text{PM}_{2.5}$ meaning particulate matter with a diameter less than or equal to 2.5 microns) which cause or aggravate respiratory diseases and have also been linked to premature death (American Lung Association, 2006).

While livestock housing is a major source of NH_3 emissions, emissions from soil following spreading of livestock manure is also a major source that must be considered (Anderson et al., 2003). The environmental and health impacts associated with these emissions require that emission inventories be developed to monitor emission trends, assess emission reduction measures, and to serve as input data for models of atmospheric transport and deposition. The processes of soil nitrogen transformations and transport are complex and are controlled by site specific factors influenced by weather, vegetation, soil properties, and land management. These influences imply that nitrogen gas emissions can be highly spatially and temporally variable. For ammonia in particular, soils and vegetation can act as both sources and sinks under different conditions. This is known as

bidirectional exchange meaning that ammonia emissions can be transported, deposited and re-emitted. Implementing measurement programs to develop inventories becomes expensive and labour intensive, thus the current approach to emission inventories for NH_3 from agricultural soils is the use of empirically-based emission factors.

The problem with existing agricultural NH_3 emission factors is that they have poor temporal resolution typically starting at a daily scale (i.e. Misselbrook et al., 2000). Most emission factors used to determine emissions from manure application are a percentage of nitrogen applied (i.e. de Vries et al., 2002) or are on a per livestock basis (i.e. Anderson et al., 2003). The majority of emissions following slurry application occur immediately in the hours following application and on subsequent days when variations in wind speed, air temperature, precipitation, and atmospheric stability govern emissions. Current empirically-based inventories cannot capture these peak emissions and diurnal trends.

Process-based or mechanistic models can better account for emission variations because these models can simulate process responses to meteorological drivers. A literature review of current models found existing process models that account for biological, chemical and physical processes but that lack direct estimation of NH_3 emissions (i.e. Hansen et al., 1990) or use an empirical approach for emissions (i.e. Li, 2000). While current process models of agricultural NH_3 emissions exist (Génermont and Cellier, 1997; Hutchings et al., 1995; Pinder et al., 2004; Rachhpal-Singh and Nye, 1986; Roelle and Aneja, 2005; Van Der Molen et al., 1990), none of them consider all of

the belowground biological, chemical and physical processes that control nitrogen dynamics during and after application events.

This thesis presents a process-based model, AGRIN, which seeks to account for the peak emissions and diurnal trends of NH_3 emissions following slurry application by using a refined temporal scale. AGRIN is a one-dimensional (vertical), time-dependent mechanistic or process-based model that predicts hourly nitrogen trace gas emissions after slurry application to a bare soil in a southeastern Ontario climate. Current model theory of belowground soil processes (i.e. Li et al., 1992) are combined with models of NH_3 volatilization at the soil surface (i.e. Van Der Molen et al., 1990) and new concepts such as a separate slurry layer are introduced to improve model performance. While the model has been developed for prediction of all nitrogen trace gas emissions, there has been an emphasis on ammonia emissions in model testing through the use of ammonia emission datasets.

The development of process models also requires data sets to validate the predicted soil conditions and emission trends. A dataset of NH_3 bare soil emissions following slurry application provided by Agriculture and Agri-Food Canada (AAFC) is used for model development while data derived from field work completed in the summer of 2005 is used for model validation of AGRIN. The dataset used forms part of the research undertaken to develop the model and this thesis.

This thesis will first present background and a literature review concerning the nitrogen cycle and existing process models. Development of the theoretical equations that the model is based on will be outlined as will the structure of the program used to implement these equations. Model testing and results using AAFC's data are presented and compared to emission factors while an example application is used to show the model's performance over longer time periods. Finally, conclusions and recommendations are presented based on the model development, testing and simulations.

2.0 BACKGROUND AND LITERATURE REVIEW

2.1 Environmental and Health Impacts of Nitrogen Emissions

The increasing levels of human activity concerning agriculture, traffic, and industrialization have resulted in enhanced levels of nitrogen within the atmosphere (de Vries et al., 2002). These enhanced levels have adverse impacts on the natural environment including climate change, groundwater pollution, eutrophication, and soil acidification. Nitrous oxide is a greenhouse gas that contributes 5% of the global warming potential (Rodhe, 1990) and also influences stratospheric ozone chemistry (Crutzen, 1974). Nitrate leaching from agricultural soils causes pollution of groundwater (Fraters et al., 1997, 1998). Increased levels of nitrogen compounds introduced to terrestrial and aquatic ecosystems contribute to eutrophication (Walker et al., 2000).

Ammonia emissions in particular contribute to soil acidification when deposited (Sutton et al., 1995) and may lead to global warming (Bouwman et al., 1997). Ammonia is also a precursor to atmospheric aerosols as it can combine with nitrogen and sulfur oxides (i.e. nitrogen dioxide or sulfur dioxide) to form ammonium sulfate and ammonium nitrate particles (Goebes et al., 2003). The particles formed are components of airborne fine particulate matter, or PM_{2.5} (particulate matter with a diameter equal or less than 2.5 microns), which has been linked to adverse human health impacts. Human exposure to high concentrations of PM_{2.5} can result in respiratory diseases and research has also linked low concentrations with premature death (American Lung Association, 2006).

Particulate matter also reduces visibility by up to 70% (US EPA, 1997), influences climate and causes degradation of aquatic and terrestrial ecosystems when deposited.

2.2 Soil Nitrogen Cycle

2.2.1 General Overview

The soil nitrogen cycle (Figure 2-1) involves various nitrogen (N) forms including dinitrogen (N_2), ammonia (NH_3), ammonium (NH_4^+), nitrate (NO_3^-), nitrite (NO_2^{2-}), nitric oxide (NO) and nitrous oxide (N_2O). The major source of nitrogen in soils where the nitrogen supply is not augmented is biological fixation of atmospheric N_2 while precipitation is a secondary source (Simpson and Steele, 1983). Nitrogen can be lost from the soil cycle via volatilization, leaching, soil removal, and plant uptake. In an agricultural soil system nitrogen fixation alone cannot sustain high crop yields and applications of animal manure or commercial inorganic fertilizer are used to augment the soil nitrogen supply and increase yields and improve crop quality (Stevenson, 1965). In addition to sources and sinks, Figure 2-1 illustrates the major belowground microbial processes controlling nitrogen transformations: mineralization, immobilization, nitrification, and denitrification.

Figure 2-1: Nitrogen cycle.
(Penn State, 2004)

2.2.2 Mineralization and Immobilization

Crop residues in the soil surface layers introduce organic forms of nitrogen into the soil which are then converted into inorganic forms and back again through mineralization and immobilization. Benbi and Richter (2002) describe mineralization as the decomposition of soil organic matter by microbes resulting in the release of mineral nitrogen in the process. The mineralization process in reverse is called immobilization. This is the process where soil microbial biomass assimilates inorganic nitrogen forms and transforms them into organic nitrogen during oxidation of suitable carbon substrates (Batholomew, 1965). As

Figure 2-2 shows, a give-and-take relationship forms where immobilized nitrogen becomes available for mineralization which in turn produces the inorganic nitrogen

assimilated in immobilization. Gross mineralization is the total release of ammonium through microbial activity prior to any immobilization; however, this is difficult to measure so net mineralization is usually estimated as the difference between gross mineralization and immobilization (Benbi and Richter, 2002).

Figure 2-2: Mineralization-immobilization turnover.

The C:N (carbon-to-nitrogen) ratio of the soil organic matter dictates which direction (mineralization or immobilization) the process will proceed. There will be a net release of nitrogen if the nitrogen content in the organic matter exceeds the needs of microbes while immobilization occurs when there is a high C:N ratio and microbes must use soil nitrogen in competition with crops (Bartholomew, 1965). There are also various other soil conditions and management practices that can alter mineralization, immobilization and decomposition rates. Mineralization is optimal at a soil moisture content of field capacity. Rates reach a maximum at 40° to 50°C and a minimum at 5 to 10°C (Penn State, 2004). Soil clay content affects the decomposition of organic matter because clays can adsorb organic carbon and shelter it from decomposition (Bouwman, 1990). Tivy (1990) states that soil tillage can change decomposition rates and

distribution of organic matter by physically mixing the soil and by increasing oxygen activity.

2.2.3 *Nitrification and Denitrification*

Nitrification is the oxidation of NH_4^+ to NO_3^- by nitrifying bacteria under aerobic conditions where N_2O and NO are gaseous intermediates (Mosier et al., 1998). In general, nitrous oxide emissions are only considered from biological nitrification (Grant, 1995) and those emissions produced by non-biological processes are considered negligible (Bremner, 1997). Nitrification occurs according to the following sequence (Li, 2000):

Regulators of nitrification include temperature, moisture, pH, aeration and substrate availability (Li and Aber, 2000). Alexander (1965) details the optimum ranges for environmental parameters such as temperature (between 30° and 35°C), pH (between 7 and 9), and nitrifying activity (greatest at about half to two-thirds of a soil's moisture-holding capacity). While nitrification is an aerobic process, Alexander (1965) states that high rates of aeration are not required for nitrifying bacteria. Nitrification rates are generally limited by the rate of mineralization which is a slower process than ammonium and nitrite oxidation.

Denitrification is another major source of soil N_2O and NO . Denitrification is the reduction of nitrogen oxides to dinitrogen gas in the absence of oxygen (anaerobic conditions) by denitrifying bacteria. The process follows the reduction sequence NO_3^- to NO_2^{2-} to NO to N_2O to N_2 indicating that nitrous oxide and nitric oxide are intermediates as in nitrification (Li, 2000). Denitrification rates in soil are controlled by temperature, moisture, pH, aeration and substrate availability. Li et al. (1992) state that N oxide transformation rates are affected by low pH where denitrification stops at N_2O instead of N_2 , meaning that total denitrification decreases as pH decreases. The authors also state that the denitrification rate is very temperature dependent in the 10° to 35°C range and the rate increases to a maximum at 60° to 75°C . Denitrification stops at temperatures below 10°C . Alexander (1965) points out that it is difficult to distinguish between moisture's influence on nitrifiers and denitrifiers, but generally increasing soil moisture will cause oxygen deficiencies favouring denitrification.

2.3 Agricultural Ammonia Emissions

2.3.1 Sources

Emission inventories in the United States indicate that over 60% of anthropogenic NH_3 emissions come from agriculture (Anderson et al., 2003) while it is estimated that approximately 50% of global NH_3 emissions come from agriculture (Schlesinger and Hartley, 1992). In 1995, the Canadian National Inventory of Ammonia Emissions estimated that agricultural NH_3 emissions represented 95% of all anthropogenic sources

and 56% of total emissions (Agriculture and Agri-Food Canada, 2003). The sources of these agricultural emissions include livestock housing, manure storage, livestock grazing, manure application and inorganic fertilizer application. NH_3 emissions from manure application in particular can contribute up to 30% of a livestock's farm nitrogen emissions (Sommer et al., 2003).

Ammonia losses following manure (or fertilizer) application occur because of the aqueous total ammoniacal nitrogen, or TAN (sum of ammonia and ammonium forms), introduced to the soil surface. An emission occurs when there is a transfer from the ammonia air-phase in immediate contact with the ammoniacal solution to the free air phase (Sommer et al., 2001). The NH_3 air-phase concentration at the soil/manure surface is in equilibrium with the dissolved NH_3 in the ammoniacal solution (Générmont and Cellier, 1997). Emission rates will be highest immediately following manure application and then fall rapidly reaching low rates after 2 days for slurries or after longer periods for solid manures (Sommer et al., 2003).

2.3.2 Factors Influencing Soil Emissions

The two major groups of factors that control soil ammonia emissions are those that influence how much ammoniacal nitrogen is available at the soil/manure surface and those that influence the rate of ammonia transfer from the surface to the atmosphere. Factors that influence the amount of TAN at the soil surface include the amount of manure applied, air temperature, pH, infiltration rate, application technique, evaporation rate (Sommer and Hutchings, 2001), and microbial processes (Sommer et al., 2003).

The rate of ammonia transfer to the atmosphere is controlled by canopy characteristics, crust formation, surface roughness, wind speed, and solar radiation (Sommer and Hutchings, 2001; Huijsmans et al., 2003).

Sommer and Hutchings (2001) discuss the influence of climate on NH_3 emissions following manure application by examining solar radiation, wind speed, and precipitation. Solar radiation will enhance NH_3 emissions by increasing turbulence, driving water evaporation which will increase aqueous ammoniacal concentrations, and increasing the surface temperature. The authors state that wind speed will enhance emissions and transport through turbulent transport and advection as found in a study by Sommer et al. (1997). Sommer and Hutchings (2001) also state that rainfall will dilute TAN concentrations and increase the rate of infiltration resulting in lower emission rates. The soil/manure surface pH is also a major factor controlling NH_3 emission rates. Sommer and Hutchings (2001) point out that a change in pH from 7.7 to 8 will double the emission. Concerning application technique, volatilization losses can be minimized through immediate soil incorporation by injection or tillage (Olesen and Sommer, 1993).

2.3.3 Emission Inventories

The environmental and health impacts of agricultural ammonia emissions have prompted the creation of policies aimed at emission reductions in countries such as the Netherlands (de Vries et al., 2002). Accurate emission inventories are an essential tool in determining the effectiveness of these abatement tools (Dragosits et al., 2002) and are needed as high

quality input data for air quality models (Anderson et al., 2003). Due to the factors influencing ammonia emissions, emissions are highly spatially and temporally variable such that models are needed to generate emission inventories.

Empirical emission factors (i.e. Hyde et al., 2002; Lenemen et al., 1998; Van Der Hoek, 1998) are the current approach to deriving ammonia emission inventories. An emission factor is simply the mass of a compound emitted per unit of activity and is multiplied by an activity level such as the mass of a material produced per time (Anderson et al., 2003). The problem with using emission factors for ammonia and other nitrogen trace gases is that these factors cannot capture the spatial and temporal variability associated with emission rates. Goebes et al. (2003) outline the issues with current ammonia inventories concerning fertilizer application in the United States:

1. Inventories are based on poor spatial resolution (i.e. a single value for an entire state).
2. There is not adequate temporal resolution in that many inventories use annual values.

There are also empirical models of ammonia emissions based on statistical analysis of experimental data (i.e. Braschkat et al., 1997; Sommer and Olesen, 2000; Søgaaard et al., 2002). In these types of models, empirical relationships between emissions and climatic and soil variables are developed based on regression analysis. Sommer et al. (2003) found that simple empirical regression models can give improbable results based on valid

input data because the mechanisms controlling NH_3 emissions are too complex to be represented by these types of models.

A more detailed approach to emission inventories has been mechanistic or process-based models which attempt to describe as many processes as possible while maintaining applicability at a variety of scales. The advantages of this type of modelling are that it can assess the impact of contrasting soils, crops, climates and farming practices, it can be applied at many scales, and it can simulate process interactions between different components (Langeveld and Leffelaar, 2002).

2.4 Process-Based Models of Soil Nitrogen Dynamics

A literature review of existing process-based models focused on two types of models: (1) models that simulate the major belowground soil nitrogen dynamics but lack direct non-empirical estimation of ammonia emissions and (2) models that predict emissions using a process-based approach. The first set of models simulate the microbial, chemical, and physical processes controlling nitrogen transformations and transport but may not necessarily simulate trace nitrogen gas emissions. The list of soil nitrogen dynamic models is quite exhaustive and only models frequently cited in literature are considered: ANIMO, CENTURY/DAYCENT, DAISY, DNDC, and NASA CASA which were each developed for different purposes and applied to different ecosystems. In general, all of these models use weather data, soil data, and agricultural practices as input. Process-

based models of ammonia emissions are considered separately in Section 2.5 as there was no comprehensive model that simulated all of the soil nitrogen dynamics and surface ammonia volatilization.

2.4.1 ANIMO

The Agricultural Nitrogen Model (ANIMO) was developed by Rijtema and Kroes (1991) and can simulate nitrogen management in agricultural areas while operating on a daily or weekly scale (Wu and McGechan, 1998). ECOBAS (2002) describes the main inputs being fertilizer management, soil properties, and soil water balance. The environmental influences included in the model are soil temperature, pH, moisture, and oxygen content (Rijtema and Kroes, 1991). Figure 2-3 shows schematic of the model outlining the transport and transformation processes simulated.

Rijtema and Kroes (1991) describe the main processes modelled as being mineralization and immobilization, nitrogen uptake by plants, nitrification, denitrification, soil moisture dynamics and nitrogen transport. No equations for direct estimation of nitrogen trace gas emissions were found, but the model simulates ammonia volatilization in a limited way (Wu and McGechan, 1998) as a fraction of the ammonium input by animal manure (Groenendijk and Kroes, 1999). ANIMO approaches soil heterogeneity slightly different from other process-based models. While most models apply Michaelis-Menten kinetics to account for soil heterogeneity in denitrification, ANIMO assumes randomly scattered air-filled pores with associated oxygenated zones (Arah and Vinten, 1995). Unlike other models, ANIMO does not include a hydrological

model and must be linked to a separate model to simulate the soil water balance (Rijtema and Kroes, 1991). ANIMO also cannot use weather data directly, and a separate model must be used as input (Wu and McGechan, 1998).

Figure 2-3: Nitrogen dynamics in ANIMO.
(Wu and McGechan, 1998)

2.4.2 CENTURY and DAYCENT

CENTURY is a general model of plant-soil nutrient cycling developed by Parton et al. (1992) to simulate carbon and nitrogen dynamics for different ecosystems including grasslands, agricultural lands, forests, and savannas (Parton et al. 1992, 1993, 1994). Figure 2-4 shows the general structure of the model which illustrates the emphasis on soil organic matter. The main purpose of the model is to analyze soil organic matter dynamics

in response to management and climate changes (ECOBAS, 2002) which requires the simulation of decomposition, nitrification and denitrification. The model functions at the scale of a square meter (Pennock and Frick, 2001), operates on a monthly time-step (NREL, 2000), and has a regional spatial extent (ECOBAS, 2002).

Figure 2-4: CENTURY model structure.
(Gilmanov et al., 1997)

CENTURY uses ecological and management-based drivers as inputs while outputs include carbon and nitrogen (NO, N₂O) fluxes (ECOBAS, 2002). Although the model was originally developed and tested on data sets from grassland and wheat-fallow agriculture in the United States (Parton et al., 1992), it has been successfully adapted to other ecosystems such as tropical agroecosystems (Liu et al., 2000; Leite et al., 2004). Detailed model description can be found in Parton et al. (1987) while model refinements can be found in Parton et al. (1993).

Many studies have used CENTURY to either simulate nitrous oxide emissions (i.e. Leite et al., 2004) or for model validation with measured emissions (i.e. Mikhailova et al., 2000). The major shortcomings of using CENTURY to estimate trace nitrogen gas emissions include the model's intended spatial scale, omission of the impact of low temperatures, failure to account for gaseous loss of NH_3 (Frolking et al., 1998), and the large temporal scale (Leite et al., 2004; Liu et al., 2000). A model comparison study by Frolking et al. (1998) concluded that models wishing to evaluate ecosystem productivity and sustainable agriculture must account for all nitrogen losses with equal weight – including ammonia. Trace gas emissions that are included are simulated as “leaky pipe” emissions meaning they are calculated as a percentage of process rates as opposed to being calculated based on atmospheric transport processes.

The issue of temporal resolution has been addressed through the introduction of a daily version of CENTURY, called DAYCENT (Parton et al., 1998). The model represents the same ecosystem processes as CENTURY but uses a daily land surface submodel and includes more detailed simulation of factors influencing trace gas fluxes (Parton et al., 1998). The model has been validated by various studies (i.e. Kelly et al., 2000) but Del Grosso et al. (2002) found that the model cannot reliably simulate daily N_2O emission patterns and is only capable of capturing seasonal patterns. Parton et al. (1998) found DAYCENT could accurately predict the impact of different management practices on N_2O emissions.

2.4.3 DAISY

DAISY is a soil-plant system model developed by Hansen et al. (1991) that operates using a weekly time step. The model simulates crop production, soil water dynamics and nitrogen dynamics based on various agricultural management practices and can facilitate both field level and regional simulations (Hansen et al., 1991). Based on inputs concerning weather, soil, and agricultural management, DAISY can estimate nitrogen concentration profiles and CO₂ fluxes (ECOBAS, 2002). The model has performed well in model comparisons (de Willigen, 1991; Diekkruger et al., 1995) and has also been validated for simulating long-term trends (Jensen et al., 1997). Hansen et al. (1990, 1991) describe the main modules as being hydrological, nitrogen dynamics, soil heat, and crop growth. Concerning nitrogen dynamics, the model includes the same major processes as other process-based models: immobilization, mineralization, nitrification, denitrification, plant uptake and leaching. These transport and transformation processes can be seen in Figure 2-5.

Figure 2-5: Nitrogen dynamics in DAISY.
(Wu and McGechan, 1998)

DAISY has successfully been validated (Abrahamsen and Hansen, 2000; Svendsen et al., 1995) and used for simulations (i.e. Mueller et al., 1997). However, an extensive literature review showed that none of these studies used DAISY to estimate trace gas emissions or ammonia volatilization. Other shortcomings include that DAISY is intended for the plot scale (Jensen et al., 1997) and that it includes some empirically derived relationships (Bruun et al., 2003). There are also questions about the quality of data used in studies that validated the model (Bruun et al., 2003).

2.4.4 DNDC

The DeNitrification and DeComposition (DNDC) model estimates the impacts of agricultural management on trace gases including N_2O , NH_3 and CO_2 (Li et al., 1992). The model can predict soil conditions such as temperature, moisture, pH, redox potential, and substrate concentration profiles and, based on these conditions, the model can predict trace gas emissions (EOS, 2003). Figure 2-6 shows the model's structure which includes modules of decomposition (and mineralization/immobilization), nitrification and denitrification. Li (2000) describes DNDC as paralleling the concept of a biogeochemical cycle where a biogeochemical field is an assembly of environmental forces that drive biogeochemical reactions in an ecosystem.

Figure 2-6: Structure of the DNDC model.
(EOS, 2003)

DNDC has been applied frequently in literature for both simulation and validation of nitrogen and carbon trace gas emissions. The model has been used to produce regional estimate of trace gas emissions for both the United States (Li et al., 1996) and Canada (Smith et al., 2004). Unlike other process-based models, DNDC has the advantage of predicting trace gas emissions simultaneously which is valuable in assessing the net impact of alternative agricultural management on the atmosphere and/or agriculture (Li, 2000). Another advantage is the fact that DNDC is linked to GIS databases (Li et al., 1996), making it capable of regional estimation for trace gas emissions (Li, 2000). Unlike other models of trace gas emissions, DNDC can estimate ammonia volatilization through modelling the NH_3 concentration in the soil water phase and the effect of soil environmental factors (Li, 2000). However, model equations indicate that ammonia volatilization is empirically calculated based on soil moisture, temperature and clay content rather than atmospheric processes.

Various studies have pointed out some of DNDC's shortcomings. Ri et al. (2003) discuss two major shortcomings with the first being that the model does not consider the effect of high initial NH_4^+ levels in the soils. Secondly, the study states that DNDC assumes that N_2O fluxes to the atmosphere are zero when the soil is snow covered or frozen which is inconsistent with published data (Rover et al., 1998; Sommerfeld et al., 1993). A study by Saggar et al. (2004) found that the model underestimates winter emissions, overestimates spring emissions, and has limited success in predicting the size and timing of high emissions observed after a summer rainfall event. Similar to CENTURY, trace gas emissions are simulated as "leaky pipe" emissions as opposed to

being simulated based on underlying processes. Finally, Frolking et al. (1998) point out that DNDC's original objective was field scale simulation and that the model does not simulate soil freeze/thaw.

2.4.5 NASA CASA

The Carnegie-Ames-Stanford (CASA) modeling approach is based on the derived NASA CASA version by Potter et al. (1993). The model was designed to simulate seasonal patterns in carbon fixation, nitrogen mineralization and trace gas production and emissions using a daily time step (Potter et al., 1997). NASA CASA was designed to run with a minimum number of inputs and is driven, in part, by satellite remotely sensed data that allow it to simulate processes at a regional to global scale (Frolking et al., 1998). Figure 2-7 shows the model's structure and indicate that the model simulates soil organic matter dynamics to estimate trace gas emissions, but omits the major processes of nitrification and denitrification.

A literature review showed few studies used the NASA CASA version to simulate N₂O emissions and that the model is likely not capable of estimating NH₃ emissions. CASA has been used to simulate global N₂O fluxes, but at a coarse resolution and without detailed agricultural management data (Parton et al., 1998). When Potter et al. (1997) developed the NASA CASA version, the study found that the model could predict maximum daily N₂O fluxes but consistently overestimated mean daily fluxes. The Frolking et al. (1998) study found that NASA CASA has a clear advantage in its use of remote sensing drivers which allows for scaling up to regional estimates. However, the

study found the model's shortcomings to include its omissions of ammonia volatilization loss, soil freeze/thaw and the low temperature effect on $N_2O:N_2$ ratios as well as the fact that the model does not separate the nitrification and denitrification processes. Similar to previously discussed models, the trace gas emissions are based on the "leaky pipe" assumption.

Figure 2-7: Structure of NASA CASA model.
(Potter, 2004)

2.4.6 Other Models

Other models found in the literature, but not as frequently cited as the previously described models, include SOILN, ExpertN and CANDY. SOILN was developed by Jansson (1991) to simulate nitrogen conditions in soil by looking at the transport and transformations of nitrogen in the soil as well as uptake by plants. It does not, however, simulate trace gas emissions. ExpertN is a soil-plant system model developed by Engle and Priesack (1993) as a development system for nitrogen turnover models to simulate the nitrogen cycle in arable agriculture. The model can incorporate agricultural

management activities and has been applied to estimate N₂O emissions from temperate agricultural soils (Frolking et al., 1998). The Carbon and Nitrogen Dynamics (CANDY) model was developed by Franko et al. (1995) to simulate carbon and nitrogen dynamics in agricultural soils but it does not simulate trace gas emissions.

Other models in the literature haven't been thoroughly tested but may have the potential to become accepted models in the future. The *ecosys* model (Grant, 1995) has been used as the basis for a modelling program (Grant, 2001) in order to create a comprehensive, detailed model for use in land management and climate change research (Grant and Pattey, 2003). The model is capable of looking at N₂O emissions (Grant, 1995) and can work in up to three dimensions (Grant and Pattey, 2003). The model of Langeveld and Leffelaar (2002) looks at microbiological transformations in denitrification and aerobic respiration in conjunction with the transport of gases, water, and solutes. Bear et al. (1998) developed a comprehensive N-dynamics model to describe N transport and transformation in soils under *environmentally friendly fertilization practices* (EFFPs). This model shows a lot of promise in that it includes all belowground processes and model design allows for easy introduction of an atmospheric transport submodel. It has been used to validate N₂O concentrations within the soil profile (Wang et al., 1998) but not for trace gas emissions at the soil surface.

2.5 Models of Ammonia Volatilization

Mechanistic models of ammonia emissions from field applied nitrogen that currently exist have high temporal resolution in both inputs and outputs, although the models do not consider all of the processes controlling soil nitrogen dynamics. These existing models either specifically examine emissions following nitrogen application or include the emissions in an integrated model of an entire farm. All of the models consider the chemical and physical aspects which control TAN equilibrium (Henry's Law, ammonium dissociation) and movement in the soil due to convection and diffusion. The models also take into account environmental controls on soil surface to atmosphere transport of ammonia. Convection, diffusion and surface to atmosphere transport controls on trace gas emissions are neglected in the nitrogen dynamics models discussed in Section 2.4.

Rachhpal-Singh and Nye (1986) detail one of the earlier models that took a mechanistic approach to predicting ammonia volatilization following urea application. Processes simulated include urea hydrolysis, urea diffusion within the soil and diffusion of soil alkalinity. The model of Van Der Molen et al. (1990) simulates ammonia volatilization from arable land after cattle slurry application by simulating convection and diffusion of TAN in the soil and the atmospheric transfer from the soil surface. Géniermont and Cellier (1997) develop a mechanistic model of ammonia volatilization following slurry application to a bare soil that accounts for the transfers and equilibriums near the soil surface, between soil layers and between the soil and the atmosphere. PaSim is a process-based grassland model (Riedo et al., 2002) that takes the estimation of ammonia emissions one step further by incorporating bi-directional exchange. PaSim

differs from the other models in that it includes microbial processes in its theory development of equations of TAN dynamics, but because there is no simulation of these processes it appears that they are defined empirically. Temporal resolution in these models is only limited by the input data.

Integrated farm models look at all sources of ammonia emissions including housing, grazing, storage, and application. The model of Hutchings et al. (1995) takes a unique approach in that it is based on the underlying physical and chemical processes but also uses empirically based factors to reduce input data demand. One important assumption is that any upward movement of ammonium in the soil is ignored. The integrated process-based model of Pinder et al. (2004) also uses a process-based approach to ultimately develop emission factors for manure application on a per cow basis. It should be noted that temporal resolution in the integrated farm models is poor in that it starts with a daily scale.

2.6 Summary and Objectives

While there are many models capable of simulating all of the processes involved in soil nitrogen dynamics, a literature review showed that few of these models simulated nitrogen trace gas emissions and even fewer considered ammonia emissions. The poor temporal resolution in the models means that trace gas emissions are simulated using an empirical “leaky pipe” approach as opposed to a process-based approach. In general,

most of the models reviewed consider the major nitrogen processes to be mineralization and immobilization, nitrification, and denitrification. All of the inputs tend to relate to weather data (i.e. precipitation, solar radiation), soil data (i.e. clay content, water holding capacity), and agricultural practices (i.e. crop rotation, fertilization). There are also issues with temporal refinement in these models in that time steps are daily or are hourly but based on daily input data.

Models that did simulate ammonia volatilization using a process-based approach had the capability of high temporal resolution and were based on underlying chemical and physical processes. However, the models lacked inclusion of biological processes and consideration of other nitrogen trace gases. Decomposition processes can deplete TAN by converting it to organic nitrogen forms while mineralization can increase TAN by doing the reverse. Nitrification can deplete TAN through oxidation to nitrate while denitrification must be simulated to examine other nitrogen trace gas emissions. Sommer et al. (2003) suggest that some microbial processes such as mineralization and nitrification are slow enough not to influence ammonia emissions in the days following nitrogen application. However, the authors state that it can be difficult to assess the contribution of microbial activity to ammonia emissions, and limit their discussion to the 7 to 14 days following application. If a model is to be applied over a longer period of time the influence of these processes must be considered.

Based on the literature review, the research objectives are:

1. To develop a process-based model capable of predicting nitrogen trace gas emissions from bare soil following manure application with emphasis on ammonia emissions.
2. To develop a tool to facilitate a better understanding of the processes controlling agricultural nitrogen trace gas emissions by implementing higher temporal resolution, including the influence of soil physical processes on species transport and emission and including the influence of soil microbial processes on ammonia emissions.
3. To refine and validate the model with experimental data and sensitivity analyses.

3.0 MODEL DEVELOPMENT

3.1 Model Overview

AGRIN consists of five main submodels: soil heat and moisture, decomposition, nitrification, denitrification, and chemical species transport. These submodels simulate the major processes and influences on soil nitrogen transformations as well as the convection and diffusion of various species (H^+ , CO_2 , O_2 , NO_3^- , NO_2^- , NH_4^+ , NH_3 , N_2O , NO , N_2) movement through the soil profile. Figure 3-1 shows a schematic of how the submodels are linked while Table 3-1 summarizes each submodel. This chapter will detail the theory behind each submodel as well as list default model parameters.

General limitations of the model are that it is one-dimensional, does not simulate the crop canopy and does not incorporate snowmelt or the influence of freeze / thaw cycle(s) experienced in colder climates.

Figure 3-1: Schematic of AGRIN model.
Framework adapted from Scholtz et al. (2002a) and Li et al. (1992).

Table 3-1: Summary of AGRIN submodels and corresponding theory basis.

Submodel	Description	Input requirements	Theory based on
Soil heat and moisture	Calculates soil temperature and moisture profiles and soil water fluxes between nodes	<i>Meteorological data:</i> air temperature, dew point temperature, wind speed, net radiation (or incoming solar radiation and cloud cover), precipitation <i>Soil data:</i> water retention parameters, particle heat capacity, porosity	Clapp and Hornberger (1978); Li et al. (1992); Mahrt and Pan (1984); McCumber and Pielke (1981); Scholtz et al. (2002a)
Decomposition	Calculates decomposition in organic matter pools and net mineralization rates	<i>Soil data:</i> initial organic C profiles, clay content, any added organic matter, soil temperature profile, moisture profile, pH	Hansen et al. (1990); Li et al. (1992); Molina et al. (1983)
Nitrification	Calculates rate of oxidation of ammonium to nitrate; also determines anaerobic fraction of soil for substrate allocation	<i>Soil data:</i> dissolved organic C profile, temperature profile, moisture profile, pH profile, O ₂ profile	Arah and Vinten (1995); Blagodatsky and Richter (1998); Blagodatsky et al. (1998); Li (2000)
Denitrification	Calculates the rate of reduction of nitrate to dinitrogen gas by denitrifiers	<i>Soil data:</i> anaerobic fraction, moisture profile, temperature profile, dissolved organic carbon profile, pH profile	Leffelaar and Wessel (1988); Li et al. (1992)
Transport	Calculates species concentration profiles and N trace gas volatilization	<i>Soil data:</i> temperature profile, moisture profile, soil water flux profile, net mineralization rate, nitrification rate, denitrification rates <i>Application data:</i> density, rate, N species concentrations, pH, organic matter content, dry matter content, C:N ratio	Jury et al. (1983); Smith et al. (2000); Sommer and Olesen (2000); Van Der Molen (1990)

3.2 Soil Heat and Moisture

The soil heat and moisture submodel structure is based on Fayer (2000) which describes the theoretical development and implementation of the UNSAT-H model. While AGRIN follows UNSAT-H's structure concerning input requirements, heat and mass balance error, boundary conditions, time step convergence and solving technique, AGRIN's theoretical equations are developed based on various literature sources. The model also improves upon UNSAT-H's temporal resolution by simulating conditions based on hourly meteorological inputs of air temperature, dew point temperature, precipitation, wind speed and either net radiation or solar radiation and cloud cover. Soil inputs are based on soil texture class and include saturated water content, saturated hydraulic conductivity, saturation matric potential and volumetric heat capacity. The submodel yields soil temperature and moisture soil profiles and surface heat fluxes over time.

Table 3-2 summarizes the inputs, processes simulated and outputs.

Table 3-2: Soil heat and moisture submodel inputs, simulated processes and outputs		
Inputs	Processes Simulated	Outputs
Soil profile depth and node spacing	Soil water retention relationships	Surface heat fluxes
Hourly meteorological data	Surface energy balance	Soil water and heat fluxes at each node
Soil moisture and temperature profiles at end of previous time step	Soil water and heat storage	Soil moisture and temperature profiles at end of time step

3.2.1 Soil Moisture and Heat Transport

One-dimensional, transient equations are used to describe the transport of heat and moisture in soil. The partial differential equation describing the diffusion and convection of soil moisture is:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D_L(\theta) \frac{\partial \theta}{\partial z} - K_L(\theta) \right] \quad (3.1)$$

where θ is the soil volumetric moisture content, t is time, z is the depth below the soil surface which is positive downwards, D_L is the soil water diffusivity and K_L is the soil hydraulic conductivity. The equation is a common modified form of Richards' equation which assumes that the fluid is incompressible, the air phase is continuous, liquid water flow is isothermal and vapor flow is negligible (Fayer, 2000).

The equation describing the diffusion of soil heat is:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left[\frac{k_H(\theta)}{C_{ps}(\theta)} \frac{\partial T}{\partial z} \right] \quad (3.2)$$

where T is the soil temperature, k_H is the soil thermal conductivity as a function of soil water content and C_{ps} is the soil volumetric heat capacity as a function of soil water content. The equation assumes several heat processes to be negligible: convective transfer of latent heat of melting ice by liquid water, convective transfer of sensible heat by soil gas phase, heat transfer by radiation and heat of wetting effects (Fayer, 2000).

3.2.2 Soil Properties

The soil's hydraulic conductivity and liquid water diffusivity are calculated from Clapp and Hornberger's (1978) empirical relationships. The hydraulic conductivity is calculated as:

$$K_L(\theta) = K_s \left(\frac{\theta}{\theta_s} \right)^{2b+3} \quad (3.3)$$

where K_s is the soil's saturated hydraulic conductivity, θ_s is the soil's saturated moisture content and b is a soil constant found by plotting the soil water retention curve. The liquid water diffusivity is calculated as:

$$D_L(\theta) = \frac{bK_s\psi_s}{\theta_s} \left(\frac{\theta}{\theta_s} \right)^{b+3} \quad (3.4)$$

where ψ_s is the soil's saturation matric potential. While the soil moisture content is simulated by the model, the other values are input by the user. Typical values can be found in Table 3-3 which contains the soil properties based on soil texture class.

The soil thermal conductivity equation applied comes from Campbell (1985) which uses an equation from McInnes (1981) to model the variable as a function of the soil's moisture content:

$$k_H(\theta) = A + B\theta - (A - D)\exp[-(C\theta)^4] \quad (3.5)$$

where A , B , C and D are curve fitting coefficients found by:

$$A = 0.65 - 0.78\rho_b + 0.60\rho_b^2 \quad (3.6)$$

$$B = 1.06\rho_b\theta \quad (3.7)$$

$$C = 1 + 1.26X_c^{-0.5} \quad (3.8)$$

$$D = 0.03 + 0.1\rho_b^2 \quad (3.9)$$

where ρ_b is the soil's bulk density and X_c is the soil's clay fraction. Both of these values are provided by the user in the input file, but typical clay fractions are presented as percentages in Table 3-3. Equation 3.5 gives the thermal conductivity in units of $\text{J s}^{-1} \text{m}^{-1} \text{K}^{-1}$. The volumetric heat capacity is from Campbell (1985):

$$C_{ps} = (1 - \eta)C_{p,part} + \theta C_{pw} \quad (3.10)$$

where η is the void fraction or porosity and $C_{p,part}$ and C_{pw} are the volumetric specific heats of soil particulates and water respectively. The soil's porosity is assumed to equal the saturated moisture content while $C_{p,part}$ is defined by the user in the input file but a typical value for mineral soils is 2.39 J cm^{-3} (Campbell, 1985 after de Vries, 1963).

3.2.3 Boundary Conditions

Surface heat and moisture fluxes are the upper boundary conditions to the partial differential equations of transport. If there is precipitation then the soil surface moisture flux is set equal to the rainfall rate, otherwise evaporation is the upper boundary condition and is calculated based on an integrated form of Fick's law of diffusion (Fayer, 2000 based on Campbell, 1977):

$$E = \frac{-(\rho_{vss} - \rho_{va})}{\rho_w r_v} \quad (3.11)$$

where E is the soil evaporation flux, ρ_{vss} is the vapour density at the soil surface, ρ_{va} is the atmospheric vapour density, ρ_w is the density of water and r_v is the resistance to vapour transport. The negative sign follows sign convention that positive flux is downward.

Table 3-3: Typical soil properties based on texture class.

Texture Class	Saturated Water Content θ_s (cm ³ cm ⁻³)	Saturated Hydraulic Conductivity K_s (cm h ⁻¹)	Soil Constant b	Saturation Matric Potential ψ_s (m)	Clay content X_c (%)
Sand	0.395	63.4	4.05	0.121	3
Loamy sand	0.410	56.3	4.38	0.090	6
Sandy loam	0.435	12.5	4.9	0.218	9
Silt loam	0.485	2.6	5.3	0.786	14
Loam	0.451	2.5	5.39	0.478	19
Sandy clay loam	0.420	2.3	7.12	0.299	28
Silty clay loam	0.477	0.6	7.75	0.356	34
Clay loam	0.476	0.9	8.52	0.63	34
Sandy clay	0.426	0.8	10.4	0.153	43
Silty clay	0.492	0.4	10.4	0.49	49
Clay	0.482	0.5	11.4	0.405	63

All values from Li et al. (1992) based on Clapp and Hornberger (1978).

The atmospheric vapour density is calculated as a function of the dew point temperature using a modified empirical relationship from Doorenbos and Pruitt (1977):

$$\rho_{va} = \exp \left(46.440973 - \frac{6790.4985}{T_{dew}} - 6.02808 \ln T_{dew} \right) \quad (3.12)$$

Calculation of the soil surface vapour density requires the saturated surface vapour density and relative humidity values. The saturated vapour density is calculated using:

$$\rho_{vss} = RH\rho_{vsat} \quad (3.13)$$

where RH is the relative humidity at the soil surface and ρ_{vsat} is the saturated vapour density at the soil surface. The relative humidity is calculated following Campbell (1985):

$$RH = \exp\left(\frac{-h_l M_w}{RT_l}\right) \quad (3.14)$$

where

$$h_l = \psi_s \left(\frac{\theta}{\theta_s}\right)^{-b} \quad (3.15)$$

where h_l is the soil surface matric potential, M_w is the molecular weight of water, R is the gas constant and T_l is the soil surface temperature.

The resistance to vapour transport, r_v , is the sum of the turbulent layer, laminar boundary sub-layer and surface resistances. The laminar boundary sub-layer resistance, r_b , is from Sommer and Olesen (2000) where an empirical relationship by Thom (1972) is used:

$$r_b = 6.2u^{*(-0.67)} \quad (3.16)$$

The surface resistance, r_c , is calculated based on Ács (2003) following Sun (1982):

$$r_c = 30 + 3.5 \left(\theta_s / \theta \right)^{2.3} \quad (3.17)$$

The turbulent layer resistance, r_a , is assumed to equal that for heat transport and is calculated following Campbell (1985) and Campbell (1977):

$$r_a = \frac{\ln \left[\frac{(z_T - d + z_h)}{z_h} \right] + \Psi_h}{\kappa u^*} \quad (3.18)$$

where z_T is the height above the surface at which temperature is measured, d is the zero plane displacement, z_h is a surface roughness parameter for heat, κ is von Karman's constant, u^* is the friction velocity and Ψ_h is a stability correction factor for heat. The z_T , d and z_h values depend on the site conditions and are input by the user. The friction velocity is found by:

$$u^* = \frac{\kappa u}{\ln \left[\frac{(z_u - d + z_m)}{z_m} \right] + \Psi_m} \quad (3.19)$$

where u is the mean wind speed measured at height z_u , z_m is a surface roughness parameter for momentum and Ψ_m is a stability correction factor for momentum.

This leaves the stability correction factors which account for the effects of atmospheric stability on mixing. The stability parameter ζ is used by Campbell (1985) to quantify the relative importance of thermal and mechanical turbulence in boundary layer transport:

$$\zeta = \frac{-\kappa z_T g H}{C_{ha} T_a u_*^3} \quad (3.20)$$

where H is the sensible heat flux in the boundary layer, C_{ha} is the volumetric heat capacity of air and T_a is the air temperature at z_T . The sensible heat flux at the soil surface is calculated as:

$$H = \frac{C_{ha}(T_l - T_a)}{r_a} \quad (3.21)$$

The stability parameter is used to calculate the stability correction factors and the relationships for the different stability conditions found in Campbell (1985) are based on Businger (1975). When the soil surface temperature is cooler than the air temperature (stable conditions) the factors are given by:

$$\Psi_m = \Psi_h = 4.7\zeta \quad (3.22)$$

When the soil surface temperature is higher than the air temperature (unstable conditions) the factors are given by:

$$\Psi_h = -2 \ln \left[\frac{1 + (1 - 16\zeta)^{0.5}}{2} \right] \quad (3.23)$$

$$\Psi_m = 0.6\Psi_h \quad (3.24)$$

Solving for the boundary layer resistance requires an iterative procedure because calculation of the sensible heat flux requires the boundary layer resistance while the resistance calculation requires the heat flux.

The upper boundary condition for soil heat transport is the soil heat flux, G , found by solving the surface heat balance:

$$G = R_n - H - LE \quad (3.25)$$

where R_n is the net radiation, H is the sensible heat flux and LE is the latent heat flux. The sensible heat calculation has already been described while the latent heat flux is simply the product of the rate of evaporation, E , from Equation 3.11 and the latent heat of vapourization, LHV . The net radiation is either supplied as hourly inputs by the user or is calculated based on hourly solar radiation and cloud cover data provided by the user. For the latter case, net radiation is calculated following Campbell (1985):

$$R_n = (1 - \alpha_s)S_t + \varepsilon_a \sigma T_a^4 - \varepsilon_s \sigma T_l^4 \quad (3.26)$$

where α_s is the surface albedo, S_t is the measured solar radiation, ε_a is the atmospheric emissivity, σ is the Stephan-Boltzmann constant and ε_s is the soil emissivity. Similar to Fayer (2000), the change in surface albedo includes the relationship with surface drying found in van Bavel and Hillel (1976):

$$\alpha_s = 0.1 + (0.25 - \theta_l) \quad (3.27)$$

where θ_l is the surface moisture content. Clear sky atmospheric emissivity is calculated based on Campbell (1985) after Brutsaert (1975):

$$\varepsilon_a = 4.174 \rho_{va}^{1/7} \quad (3.28)$$

For cloudy skies, an equation from Unsworth and Monteith (1975) is used to calculate the emissivity:

$$\varepsilon_{ac} = (1 - 0.84c)\varepsilon_a + 0.84c \quad (3.29)$$

where c is the fractional cloud cover.

For soil moisture transport the lower boundary condition is a unit hydraulic gradient such that diffusion of moisture becomes negligible ($\partial\theta/\partial z = 0$). For soil heat transport the soil temperature is assumed to be constant at the deepest node.

3.2.4 Slurry Infiltration

When slurry application occurs at the soil surface the slurry layer is modelled as a separate surface layer and slurry infiltration becomes the upper boundary condition for the upper soil layer. The infiltration rate is based on Philip's Two-Term Model (Philip, 1957) described by Williams et al. (1998):

$$I_s = \mu_{vixc} \left(0.5S(t)^{-0.5} + AK_s \right) \quad (3.30)$$

where I_s is the slurry infiltration rate, S is the sorptivity, A is a soil constant and μ_{visc} is the reduction on infiltration due to slurry viscosity (Sommer and Olesen, 1991). The sorptivity is assumed to equal 0.5 based on Philip (1969) and the soil constant A is assumed to equal 0.363 based on Philip (1974). This infiltration rate is constrained by the amount of water available at the surface such that the infiltration cannot surpass the difference between the water applied and evaporative losses over the time step.

While application timing is governed by the application rate, the model averages the infiltration over the entire field.

3.2.5 Numerical Simulation of Soil Moisture

The Richards' equation used to describe soil moisture transport is solved numerically using the finite difference method which has also been used frequently by other models (i.e. Fayer, 2000; Warrick, 2000). The finite difference approximation applied is adopted from Warrick (2000). Equation 3.1 is rearranged to solve for soil moisture content at the end of each time step by forming a system of equations:

$$A_i \theta_{i-1}^j + B_i \theta_i^j + C_i \theta_{i+1}^j = D_i \quad i = 1, \dots, n \quad (3.31)$$

where i represents the node, n represents the bottom node and j represents the time step. The general equation form and coefficients are modified based on the nodes being considered (surface, interior or lower).

For interior nodes ($i = 2, \dots, n-1$) and the coefficients are calculated as:

$$\begin{aligned}
A_i &= \frac{-D_{L,i-0.5}^j}{\Delta z_i(z_i - z_{i-1})} \\
B_i &= \frac{1}{\Delta t} + \frac{1}{\Delta z_i} \left[\frac{D_{L,i+0.5}^j}{(z_{i+1} - z_i)} + \frac{D_{L,i-0.5}^j}{(z_i - z_{i-1})} \right] \\
C_i &= \frac{-D_{L,i+0.5}^j}{\Delta z_i(z_{i+1} - z_i)} \\
D_i &= \frac{\theta_i^{j-1}}{\Delta t} - \frac{1}{\Delta z_i} \left[K_{L,i+0.5}^j - K_{L,i-0.5}^j \right]
\end{aligned} \tag{3.32}$$

where Δz_i is the node thickness and $i+0.5$ and $i-0.5$ indicate internodal values. The model calculates the internodal values as arithmetic averages such that:

$$\begin{aligned}
D_{L,i+0.5} &= 0.5(D_{L,i+1} + D_{L,i}) \\
D_{L,i-0.5} &= 0.5(D_{L,i} + D_{L,i-1})
\end{aligned} \tag{3.33}$$

The same arithmetic averaging is used for internodal hydraulic conductivities.

For the surface boundary node ($i = 1$), the surface boundary condition is a flux based on the surface moisture and meteorological conditions which determine whether there is infiltration or evaporation. The coefficients become:

$$A_1 = 0$$

$$B_1 = \frac{1}{\Delta t} + \frac{D_{L,1.5}^j}{\Delta z_1(z_2 - z_1)} \quad (3.34)$$

$$C_1 = \frac{-D_{L,1.5}^j}{\Delta z_1(z_2 - z_1)}$$

$$D_1 = \frac{\theta_1^{j-1}}{\Delta t} - \frac{1}{\Delta z_1} [K_{L,1.5}^j - q_{L,1}^j]$$

where $q_{L,1}$ is the surface flux term which is evaporation or the difference between infiltration and evaporation. Infiltration is set equal to the precipitation rate.

For the lower boundary node ($i = n$), the unit hydraulic gradient approach is taken ($\partial\theta/\partial z = 0$). The coefficients become:

$$\begin{aligned} A_n &= \frac{-D_{L,n-0.5}^j}{\Delta z_n(z_n - z_{n-1})} \\ B_n &= \frac{1}{\Delta t} + \frac{D_{L,n-0.5}^j}{\Delta z_n(z_n - z_{n-1})} \\ C_n &= 0 \end{aligned} \quad (3.35)$$

$$D_n = \frac{\theta_n^{j-1}}{\Delta t} - \frac{1}{\Delta z_n} [q_{L,n}^j - K_{L,n-0.5}^j]$$

where $q_{L,n}$ is the bottom flux and is taken to be the hydraulic conductivity of the last node.

The system of equations forms a linear tri-diagonal matrix which can be solved using the Thomas algorithm described by von Rosenberg (1969). A mass balance error is calculated by examining the moisture flux conditions at the lower and upper boundaries and the change in soil moisture storage over the time step. The moisture storage, S_w , is given by:

$$S_w = \theta_1 \left(\frac{z_2 - z_1}{2} \right) + \theta_n \left(\frac{z_n - z_{n-1}}{2} \right) + \sum_{i=2}^{n-1} \theta_i \left(\frac{z_{i+1} - z_{i-1}}{2} \right) \quad (3.36)$$

The mass balance error, MBE , is then calculated as:

$$MBE^j = q_{L,1}^j \Delta t - q_{L,n}^j \Delta t - (S_w^j - S_w^{j-1}) \quad (3.37)$$

3.2.6 Numerical Simulation of Soil Heat

The numerical implementation of the soil heat transport equation is a similar approach to that taken for moisture. The partial differential equation (Equation 3.2) is rearranged to solve for temperature at the end of each time step by forming a system of equations:

$$A_i T_{i-1}^j + B_i T_i^j + C_i T_{i+1}^j = D_i \quad i = 1, \dots, n \quad (3.38)$$

For interior nodes ($i = 2, \dots, n-1$) the coefficients for the solution are:

$$\begin{aligned}
A_i &= \frac{-k_{H,i-0.5}^j}{\Delta z_i(z_i - z_{i-1})} \\
B_i &= \frac{C_{ps,i}^j}{\Delta t} + \frac{1}{\Delta z_i} \left[\frac{k_{H,i+0.5}^j}{(z_{i+1} - z_i)} + \frac{k_{H,i-0.5}^j}{(z_i - z_{i-1})} \right] \\
C_i &= \frac{-k_{H,i+0.5}^j}{\Delta z_i(z_{i+1} - z_i)} \\
D_i &= \frac{C_{ps,i}^j T_i^{j-1}}{\Delta t}
\end{aligned} \tag{3.39}$$

The soil thermal conductivity between nodes is calculated as an arithmetic average was done for internodal soil water diffusivity and hydraulic conductivity.

For the surface boundary node ($i = 1$), the surface boundary condition is the soil heat flux through surface node using calculated as G in the surface energy balance from Equation 3.25. The coefficients for the surface node solution are:

$$\begin{aligned}
A_1 &= 0 \\
B_1 &= \frac{C_{ps,1}^j}{\Delta t} + \frac{k_{H,1.5}^j}{\Delta z_1(z_2 - z_1)} \\
C_1 &= \frac{-k_{H,1.5}^j}{\Delta z_1(z_2 - z_1)} \\
D_1 &= \frac{C_{ps,1}^j T_1^{j-1}}{\Delta t} + \frac{G^j}{\Delta z_1}
\end{aligned} \tag{3.40}$$

For the lower boundary node ($i = n$), a constant temperature is specified and the following equation is used for node n :

$$A_{n-1}T_{n-2}^j + B_{n-1}T_{n-1}^j = D_{n-1} - C_{n-1}T_n^j \quad (3.41)$$

Similar to soil moisture, the system of equations forms a linear tri-diagonal matrix which can be solved using the Thomas algorithm described by von Rosenberg (1969). A heat balance error is calculated by examining the heat flux conditions at the lower and upper boundaries and the change in soil heat storage over the time step. The soil heat storage is given by:

$$S_h = C_{ps,1}(T_1 - T_0)\left(\frac{z_2 - z_1}{2}\right) + C_{ps,n}(T_n - T_0)\left(\frac{z_n - z_{n-1}}{2}\right) + \sum_{i=2}^{n-1} C_{ps,i}(T_i - T_0)\left(\frac{z_{i+1} - z_{i-1}}{2}\right) \quad (3.42)$$

The heat balance error, HBE , is given by:

$$HBE^j = G^j \Delta t - q_{h,n}^j \Delta t - (S_h^j - S_h^{j-1}) \quad (3.43)$$

where $q_{h,n}$ is the heat flow at the lower boundary calculated as:

$$q_{h,n} = q_{h,n-1} = \frac{k_{H,n-1}(T_n - T_{n-1})}{z_n - z_{n-1}} \quad (3.44)$$

3.3 Decomposition

The decomposition submodel simulates decomposition including the mineralization/immobilization of nitrogen. The theory is based on NCSOIL described by Molina et al. (1983) which was also used to develop DNDC's decomposition submodel. Based on profiles of soil temperature, water content and substrate concentration, the model calculates carbon and nitrogen flows between organic matter pools. It is assumed that N₂ fixation is a negligible source of organic nitrogen in agricultural soils and, since there is insufficient understanding of fixation mechanisms (Smith, 1982), the process is not modelled. Table 3-4 lists the inputs, simulated processes and outputs.

Table 3-4: Decomposition submodel inputs, simulated processes and outputs

Inputs	Processes Simulated	Outputs
Soil temperature and moisture profile	Decomposition of soil organic matter and subsequent C and N flows between pools	Soil organic carbon and residue profiles at end of time step
Soil ammonium, nitrate, nitrite profiles	Net mineralization of N	
Soil organic carbon and residue profiles from previous time step	CO ₂ production	Organic N profile at end of time step
Organic C from any added organic material		Net mineralization rate
Option: C:N, decomposition rates of any added organic material		

3.3.1 Organic Matter Pool Transformations

The model of decomposition and carbon and nitrogen flows is based on NCSOIL's (Molina et al., 1983) three major organic matter pools: the organic residues, microbial

biomass and humads pools which are each divided into labile and resistant fractions. The model structure is shown in Figure 3-2 where carbon flow partitioning between pools is

Figure 3-2: Organic matter pools and C, N flows. Partitioning based on Li (1992) and Molina et al. (1983).

noted as fractions. Each of the pools decomposes following first-order kinetics. The microbial biomass receives all of the decomposition products from the residue pool and a

fraction from itself as well as the humads pools. The humads pools receive the decomposition products from the microbial biomass which are not recycled. A fourth passive pool exists to receive a portion of the decomposed products from the humads pool. However, the turnover time is considered long enough (when considering the growing season only) such that decomposition in this passive pool can be neglected.

Molina et al. (1983) describe the rate of decomposition for each major pool as:

$$\frac{dC}{dt} = \mu_{dec} [Sk_{dec}C + (1-S)h_{dec}C] \quad (3.45)$$

where C is the carbon concentration of the substrate at time t , S and $(1-S)$ are the labile and resistant proportions, and k and h are the rates of decomposition for each component at standard conditions (optimum water and temperature, no clay content). In the above equation, μ_{dec} is a reduction factor for decomposition that accounts for the influence of soil temperature, soil water and clay content on soil organic matter movement. The decomposition rates and labile and resistant fractions are based on literature values found in Table 3-5.

Hansen et al. (1990) state that the influence of clay content on decomposition can be described by the function:

$$\begin{aligned} \mu_c &= 1 - 0.02X_c & \text{for } 0 < X_c \leq 0.25 \\ \mu_c &= 0.995 & \text{for } X_c > 0.25 \end{aligned} \quad (3.46)$$

where X_c is the fractional soil clay content. It is assumed that clay content only affects the humads pools and the resistant component of the microbial biomass (i.e. $\mu_c = 1$ for all

other pools). The effect of temperature on microbial activity is simulated using reduction factors from Li et al. (1992) based on Nyhan (1976):

$$\begin{aligned}
 \mu_T &= 0 & \text{for } T \leq 0 \\
 \mu_T &= 0.033T & \text{for } 0 < T \leq 30 \\
 \mu_T &= 1.0 & \text{for } 30 < T \leq 40 \\
 \mu_T &= -0.04T + 2.6 & \text{for } 40 < T
 \end{aligned} \tag{3.47}$$

Note that the temperature is in degrees Celsius. The model also follows the Li et al. (1992) model of soil water correction based on Clay et al. (1985):

$$\begin{aligned}
 \mu_W &= 0 & \text{for } (\theta/\eta) \leq 0.1 \\
 \mu_W &= 2\left(\frac{\theta}{\eta}\right) - 0.2 & \text{for } 0.1 < (\theta/\eta) < 0.6 \\
 \mu_W &= 1.0 & \text{for } \theta/\eta = 0.6 \\
 \mu_W &= -2.5\left(\frac{\theta}{\eta}\right) + 2.5 & \text{for } 0.6 < \theta/\eta \leq 0.8 \\
 \mu_W &= -0.5\left(\frac{\theta}{\eta}\right) + 0.9 & \text{for } 0.8 < \theta/\eta
 \end{aligned} \tag{3.48}$$

These equations indicate that decomposition is reduced at saturated conditions and ceases at completely dry conditions.

As Figure 3-2 shows, decomposition of organic C in the residue pools results in C respired as CO₂ or transferred to the microbial biomass pool. The amount of carbon respired as CO₂ is determined by the efficiency of the microbial biomass (Li et al., 1992) and the decomposed products entering the microbial biomass pools are then divided into the labile and resistant fractions. Partitioning of carbon flows is based on Li et al. (1992). As the residue pools decompose, 40% of the carbon is respired as CO₂ and 60% flows

into the biomass pools. As the microbial biomass pools decompose, 20% of the carbon is respired as CO₂, 60% is recycled into the biomass pools, and 20% flows into the resistant humads pool (Gilmour et al., 1985; Molina et al., 1983). As the humads pool decompose, 40% of the carbon produced flows into the passive humus pool, 40% is respired as CO₂ and 20% is recycled into the microbial biomass.

3.3.2 Mineralization and Immobilization

Nitrogen behaviour is closely linked to carbon flows during decomposition through C:N ratios. All N associated with organic C lost to CO₂ is mineralized to NH₄⁺ and then consideration is given to mineralization/immobilization depending on the C flows between the pools and the associated C:N ratios. For example, if there is C flow from a low C:N pool to a high C:N pool, there will be excess N in the receiving pool such that N mineralization (organic N to NH₄⁺) occurs. If the reverse occurs, there will not be enough N available and immobilization (NH₄⁺ to organic N) occurs. Immobilization may not be able to provide enough N if there is not enough available inorganic N. If this is the case, the C flow is reduced. The net mineralization of N in each pool, R_{min} , can be described by:

$$R_{min} = -\frac{\frac{dC}{dt}}{(C:N)}$$

As this represents a net mineralization, a negative value indicates immobilization.

3.3.3 Parameterization

The decomposition module requires many parameters that typical site data will not include. Based on a literature review of current soil organic matter models, values were parameterized according to Table 3-5. While initial residue and soil organic carbon (SOC) are usually provided in a soil analysis, the partitioning of the soil organic carbon amongst the organic matter pools is not. Thus, soil organic carbon is partitioned based on Parton et al. (1987).

In discussion of residue pool it is assumed the pool is mainly composed of plant residue, however any added organic matter (i.e. manure) can also be considered residue matter. This material will still follow residue pool behaviour but will have different properties such as C:N ratio and decomposition rates which are assumed to dominate the properties of any plant residues in the surface layer. Table 3-6 shows how values for the residue pool might change if different plant residues were present or slurry application occurred. The user may want to apply residue decomposition parameters other than the default values. There is the option to include user-defined values relating to the residue pool.

Table 3-5: Decomposition default parameters

Parameter	Value	Source
Labile fraction of residue pool, S^a	0.4	Gilmour et al. (1985)
Resistant fraction of residue pool, $1-S^a$	0.6	Gilmour et al. (1985)
Labile fraction of biomass pool, S_{bio}	0.9	Gilmour et al. (1985)
Resistant fraction of biomass pool, $1-S_{bio}$	0.1	Gilmour et al. (1985)
Labile fraction of humads pool, S_{hum}	0.16	Molina et al. (1983)
Resistant fraction of humads pool, $1-S_{hum}$	0.84	Molina et al. (1983)
Specific decomposition rate for labile fraction of residue pool, k_{res}	0.00185 d ⁻¹	Gilmour et al. (1985)
Specific decomposition rate for resistant fraction of residue pool, h_{res}	0.0005 d ⁻¹	Gilmour et al. (1985)
Specific decomposition rate for labile fraction of biomass pool, k_{bio}	0.00825 d ⁻¹	Molina et al. (1983)
Specific decomposition rate for resistant fraction of biomass pool, h_{bio}	0.001 d ⁻¹	Molina et al. (1983)
Specific decomposition rate for labile fraction of humads pool, k_{hum}	0.004 d ⁻¹	Molina et al. (1983)
Specific decomposition rate for resistant fraction of humads pool, h_{hum}	0.00015 d ⁻¹	Molina et al. (1983)
Fraction of total SOC allocated to biomass pool, F_{bio}	0.03	Colorado State University (2005)
Fraction of total SOC allocated to humads pool, F_{hum}	0.47	Colorado State University (2005)
Fraction of total SOC allocated to passive humus pool, F_{pass}	0.5	Colorado State University (2005)
C:N ratio of residue pool, CN_{res}	20	Gilmour et al. (1985)
C:N ratio of biomass pool, CN_{bio}	8	Knapp et al. (1983)
C:N ratio of humads pool, CN_{hum}	8	Stevenson (1982)

All values from Li et al. (1992) except SOC fractions.

Table 3-6: Plant residue and added organic matter properties

Added Organic Matter	k (d⁻¹)	h (d⁻¹)	S	$1-S$	$C:N$
Grass ^a	0.005	0.0005	0.6	0.4	80
Straw ^a	0.1	0.01	0.55	0.45	80
Pig slurry ^a	0.1	0.005	0	1	80
Barley straw ^b	default value	default value	0.06	0.94	72
Blue grass ^b	default value	default value	0.12	0.88	22
Maize ^b	default value	default value	0.23	0.77	32

^aHansen et al. (1990) based on Lind et al. (1990)

^bMueller et al. (1997,1998)

3.3.4 Slurry Application Considerations

If slurry application occurs, the rate of organic carbon added is determined from the manure's organic matter content and application rate:

$$I_c = \frac{OM\rho_s R_{appn}\Delta t}{\Delta z_i} \quad (3.49)$$

where I_c is the amount of organic C added, OM is the slurry's organic matter content, ρ_s is density of the slurry and R_{appn} is the rate of application. This organic carbon addition is assumed to take place at the surface node.

3.3.5 Numerical Simulation

Before decomposition can be simulated, the carbon and nitrogen profiles are initialized based on input data. Values of initial residue C, soil organic C, nitrate, ammonium, nitrite, uniform surface depth and concentration gradients are used to derive profiles. Carbon and nitrogen profiles are assumed to be uniform to a user-specified depth after which the concentrations are calculated based on user-specified gradients. The following equations illustrate initial profile development:

$$\begin{aligned} X_i &= X_{init} & \text{for } 0 \leq z < z_{sur} \\ X_i &= X_{i-1} + X_{rate} \Delta z_i & \text{for } z \geq z_{sur} \end{aligned} \quad (3.50)$$

where X_i is the concentration of the species (i.e. nitrate) at node i , z is the depth below the soil surface, X_{init} is the initial concentration specified in the input file, z_{sur} is the specified uniform surface depth, X_{rate} is the rate of increase or decrease of the species within the profile and Δz_i is the thickness of the node layer.

The movement of carbon throughout the organic matter pools and soil profile is simulated through the implementation of the decomposition equation. The equation is integrated and rearranged to solve for the carbon concentration in each pool at each node at time t :

$$C_i^j = C_i^{j-1} S_i^j e^{-\mu k \Delta t} + C_i^{j-1} (1 - S_i^j) e^{-\mu h \Delta t} + I_{c,i} \quad (3.51)$$

where i denotes the node, C is the carbon concentration at end of time step j or previous time step $j-1$ and I_c is organic input either from added organic matter to the residue pool or from other pools as would be the case for the biomass and humads pools. The rest of the variables (S , μ , k , h) have been previously described. The decomposed or decayed portion is then allocated to CO_2 production (with the corresponding organic N mineralized as NH_4^+) and other pools. The incoming organic C and N are used to determine whether mineralization or immobilization will occur in the receiving pool based on that pool's C:N ratio. It is assumed that organic N is mineralized to NH_4^+ and that immobilization of NH_4^+ is preferred over NO_3^- .

At the end of each time step the CO₂, organic C (biomass, humads, and passive humus) and residue C profiles are generated. The CO₂ at each node is the sum of the CO₂ produced by each pool and the SOC profile is a sum of the carbon available in each pool. The residue profile is simply the residue carbon concentration at each node (C_{res}). Based on Li et al. (1992), the soluble or dissolved organic carbon (DOC) profile is based on the carbon produced from microbial biomass and humads decomposition that is recycled into the microbial biomass (see Figure 3-2). The changes in organic and inorganic nitrogen concentrations due to net mineralization are also considered at each node. The organic nitrogen concentration at the end of the time step is determined by dividing the organic carbon in each pool by the pool's C:N ratio. The change in inorganic nitrogen concentrations is set equal to the total net mineralization at that node.

3.4 Nitrification

In addition to net mineralization, ammonium can undergo nitrification which is the oxidation to nitrite and nitrate under aerobic conditions. The nitrification submodel calculates the NO₃⁻ produced by nitrification as a function of soil temperature, redox status, moisture status, pH, nitrifier biomass dynamics and substrate concentrations. Outputs include nitrate production and N trace gas production (N₂O, NO) resulting from nitrification. Table 3-7 summarizes the submodel.

Table 3-7: Nitrification submodel inputs, simulated processes and outputs

Inputs	Processes Simulated	Outputs
Soil aqueous ammonium profile	Soil aeration status	Soil anaerobic fraction
Soil temperature and moisture profiles	Substrate allocation to nitrification	Nitrification rate
Soil DOC profile	Nitrifier biomass dynamics	Nitrifier biomass profile at end of time step
Soil O ₂ profile	Nitrification rate	NO and N ₂ O gas production from nitrification
Soil pH profile	NO and N ₂ O gas production	
Nitrifier biomass profile from previous time step		

3.4.1 Anaerobic Soil Fraction

An aerobic soil can still have anaerobic microsites that cannot support processes such as nitrification. AGRIN simulates the soil redox status to determine the anaerobic fraction of the soil which will govern allocation of substrates to nitrification and denitrification. The model assumes that the soil redox status is dominated by oxygen since it is the reducing species which possesses the lowest Gibbs free energy change to accept electrons (Li and Aber, 2000). AGRIN models oxygen concentrations by applying Fick's Law and the continuity principle outlined in Section 3.6 which details theory behind simulating species transport.

Based on the soil's oxygen profile, soil anaerobicity can be modelled to simulate the anaerobic fraction where nitrification cannot occur (and denitrification does occur). This concept has not been explicitly modelled in many existing process models of N trace

gas emissions. Arah and Vinten (1995) developed simplified models of anaerobicity based on two complex models. The first model is based on physical aggregates and Michaelis-Menten kinetics (Arah and Smith, 1989) while the second model assumes a random distribution of cylindrical air-filled pores, uniform metabolic activity and zero-order reaction kinetics (Rijtema and Kroes, 1991). AGRIN bases its anaerobic fraction calculation on Arah and Vinten's (1995) functional approximation of the simple-structure model since it does not require knowledge of a soil's intra-aggregate conditions. The soil anaerobic fraction is calculated as:

$$\Phi = \exp\left(-a' r_{\psi}^{-\alpha} R_{O_2}^{-\beta} [O_2]^{\gamma} [\theta + a\chi]^{\delta}\right) \quad (3.52)$$

where Φ is the anaerobic soil fraction, r_{ψ} is the radius of typical air-filled pore at moisture tension ψ , R_{O_2} is the oxygen reaction potential in the soil, and χ is the ratio between the oxygen diffusion coefficient in air and the oxygen diffusion coefficient in water. The oxygen concentration is the molar concentration in mol m^{-3} . The parameters a' , α , β , γ and δ are curve fitting parameters. Table 3-8 lists the default parameter values used in the submodel. AGRIN's anaerobic fraction controls substrate allocation similar to the postulated "anaerobic balloon" of Li and Aber (2000). Nitrification is only allowed to occur outside of the anaerobic fraction such that as the balloon swells less substrates will be allocated for nitrification and more will be allocated as the balloon shrinks.

3.4.2 Nitrifier Biomass and Nitrification Rate

The main approach to modelling nitrification rates has been through the application of first-order Michaelis-Menten kinetics and/or the Monod growth curve. As discussed in the Section 2.0, the factors influencing the nitrification rate are soil redox status, moisture, temperature, substrate concentration and pH. Few models consider each of these factors and AGRIN attempts to model nitrification rates and nitrifier biomass using Monod-Michaelis-Menten kinetics while accounting for all influencing factors. Note that soil redox status is addressed by only allowing nitrification to occur in the aerobic fraction of the soil.

Nitrifier dynamics control the nitrification rate and are governed by the growth and death rates of the nitrifying microorganisms. AGRIN models the nitrifier dynamics following Li (2000) where growth and death rates are based on Monod kinetics proposed by Blagodatsky and Richter (1998). The relative growth rate of the nitrifiers is modelled as:

$$G_{nit} = \mu_{max,nit} \left[\frac{[DOC]}{1+[DOC]} + \frac{\mu_w}{1+\mu_w} \right] \quad (3.53)$$

where G_{nit} is the growth rate, $\mu_{max,nit}$ is the maximum growth rate for nitrifiers (see Table 3-8), DOC is the dissolved organic carbon concentration outside of the anaerobic balloon, and μ_w is the moisture factor. The relative death rate of nitrifiers is:

$$D_{nit} = a_{max,nit} \left[\frac{B_{nit}/(5+[DOC])}{1+\mu_w} \right] \quad (3.54)$$

where D_{nit} is the death rate, B_{nit} is the nitrifier biomass and a_{max} is the maximum death rate for nitrifiers (see Table 3-8). The net increase in nitrifiers biomass is then calculated using the growth and death rates:

$$\frac{dB_{nit}}{dt} = (G_{nit} - D_{nit})B_{nit}\mu_w\mu_T \quad (3.55)$$

where μ_T is the temperature factor.

It is widely accepted that nitrification increases with temperature and Li (2000) use a temperature function based on various experimental observations. AGRIN adopts the following function based on an optimum temperature of 35°C and exponential increase in the range 15° to 35°C:

$$\mu_T = 3.503^{((60-T)/25.78)} e^{3.503((T-34.22)/25.78)} \quad (3.56)$$

where T is the soil temperature in degrees Celsius. Li (2000) also applies a moisture function based on various observations (Anderson and Levine, 1986; Davidson, 1991; Martin et al., 1998) indicating that moisture only has a moderate effect unless the soil is extremely dry:

$$\begin{aligned} \mu_w &= 0.8 + 0.21(1.0 - \theta) & \text{if } \theta > 0.05 \\ \mu_w &= 0 & \text{if } \theta \leq 0.05 \end{aligned} \quad (3.57)$$

AGRIN assumes that nitrification is a single-step process following first-order reaction kinetics. Based on Li (2000) the nitrification rate is modelled as:

$$R_{nit} = k_{nit}[NH_4^+]_l B_{nit} pH \quad (3.58)$$

where R_{nit} is the nitrification rate, $[NH_4^+]_l$ is the concentration of aqueous ammonium in the soil allocated to the area outside of the anaerobic balloon (assumed to be in terms of soil volume not water volume), k_{nit} is the maximum nitrification rate (see Table 3-8) and pH is the soil pH. The equation shows a linear correlation with soil pH.

3.4.3 NO and N₂O Production

The nitrification process also leads to emission of the trace gases NO and N₂O. Most process models simulate the emissions as a fraction of the nitrification rate (i.e. CENTURY and DNDC). Maintaining the consistency of adopting DNDC theory for the nitrification module, AGRIN models NO and N₂O production from nitrification based on Li (2000):

$$R_{NO,nit} = 0.0025 R_{nit} \mu_T \quad (3.59)$$

$$R_{N_2O,nit} = 0.0024 R_{nit} \quad (3.60)$$

Li (2000) takes NO fluxes to be highly temperature dependent based on experimental observations (Johansson, 1984; Slemr and Seiler, 1991; Valente and Thornton, 1993).

Table 3-8: Nitrification default parameters

Parameter	Value	Source
Ratio between diffusion constant for O ₂ in air and diffusion constant in water, χ	10 ⁴	Arah and Vinten (1995)
Radius of typical air-filled pore space, r_{ψ}	10 ⁻⁴ m	Arah and Vinten (1995)
Oxygen reaction potential, R_{O_2}	20 x 10 ⁻⁶ mol m ⁻³ s ⁻¹	Riley and Matson (2000)
Regression constant for model of anaerobic fraction, α	1.5 x 10 ⁻¹⁰	Arah and Vinten (1995)
Regression constant for model of anaerobic fraction, α	1.26	Arah and Vinten (1995)
Regression constant for model of anaerobic fraction, β	0.6	Arah and Vinten (1995)
Regression constant for model of anaerobic fraction, γ	0.6	Arah and Vinten (1995)
Regression constant for model of anaerobic fraction, δ	0.85	Arah and Vinten (1995)
Maximum growth rate for nitrifiers, $\mu_{max,nit}$	0.2 hr ⁻¹	Blagodatsky et al. (1998)
Maximum death rate for nitrifiers, $a_{max,nit}$	0.008 hr ⁻¹	Blagodatsky et al. (1998)
Maximum nitrification rate, k_{nit}	0.005 d ⁻¹	Li (2000)
Initial soil nitrifier population	10% of total microbial biomass	Li and Aber (2000)

3.4.4 Numerical Simulation

Based on the soil oxygen concentration profile, the anaerobic and aerobic fractions are then calculated at each layer. The amount of substrate (DOC, NH₄⁺) allocated to nitrification is determined by multiplying the amount of the substrate by the aerobic fraction (1- Φ). The model assumes that immobilization dominates if there is insufficient ammonium to meet the demand of both immobilization and nitrification.

Similar to soil temperature and moisture the following values are solved for each soil layer: nitrifier biomass, nitrification rate, NO production, and N₂O production. The

nitrifier biomass at each node at the end of the time step is found by integrating the equation for net increase in biomass:

$$B_{nit,i}^j = B_{nit,i}^{j-1} \exp[(G_{nit,i}^j - D_{nit,i}^j) \mu_{T,i}^j \mu_{W,i}^j \Delta t] \quad (3.61)$$

where i denotes the node, j the current time step, $j-1$ the previous time step, and Δt is the time step. Nitrification will act a sink term for ammonium and a source term for nitrate, NO gas and N₂O gas.

3.5 Denitrification

The various nitrogen oxides can undergo denitrification in anaerobic conditions. The denitrification submodel calculates the reduction of NO₃⁻ to N₂ by denitrifiers while considering intermediate processes such as NO₂⁻, NO and N₂O production and consumption. Influencing factors taken into account are soil temperature, redox status, moisture status, denitrifier biomass dynamics and substrate concentrations. Note that soil redox potential is already accounted for in the calculation of the anaerobic soil fraction. Outputs include N₂ production and nitrogen oxide production resulting from denitrification. Table 3-9 summarizes the submodel.

Table 3-9: Denitrification submodel inputs, simulated processes and outputs

Inputs	Processes Simulated	Outputs
Soil N oxide profiles from previous time step	Denitrifier biomass dynamics	Denitrifier biomass at end of time step
Soil moisture and temperature profiles	NO _x consumption/production	Changes in CO ₂ , DOC, and organic N profiles due to denitrification
Anaerobic fraction of soil		Changes in NO _x profiles due to denitrification
Soil DOC profile		N ₂ production from denitrification
Denitrifier biomass profile from previous time step		
Soil pH profile		

3.5.1 Denitrifier Biomass Dynamics

AGRIN bases most of its denitrification simulation on the model of Leffelaar and Wessel (1988). Their model makes several assumptions including: homogenous distribution, immobility of organisms, and non-limiting microbial population density. The net growth of denitrifier biomass is calculated as the difference between the growth and death rates of the bacteria:

$$\frac{dB_{denit}}{dt} = G_{denit} - D_{denit} \quad (3.62)$$

where B_{denit} is the denitrifier biomass, G_{denit} is the biomass growth rate and D_{denit} is the biomass death rate. The growth and death rates are calculated as:

$$G_{denit} = \mu_{total,denit} B_{denit} \quad (3.63)$$

$$D_{denit} = M_{c,denit} Y_{c,denit}^{\max} B_{denit} \quad (3.64)$$

where $\mu_{total,denit}$ is the total relative growth rate for denitrifiers, $M_{c,denit}$ is the maintenance coefficient of carbon, and $Y_{c,denit}^{max}$ is the maximum growth yield on carbon. Table 3-10 lists default parameter values.

Leffelaar and Wessel (1998) apply double-Monod kinetics to describe the multi-nutrient-dependent relative growth rate for each N oxide denitrifier:

$$\mu_{NOx} = \mu_{NOx}^{max} \frac{[DOC]_l}{K_c + [DOC]_l} \frac{[NOx]_l}{K_{NOx} + [NOx]_l} \quad (3.65)$$

where μ_{NOx}^{max} is the maximum relative growth rate of the N oxide denitrifier, DOC is the dissolved carbon concentration available for denitrification, K_c is the half-saturation value for carbon, NOx is the amount of the N oxide available for denitrification, and K_{NOx} is the half-saturation value for the N oxide. The total relative growth rate of the denitrifiers is the sum of the rates for each N oxide species.

The influence of soil temperature and pH must be accounted for in the simulation. Li (2000) and Li and Aber (2000) model this influence based on studies showing an increase in denitrification with temperature and pH. The authors also found that pH affects each type of denitrifier differently such that the total relative growth rate can be described by:

$$\mu_{total,denit} = F_{T,denit} (\mu_{NO3} F_{pH1} + \mu_{NO2} F_{pH2} + \mu_{NO} F_{pH2} + \mu_{N2O} F_{pH3}) \quad (3.66)$$

where F_T simulates the temperature effect and F_{pH} simulates the pH effect. The functions are described by:

$$\begin{aligned} F_T &= 2^{(T-22.5)/10} \\ F_{pH1} &= 0.4(pH - 2.5) \\ F_{pH2} &= 0.4(pH - 3) \\ F_{pH3} &= 0.4(pH - 3.5) \end{aligned} \quad (3.67)$$

The pH parameters are based on Focht (1974). The temperature in the temperature function is expressed in degrees Celsius.

3.5.2 Consumption Reactions and CO₂ Production

It is assumed that the decomposition module is simulating aerobic conditions such that DOC consumption and CO₂ production by denitrifiers must be considered separately. This approach is taken in Leffelaar and Wessel (1988) where aerobic conditions are neglected and in Li et al. (1992) which includes aerobic processes (i.e. nitrifier DOC consumption and CO₂ production assumed to be included in microbial biomass pool calculations) but still calculate denitrifier carbon flows separately. The consumption of DOC is described by Pirt (1965):

$$\frac{d[DOC]}{dt} = B_{denit} \left(\frac{\mu_{total,denit}}{Y_{c,denit}^{max}} + M_{c,denit} \right) \quad (3.68)$$

The assimilation of nitrogen during denitrification is determined using the C:N ratio of the denitrifiers:

$$N_{ass,denit} = \frac{G_{denit}}{CN_{denit}} \quad (3.69)$$

where $N_{ass,denit}$ is the amount of assimilated N based on the C:N ratio of the denitrifier biomass, CN_{denit} (see Table 3-10). The CO_2 production is determined from the carbon that isn't incorporated into the biomass:

$$\frac{d[CO2_{denit}]}{dt} = \frac{d[DOC]}{dt} - \frac{dB_{denit}}{dt} \quad (3.70)$$

where $CO2_{denit}$ is the CO_2 produced by denitrification.

N oxide consumption rate are also based on Pirt's equation (Pirt, 1965):

$$\frac{d[NOx]}{dt} = \left(\frac{\mu_{NOx}}{Y_{NOx}^{max}} + M_{NOx} \frac{[NOx]}{[NOx_{total}]} \right) B_{denit} \quad (3.71)$$

where NOx is the N oxide species being considered, Y_{NOx}^{max} is the maximum growth yield on the N oxide, M_{NOx} is the corresponding maintenance coefficient and NOx_{total} is the total amount of N oxides. See Table 3-10 for default parameter values.

3.5.3 NO and N₂O Movement

An important divergence between AGRIN and the DNDC model of Li et al. (1992) is that AGRIN does not use a simple scheme to describe the diffusion of NO and N₂O gases within the soil matrix. DNDC simply calculates the daily emission rates of NO and N₂O based on a gas diffusion factor, however AGRIN's temporal scale is much more refined

such that diffusion will be included in a partial differential equation describing gaseous movement within the soil profile (see Section 3.6).

Table 3-10: Denitrification default parameters

Parameter	Value
Maintenance coefficient with respect to carbon, $M_{c,denit}$	$0.21 \times 10^{-5} \text{ g g}^{-1} \text{ s}^{-1}$
Maintenance coefficient with respect to NO_3^- , M_{NO_3}	$2.5 \times 10^{-5} \text{ g g}^{-1} \text{ s}^{-1}$
Maintenance coefficient with respect to NO_2^- , M_{NO_2}	$0.97 \times 10^{-5} \text{ g g}^{-1} \text{ s}^{-1}$
Maintenance coefficient with respect to NO, M_{NO}	$2.2 \times 10^{-5} \text{ g g}^{-1} \text{ s}^{-1}$
Maintenance coefficient with respect to N_2O , $M_{\text{N}_2\text{O}}$	$2.2 \times 10^{-5} \text{ g g}^{-1} \text{ s}^{-1}$
Maximum growth yield on carbon, $Y_{c,denit}^{max}$	0.503 g g^{-1}
Maximum growth yield on NO_3^- , $Y_{\text{NO}_3}^{max}$	0.401 g g^{-1}
Maximum growth yield on NO_2^- , $Y_{\text{NO}_2}^{max}$	0.428 g g^{-1}
Maximum growth yield on NO, Y_{NO}^{max}	0.151 g g^{-1}
Maximum growth yield on N_2O , $Y_{\text{N}_2\text{O}}^{max}$	0.151 g g^{-1}
Maximum relative growth rate on NO_3^- denitrifier, $\mu_{\text{NO}_3}^{max}$	$4.8 \times 10^{-6} \text{ s}^{-1}$
Maximum relative growth rate on NO_2^- denitrifier, $\mu_{\text{NO}_2}^{max}$	$4.8 \times 10^{-6} \text{ s}^{-1}$
Maximum relative growth rate on NO denitrifier, μ_{NO}^{max}	$2.4 \times 10^{-6} \text{ s}^{-1}$
Maximum relative growth rate on N_2O denitrifier, $\mu_{\text{N}_2\text{O}}^{max}$	$2.4 \times 10^{-6} \text{ s}^{-1}$
Half-saturation value with respect to carbon, K_c	0.017 kg m^{-3}
Half-saturation value with respect of N oxides, K_{NO_x}	0.083 kg m^{-3}
C:N ratio of denitrifier biomass, CN_{denit}	3.45
Initial fraction of denitrifiers	0.02

Note: all values based on literature compilation from Leffelaar and Wessel (1988) except for C:N ratio which is from Li and Aber (2000)

3.5.4 Numerical Simulation

Substrates are allocated to the denitrification process in proportion to the soil's anaerobic fraction. These substrate portions are used to calculate the relative growth rate of each

denitrifier and rates are summed to calculate the total relative growth rate for all denitrifiers. The biomass equation is integrated to solve for the biomass at the end of the time step:

$$B_{denit,i}^j = B_{denit,i}^{j-1} \exp[(G_{denit,i}^j - D_{denit,i}^j) \Delta t] \quad (3.72)$$

Based on this biomass, the model calculates DOC consumption, CO₂ production and N assimilation. Using a separate denitrifier biomass means that the calculated carbon and N amounts must be added or subtracted from the soil profile.

The N oxide consumption and production rate equation (Equation 3.71) for each oxide is integrated using a 4th order Runge-Kutta integration scheme. This method calculates the amount of each N oxide that is consumed and then the net rate of change for each oxide (due to denitrification only) is calculated as:

$$\begin{aligned} \frac{d[NO_3^-]}{dt} &= - \left(\frac{d[NO_3^-]}{dt} \right)_{consumed} \\ \frac{d[NO_2^{2-}]}{dt} &= \left(\frac{d[NO_3^-]}{dt} \right)_{consumed} - \left(\frac{d[NO_2^{2-}]}{dt} \right)_{consumed} \\ \frac{d[NO]}{dt} &= \left(\frac{d[NO_2^{2-}]}{dt} \right)_{consumed} - \left(\frac{d[NO]}{dt} \right)_{consumed} \\ \frac{d[N_2O]}{dt} &= \left(\frac{d[NO]}{dt} \right)_{consumed} - \left(\frac{d[N_2O]}{dt} \right)_{consumed} \\ \frac{d[N_2]}{dt} &= \left(\frac{d[N_2O]}{dt} \right)_{consumed} \end{aligned} \quad (3.73)$$

3.6 Transport

This submodel simulates the movement of chemical species throughout the soil profile due to convection, diffusion and source-sink terms. Based on the output from previous submodels, the transport submodel solves for the species concentration at the end of a time step using an approach parallel to the simulation of soil water movement. Since the upper boundary condition for N trace gases is a flux condition, this submodel also simulates N trace gas fluxes from the soil surface. See Table 3-11 for the inputs, processes and outputs for the submodel.

Table 3-11: Transport submodel inputs, simulated processes and outputs

Inputs	Processes Simulated	Outputs
Soil N species profile for previous time step	Convection and diffusion of chemical species in soil profile	Soil N species profiles at end of time step
Other soil species profiles for previous time step (O ₂ , CO ₂ , H ⁺)	Net loss or gain of species due to source-sink terms	Other species profiles at end of time step (O ₂ , CO ₂ , H ⁺)
Slurry buffering capacity	TAN equilibrium	Trace gas fluxes from soil surface
Mineralization rate	Phase partitioning of each species	
Nitrification rate	Trace gas volatilization to atmosphere	
N oxide net consumption rates		
Soil moisture and temperature profiles		
Soil water flux profile		
N ₂ production from denitrification		
N ₂ O and NO production from nitrification		
TAN, NO ₃ ⁻ application rate if applicable		

3.6.1 Transport Equations

The movement of each nitrogen species is governed by vertical transport and various source and sink terms represented by the following general equation:

$$\frac{\partial [X]}{\partial t} = -\frac{\partial J_s}{\partial z} + S \quad (3.74)$$

where $[X]$ is the mass concentration of the species in the soil, J_s is the soil vertical flux, and S is the source-sink term (sum of all the sources and sinks). The mass concentration is the sum of the concentrations in all three phases:

$$[X] = \theta[X]_l + \rho_b[X]_s + a[X]_g \quad (3.75)$$

where l , s , and g denote the aqueous, sorbed, and gas phase mass concentrations respectively.

The vertical flux component is a sum of a convective flux in the liquid phase and diffusion in liquid and gas phases:

$$J_s = J_w[X]_l - D_G \frac{\partial [X]_g}{\partial z} - D_{AQ} \frac{\partial [X]_l}{\partial z} \quad (3.76)$$

where J_w is the vertical water flux, D_G is the gaseous diffusion coefficient and D_{AQ} is the aqueous diffusion coefficient. Convection is assumed to be negligible for the gaseous phase. The diffusion coefficients in soil can be determined by using the Millington-Quirk model (Jury et al., 1983):

$$D_G = \left(\frac{a^{10/3}}{\eta^2} \right) D_G^{air} \quad (3.77)$$

$$D_{AQ} = \left(\frac{\theta^{10/3}}{\eta^2} \right) D_{AQ}^{water} \quad (3.78)$$

where D_{AQ}^{water} and D_G^{air} are the molecular diffusivities of the species in water and air and η is the porosity. See Table 3-12 for the diffusivity values for the various species.

Equations 3.74 though 3.76 can be combined to write an equation in terms of the aqueous concentration only:

$$(\theta + \rho_b K_d + a K_h) \frac{\partial [X]_l}{\partial t} = - \frac{\partial}{\partial z} \left[- D_{AQ} \frac{\partial [X]_l}{\partial z} - D_G K_h \frac{\partial [X]_l}{\partial z} + J_w [X]_l \right] + S \quad (3.79)$$

where K_d is the liquid-solid partitioning coefficient and K_h is the Henry's Law constant that partitions the species between gas and liquid phases. The various parameter values required to solve the transport equations for each species can be found in Table 3-12.

The source-sink terms are based on calculations from the previous submodels. The source term for TAN is mineralization while the sink terms are immobilization and nitrification. Nitrification is a source term for nitrate, nitrous oxide and nitric oxide. Denitrification is a sink term for nitrate but may act as a sink or source term for the other N oxides depending on net consumption rates. Denitrification is a source term for dinitrogen gas. The source term for oxygen is the reaction potential term R_{O_2} introduced in Section 3.4. Currently, DOC transport is not simulated because of the lack of adequate

parameters needed to implement the transport equations. Existing process models (i.e. DNDC) have also excluded DOC transport yet have shown reasonable simulation of soil C and N dynamics.

Equation 3.79 can be simplified for all species except TAN by assuming certain processes to be negligible. For chemical species predominantly in the aqueous phase (NO_3^- , NO_2^{2-}), the transport due to diffusion of the gaseous phase is assumed to be negligible. For chemical species predominantly in the gaseous phase (O_2 , NO , N_2O , N_2), the transport due to diffusion and convection of the aqueous phase is assumed to be negligible.

3.6.2 Transport of TAN

Special consideration is given to TAN as Equation 3.79 must include the ammonium/ammonia equilibrium. Aqueous total ammoniacal nitrogen (or TAN which is the sum of NH_4^+ and NH_3) is subject to the following equilibrium:

$$[\text{NH}_3]_l = \frac{[\text{TAN}]_l}{1 + \frac{[\text{H}^+]_l}{K_D}} \quad (3.81)$$

The aqueous concentrations are expressed as molar concentrations in the above equations. These equilibria are considered when applying Equation 3.79 to aqueous TAN by replacing K_h with $K_h / (1 + [\text{H}^+]/K_D)$.

3.6.3 Transport of H^+

Special consideration is given to the transport of the hydrogen ion within the soil because source-sink terms have not yet been discussed and the transport equation must be modified to account for soil buffering capacity. Several nitrogen transformation processes can influence pH while pH in turn can affect the rate constants governing those processes. It is necessary to simulate changes in pH due to major influencing factors which are nitrification, ammonia volatilization, and CO_2 volatilization. The volatilization of ammonia will decrease pH (see Equation 3.80). Nitrification will reduce pH as hydrogen ions are released in the reaction:

where l denotes the soil solution concentration and g the gas phase concentration. The carbonate system reactions show how CO_2 volatilization acts to increase pH:

Sommer et al. (2003) state that most soil inorganic carbon is in the form $[HCO_3^-]$ such that the volatilization of one mole of CO_2 will reduce the concentration of $[H^+]$ by one mole (based on Bril and Salomons, 1990; Sommer and Husted, 1995).

The described pH influencing factors act as source-sink terms for $[H^+]$ which can contribute to the movement of $[H^+]$ in the soil profile. The movement of $[H^+]$ is described by a partial differential equation (based on Wang et al., 1998; Bear et al., 1998):

$$\left(\theta + \frac{\rho_b B_s}{[H^+]_l \ln 10} \right) \frac{\partial [H^+]_l}{\partial t} = \frac{\partial}{\partial z} \left(D_{AQ}^{H^+} \frac{\partial [H^+]_l}{\partial z} - J_w [H^+]_l \right) + \frac{1}{14} R_{vol, NH_3} - \frac{1}{12} R_{vol, CO_2} + \frac{1}{7} R_{nit} \quad (3.84)$$

where H^+ is the molar concentration of protons in the soil solution, B_s is soil buffering power, R_{vol, NH_3} is the ammonia volatilization rate, R_{vol, CO_2} is the CO_2 volatilization rate, and R_{nit} is the nitrification rate. The numbers before the rates adjust for stoichiometry and conversion to moles.

3.6.4 Boundary Conditions

Volatilization to the atmosphere is treated as an upper boundary condition for gaseous species while infiltration by slurry or precipitation is the upper condition for aqueous species. The lower boundary condition for all species is a unit gradient. Volatilization of NH_3 will occur if the surface concentration surpasses the atmospheric concentration according to the equation:

$$F_{NH_3} = \frac{1}{r_a + r_b + r_c} \left[[NH_3]_{g,0} - [NH_3]_{g,air} \right] \quad (3.85)$$

where F_{NH_3} is the NH_3 flux from the soil surface, r_a is the aerodynamic resistance, r_b is the interfacial sublayer resistance, r_c is the soil surface resistance, $[NH_3]_{g,0}$ is the soil surface concentration and $[NH_3]_{g,air}$ is the atmospheric concentration which is assumed to be zero. Due to lack of experimental data and research on the soil-slurry surface resistance, r_c , to NH_3 volatilization, the model assumes this value to be zero. The other resistances have already been described in Section 3.2.3. This same equation is applied to NO , N_2O , and N_2 .

Table 3-12: Transport default parameters

Parameter	Value	Source
TAN solid-liquid partitioning coefficient, K_d	$2.2 \text{ cm}^3 \text{ g}^{-1}$	Wang et al. (1988)
All other species solid-liquid partitioning coefficient, K_d	0	Assumed
TAN dissociation constant, K_D	$10^{-(0.09018 - 2129.92T^{-1})}$	Van Der Molen et al. (1990) based on Hales and Drewes (1979)
Ammonia Henry's Law constant, K_H	$10^{(-1.69 + 1477.7T^{-1})}$ ($\text{m}^3 \text{ air m}^{-3} \text{ water}$)	Van Der Molen et al. (1990) based on Hales and Drewes (1979)
Nitrous oxide Henry's Law constant, K_H	$1.68 \text{ m}^3 \text{ water m}^{-3} \text{ air}$	Venterea and Rolston (2000) based on Wilhelm et al. (1977)
Nitric oxide Henry's Law constant, K_H	$21.2 \text{ m}^3 \text{ water m}^{-3} \text{ air}$	Venterea and Rolston (2000) based on Wilhelm et al. (1977)
Dinitrogen Henry's Law constant, K_H	$59.3 \text{ m}^3 \text{ water m}^{-3} \text{ air}$	Riley and Matson (2000)
Diffusivity of H^+ in water, D_L^{water}	$3.4 \times 10^{-6} \text{ m}^2 \text{ h}^{-1}$	Wang et al. (1998) based on Robinson and Stokes (1968)
Nitrate molecular diffusivity in water, D_L^{water}	$6.8 \times 10^{-6} \text{ m}^2 \text{ h}^{-1}$	Venterea and Rolston (2000) based on Hunick et al. (1994)
Nitrite molecular diffusivity in water, D_L^{water}	$6.9 \times 10^{-6} \text{ m}^2 \text{ h}^{-1}$	Venterea and Rolston (2000) based on Hunick et al. (1994)
Ammonia molecular diffusivity in air, D_G^{air}	$1.7 \times 10^{-5} \times 1.03^{(T-293)}$ ($\text{m}^2 \text{ s}^{-1}$)	Van Der Molen et al. (1990) based on Bruckler et al. (1989)
Nitrous oxide molecular diffusivity in air, D_G^{air}	$5.2 \times 10^{-2} \text{ m}^2 \text{ h}^{-1}$	Venterea and Rolston (2000) based on Bird et al. (1960)
Nitric oxide molecular diffusivity in air, D_G^{air}	$8.5 \times 10^{-2} \text{ m}^2 \text{ h}^{-1}$	Venterea and Rolston (2000) based on Bird et al. (1960)
Dinitrogen molecular diffusivity in air, D_G^{air}	$5.2 \times 10^{-2} \text{ m}^2 \text{ h}^{-1}$	Assumed
Carbon dioxide molecular diffusivity in air, D_G^{air}	$0.0576 \text{ m}^2 \text{ h}^{-1}$	Brokaw (1998)
Oxygen molecular diffusivity in air, D_G^{air}	$0.054 \text{ m}^2 \text{ h}^{-1}$	Weast and Astle (1980)
Soil buffering capacity, B_s	$0.07 \text{ mol kg}^{-1} \text{ soil pH}^{-1}$	Wang et al. (1998) based on Rachhpal-Singh and Kirk (1993)
Initial soil oxygen concentration	$2.0 \times 10^{-6} \text{ mol cm}^{-3} \text{ air}$	Arah and Vinten (1995)
N species rainfall concentration	0	Assumed
Carbon dioxide atmospheric concentration	$5.72 \times 10^{-7} \text{ g cm}^{-3}$	Brokaw (1998)
Oxygen atmospheric concentration	0.21 atm or $9 \times 10^{-6} \text{ mol cm}^{-3}$	Assumed
Dinitrogen gas atmospheric concentration	0.79 atm or $4.76 \times 10^{-4} \text{ g cm}^{-3}$	Assumed

3.6.5 Slurry Application Considerations

The application of slurry will introduce a source of TAN and nitrate at the soil surface.

The rate of application of each species is calculated as:

$$R_{appn,TAN} = [TAN]_{sl} R_{appn,s} \quad (3.86)$$

$$R_{appn,NO3} = [NO_3^-]_{sl} R_{appn,s} \quad (3.87)$$

where $R_{appn,TAN}$ is the rate of TAN application and $R_{appn,NO3}$ is the rate of nitrate application. Infiltration of aqueous TAN and nitrate become the upper boundary condition for the soil surface and ammonia surface fluxes are based on the slurry concentration and pH. Similar to slurry water, the masses of the two nitrogen species in the slurry layer is calculated at the end of each time step.

Following slurry application volatile fatty acids contained in the slurry are oxidized to carbon dioxide (CO₂) by microorganisms and because CO₂ will volatilize more rapidly than NH₃ an increase in the slurry pH will occur (Sommer et al., 2003). This increase in pH will encourage NH₃ volatilization. Sommer and Hutchings (2003) have pointed out that the factors controlling the magnitude of the increase in pH are complex and that NH₃ emissions may not be closely related to initial manure pH.

3.6.6 Numerical Simulation

The finite difference approximation for Equation 3.79 is the same type used for soil moisture. The partial differential equation can be rearranged to solve for concentration values at the end of each time step by forming a system of equations:

$$A_i[X]_{l,i-1}^j + B_i[X]_{l,i}^j + C_i[X]_{l,i+1}^j = D_i \quad i=1,\dots,n \quad (3.88)$$

For the interior nodes ($i = 2, \dots, n-1$) the coefficients are calculated as:

$$A_i = \frac{-D_{AQ_{i-1/2}}^j}{\Delta z_i(z_i - z_{i-1})} - \frac{K_{h,i-1/2}^j D_{G_{i-1/2}}^j}{\Delta z_i(z_i - z_{i-1})} - \frac{J_{w,i-1/2}^j}{2\Delta z_i}$$

$$B_i = \frac{Y_i^j}{\Delta t} + \frac{1}{\Delta z_i} \left[\frac{D_{AQ_{i+1/2}}^j}{(z_{i+1} - z_i)} + \frac{D_{AQ_{i-1/2}}^j}{(z_i - z_{i-1})} + \frac{K_{h,i+1/2}^j D_{G_{i+1/2}}^j}{(z_{i+1} - z_i)} + \frac{K_{h,i-1/2}^j D_{G_{i-1/2}}^j}{(z_i - z_{i-1})} \right] - \frac{J_{w,i+1/2}^j}{2} + \frac{J_{w,i-1/2}^j}{2} \quad (3.89)$$

$$C_i = \frac{-D_{AQ_{i+1/2}}^j}{\Delta z_i(z_{i+1} - z_i)} - \frac{K_{h,i+1/2}^j D_{G_{i+1/2}}^j}{\Delta z_i(z_{i+1} - z_i)} + \frac{J_{w,i+1/2}^j}{2\Delta z_i}$$

$$D_i = \frac{Y_i^j [X]_{l,i}^{j-1}}{\Delta t} + S_i^j$$

In the above set of equations, Y represents the partitioning of the species into the three phases:

$$Y_i^j = \theta_i^j + \rho_b K_d + a_i^j K_{h,i}^j \quad (3.90)$$

The internodal diffusivities are calculated as an arithmetic average. Note that TAN is the only species which is simulated by these full discretization schemes because all three phases are included. The coefficients will simplify for species that are predominantly in one phase.

For the surface boundary node ($i = 1$), the surface boundary condition is volatilization from the surface or infiltration. The coefficients become:

$$A_i = 0$$

$$B_i = \frac{Y_1^j}{\Delta t} + \frac{1}{\Delta z_1} \left[\frac{D_{AQ_{1.5}}^j}{(z_2 - z_1)} + \frac{K_{h,1.5}^j D_{G_{1.5}}^j}{(z_2 - z_1)} + \frac{J_{w,1.5}^j}{2} \right] \quad (3.91)$$

$$C_i = \frac{-D_{AQ_{1.5}}^j}{\Delta z_1 (z_2 - z_1)} - \frac{K_{h,1.5}^j D_{G_{1.5}}^j}{\Delta z_1 (z_2 - z_1)} + \frac{J_{w,1.5}^j}{2 \Delta z_1}$$

$$D_i = \frac{Y_1^j [X]_{l,1}^{j-1}}{\Delta t} + S_1^j + \frac{q_{s,1}^j}{\Delta z_1}$$

where $q_{s,1}$ is the surface flux term based on the previous time steps or any species influx associated with the infiltration of slurry.

For the lower boundary node ($i = n$), the unit hydraulic gradient approach is taken ($\partial[X]/\partial z = 0$). The coefficients become:

$$\begin{aligned}
A_i &= \frac{-D_{AQ_{n-1/2}}^j}{\Delta z_n(z_n - z_{n-1})} - \frac{K_{h,n-1/2}^j D_{G_{n-1/2}}^j}{\Delta z_n(z_n - z_{n-1})} - \frac{J_{w,n-1/2}^j}{2\Delta z_n} \\
B_i &= \frac{Y_n^j}{\Delta t} + \frac{1}{\Delta z_n} \left[\frac{D_{AQ_{n-1/2}}^j}{(z_n - z_{n-1})} + \frac{K_{h,n-1/2}^j D_{G_{n-1/2}}^j}{(z_n - z_{n-1})} - \frac{J_{w,n-1/2}^j}{2} \right] \\
C_i &= 0
\end{aligned} \tag{3.92}$$

$$D_i = \frac{Y_n^j [X]_{l,n}^{j-1}}{\Delta t} + S_n^j - \frac{q_{s,n}^j}{\Delta z_n}$$

The bottom flux, $q_{s,n}$ is taken to be:

$$q_{s,n}^j = J_{w,n}^j [X]_{l,n}^j \tag{3.93}$$

The system of equations forms a linear tri-diagonal matrix which can be solved using the Thomas algorithm described by von Rosenberg (1969). A mass balance error for each species is calculated by examining the flux conditions at the lower and upper boundaries, the net source term and the change in soil storage over the time step. For example, the TAN storage, S_{TAN} , is given by:

$$S_{TAN} = [TAN]_l \left(\frac{z_2 - z_1}{2} \right) + [TAN]_n \left(\frac{z_n - z_{n-1}}{2} \right) + \sum_{i=2}^{n-1} [TAN]_i \left(\frac{z_{i+1} - z_{i-1}}{2} \right) + \sum_{i=1}^n S_i \tag{3.94}$$

The mass balance error, MBE_{TAN} , is then calculated as:

$$MBE_{TAN}^j = q_{TAN,l}^j \Delta t - q_{TAN,n}^j \Delta t - (S_{TAN}^j - S_{TAN}^{j-1}) \tag{3.95}$$

4.0 AGRIN COMPUTER PROGRAM

4.1 Program Design

The AGRIN model was implemented into computer code using Compaq Visual Fortran which is based on American National Standard FORTRAN 77 (ANSI X3.9-1978) and FORTRAN 90 (ANSI X3.198-1992). The source code for the entire program can be found in Appendix A. This section describes the program's design and operation. Similar to the UNSAT-H (Fayer, 2000) program design, AGRIN consists of three programs: AGRIN IN, AGRIN MAIN and AGRIN OUT. A summary of each program's function and subroutines can be found in Table 4-1.

Table 4-1: AGRIN program summary

Program	Input	Output	Function	Subroutines
AGRIN IN	*.inp file	*.bin file	Processes input file prior to simulation to reduce likelihood of errors occurring during run time	timex, welcome, soilprop, polykh, thermk, etpar, etbc, precipbc, diffusivity
AGRIN MAIN	*.bin file	*.res file	Simulates soil heat, moisture and chemical species dynamics	timex, welcome, soilmod, blr, zeroa, zeroi, zeror, thermk, airdens, blr, interk, reset, diffusivity, eqmmod, netrad, soilmod, mngmtmod, decompmod, nitmod, denitmod, transmod, interk, relhum, tridag, polykh, flux, heatflow, delchk, profitan, profaq, profgas, cbalance
AGRIN OUT	*.res	Text file	Processes output file such that user can specify values to be printed to text file	welcome, listdata, readrec

4.1.1 AGRIN IN

The AGRIN IN program is responsible for processing input data to reduce the risk of errors occurring when running the main program. The program reads the input file (*.inp) by prompting the user for the filename and then performs error checking to ensure there are no input errors. The data is then written to a binary input file (*.bin). The types of error checking include ensuring that certain options exist, that data is in chronological order, that data is of the right type and that array dimensions are not exceeded. A summary of the subroutines can be found in Table 4-2.

Table 4-2: AGRIN IN subroutines

Subroutine	Description
Diffusivity	Calculates the liquid water diffusivity at each node as a function of soil moisture content.
Etbc	Reads in hourly meteorological data.
Etpar	Reads in meteorological parameters.
Polykh	Calculates hydraulic and thermal conductivities at each node as a function of moisture content.
Precipbc	Reads in precipitation data and writes meteorological and precipitation data to binary input file
Soilprop	Reads in soil moisture and heat properties.
Timex	Determines the time and date of run.
Thermk	Calculates soil volumetric heat capacity at each node.
Welcome	Writes program header and contact information.

4.1.2 AGRIN MAIN

The AGRIN MAIN program performs the actual simulation using the *.bin file created by AGRIN IN as input. The user is prompted for the filename and calculations are

performed that can simulate just soil heat and moisture or soil heat and moisture and chemical species dynamics. A list of subroutines can be found in

Table 4-3. An output file is created (*.res) which includes initial conditions, hourly values of soil water content, temperature, nitrogen species concentrations, nitrogen species volatilization, and surface heat balance values. This file serves as input for AGRIN OUT.

4.1.3 AGRIN OUT

The AGRIN OUT program processes the *.res file such that it is converted to ASCII format. The user has the option as to what parameters (moisture content, temperature, heat balance values, ammonia fluxes, etc.) are to be output versus time for surface values or output versus time and depth for soil profile values. Table 4-4 gives a list of subroutines in the program.

Table 4-3: AGRIN MAIN subroutines

Subroutine	Description
Airdens	Calculates atmospheric vapour density and saturated atmospheric vapour density.
Blr	Calculates aerodynamic boundary layer resistance based on meteorological and surface conditions.
Decompmmod	Calculates decomposition rate of organic matter, CO ₂ production from microbial respiration, and net mineralization.
Delchk	Tells user if mass and/or heat balance errors.
Denitmod	Calculates N oxide consumption/production and N ₂ production from denitrification.
Diffusivity	Calculates the liquid water diffusivity at each node as a function of soil moisture content.
Flux	Calculates water fluxes between nodes.
Heatflow	Solves heat balance equations, fluxes between nodes, and heat balance error.
Interk	Calculates internodal hydraulic conductivities.
Mngmtmod	Calculates water, nitrogen and carbon application rates if slurry application occurs.
Netrad	Calculates net radiation as a function of meteorological conditions.
Nitmod	Calculates nitrification rate and NO and N ₂ O production from nitrification.
O2status	Simulates oxygen movement in the soil and calculates the soil's anaerobic fraction.
Polykh	Calculates hydraulic and thermal conductivities at each node as a function of moisture content.
Profaq	Calculates aqueous species profile at end of time step.
Profgas	Calculates gaseous species profile at end of time step.
Proftan	Calculates TAN species profile at end of time step.
Relhum	Calculates soil surface relative humidity based on moisture content and temperature.
Reset	Stores current values as values for previous time step.
Soilmod	Calculates surface heat fluxes and soil moisture and temperature profiles based on soil properties and meteorological conditions.
Thermk	Calculates soil volumetric heat capacity at each node.
Timex	Determines the time and date of run
Transmod	Simulates chemical species movement through the soil profile including surface volatilization.
Tridag	Solves the tridiagonal solution matrix.
Welcome	Writes program header and contact information.
Zeroa, zeror and zeroi	Sets arrays, real parameters and integer parameters to zero.

Table 4-4: AGRIN OUT subroutines

Subroutine	Description
Listdata	Creates data lists versus time and depth or just time; these lists can be used for plotting purposes.
Readrec	Reads the *.res file created by AGRIN MAIN.
Welcome	Writes program header and contact information.

4.2 Using the Program

Using the AGRIN program requires the user to transform a scenario into an input file that can be processed by the numerical model. The user must specify options, specify initial conditions, spatially discretize the soil profile through nodal spacing, assign soil and slurry application properties, and define the atmospheric surface conditions. Program control variables are user-specified such that the user can control the balance between computational time requirements and solution accuracy. This may result in the need for several simulation runs during which the user may wish to test different scenarios (i.e. alter node number and spacing, time step, mass balance criteria) to achieve a solution that does not change significantly.

Initial conditions and soil properties are used to calculate initial hydraulic and thermal conductivities and soil heat and moisture storage. The initial carbon and nitrogen profiles are calculated based on surface values and user-specified profile concentration gradients. The lower boundary condition of unit hydraulic gradient is maintained for all simulations (except for heat which assumes a constant temperature) and the upper boundary condition is either a surface flux or atmospheric concentration. Hourly

meteorological data and site conditions are used to compute the atmospheric resistances to moisture, heat and solute fluxes. In the case of slurry application, application rates are used to determine the appropriate upper boundary flux condition for the soil surface.

If the program has not been compiled yet or the user alters the source files in any way, the program executable files must be created to run the simulation. The computer code must be compiled and built such that executable files are created for each program: *agrin in.exe*, *agrin main.exe*, and *agrin out.exe*. During the compiling process, the *agringlob.inc* and *agrininit.inc* files must be located in the same directory as the source code files. These files can be found in Appendix B. The *agringlob.inc* file globalizes variables and arrays while *agrininit.inc* initializes variables and arrays and also defines default values. These files can be altered by the user to re-dimension arrays and change default values.

Once the executables files have been created and are stored in the same default directory, the AGRIN IN program can be run during which the user is asked to supply the input file name. After AGRIN IN is run a summary file (*.lis) is created which presents input data in a form more easily read than the .inp file and includes preliminary calculations. Any error that occurs will be printed to the screen and if no errors are encountered a binary file will have been created having the same name as the input file and this file serves as input to the AGRIN MAIN program.

Next, the AGRIN MAIN executable program is run where the user is asked to supply the binary input file name – this file should be in the default directory. Any error that occurs will be printed to the screen and if no errors are encountered a *.res file is created having the same name as the *.inp and *.bin files and this file serves as input to the AGRIN OUT program. Finally, the AGRIN OUT program is run to process the *.res file and create an ASCII file that the user can import into other programs such as Excel for plotting purposes. The *.res file should already be located in the default directory which is where the final output file will also go.

5.0 MODEL TESTING

5.1 Soil Heat and Moisture

Testing of the soil heat and moisture submodel is essential to determining if AGRIN's theoretical equations and numerical solving technique are accurate. This submodel simulates the soil environment that drives the chemical species transport processes and controls the rate of transformation processes. Also, the equation describing the convection and diffusion of soil moisture is of the same form for the various chemical species. Thus, it is assumed that if this submodel can predict the soil heat and moisture environment then the theory and solving technique are adequate for other chemical species besides water.

5.1.1 Field Study

Heat and moisture fluxes from a field study conducted by Agriculture and Agri-Food Canada were used to test the soil submodel. The study took place over 5 days in late September 1992 and was conducted in order to make volatilization measurements of pesticides over a bare soil. This dataset was chosen because it measured a wide set of parameters and had previously been compared with numerical model predictions (Scholtz et al., 2002b). Field measurements included hourly meteorological data (wind speed, air temperature, humidity, dew point temperature, cloud cover) and heat fluxes (latent heat, net radiation, sensible heat, soil heat).

Solar radiation and net radiation measurements were averaged every hour while hourly cloud cover was estimated from observations and radiation measurements. Precipitation measurements were taken from the local airport. Heat flux plates were utilized for the soil heat flux while the eddy covariance technique was used to measure sensible and latent heat fluxes. Soil data measured included temperature (5cm depth), moisture (average over 0 to 2.5cm depth), texture (loam) and soil bulk density. A more detailed description of the field study can be found in Pattey et al. (1995).

5.1.2 Simulation

During initial test runs, initial profiles of soil moisture and heat were assumed since these data weren't available. A uniform moisture profile of $0.27 \text{ cm}^3 \text{ cm}^{-3}$ was assumed based on soil moisture measurements while the temperature profile was initialized using a typical surface temperature and profile (1992 data from Central Experimental Farm Weather Site, 2006). Soil properties were based on loam values from Clapp and Hornberger (1978). Roughness lengths of 0.001 m were assumed. The input file can be found in Appendix B (1992.inp). Figure 5-1 shows that predicted soil moisture follows the appropriate diurnal trends and responds to rainfall events which occur on Days 270 and 271. The limited field data available (daily measurements) shows that moisture trends are followed. Figure 5-2 shows that the predicted soil temperature agrees well with observed data; however, the daily maximum temperature is over predicted by a few degrees.

The predicted latent heat fluxes (Figure 5-3) were slightly higher than observed data but in general showed good agreement. Scholtz et al. (2002b) found similar results using the same set of data to validate a model of pesticide emissions. The authors concluded that the rainfall events occurring on Days 270 and 271 may explain the overestimation of latent heat fluxes on these days. Precipitation data was not measured on site, thus measurements from an airport located 6 km away were supplied in the dataset.

While predicted sensible heat fluxes (Figure 5-4) followed observed trends, the magnitudes were substantially under predicted on days with no precipitation (Julian days 268 and 269). Similarly, the soil heat fluxes (Figure 5-5) are slightly overestimated on days with no rainfall. Scholtz et al. (2002b) found similar results for these fluxes. The underestimation of sensible heat fluxes during the day is resulting in a surface energy balance which over predicts the heat flux into the soil giving higher soil temperatures. The slightly higher maximum temperatures help explain why moisture fluxes are over predicted during the daytime.

Figure 5-1: Modelled versus measured soil moisture.
Field measurements took place once a day.

Figure 5-2: Modelled versus measured soil temperature.

Figure 5-3: Modelled versus measured latent heat flux.

Figure 5-4: Modelled versus measured sensible heat flux.

Figure 5-5: Modelled versus measured soil heat flux.

5.2 Soil Ammonia Emissions

Simulating NH_3 volatilization from a soil involves simulation of all of the nitrogen transformation and transport processes. To help develop and test AGRIN's model of NH_3 volatilization datasets from Agriculture and Agri-Food Canada were used. Model testing included investigations into the influence of surface pH, slurry infiltration rate and microbial processes on NH_3 emission peaks and trends.

5.2.1 *Field Studies*

Data from two field studies conducted by Agriculture and Agri-Food Canada (AAFC) were used to test the model. The first study took place in the fall of 2004 and involved ammonia measurements following liquid dairy manure application to a bare field located at Schoeten's Farm in Richmond, Ontario. Measurement techniques included relaxed eddy accumulation (REA) and flux gradient (FG). This field study will be referred to as the Richmond Experiment. The second experiment took place in August 2005 and involved REA measurements of ammonia emissions following application of a poultry slurry to a bare soil located south of Ottawa, Ontario. This field study will be referred to as the Forage Field Experiment and was completed as part of the overall development, testing and validation of the model. More details concerning this experiment are given below. Table 5-1 and Table 5-2 summarize the inputs required for the simulations. The input files can be found Appendix B (richmond.inp and forage.inp).

The Forage Field Experiment used denuder tubes for measurement of NH_3 where the denuders act as scrubbers such that ammonia is adsorbed onto an acid coating solution on the walls of the denuder; particulate is also collected downstream. The REA technique implemented samples air according to the direction of the vertical wind fluctuation to collect updraft and downdraft air. The ammonia flux is proportional to the difference of the mean concentrations of ammonia in updrafts and downdrafts (Zhu et al., 1999).

Manure application consisted of applying a nitrogen source (poultry and pig slurries) to a bare field in a confined area. There were measurements of NH_3 emissions in the confined application area as well as short range deposition of the gases and particulate matter presumably resulting from emissions from the application area. In addition to emission measurements, meteorological data (horizontal wind speed, air temperature, precipitation, atmospheric pressure, etc.) and soil data (moisture, respiration, and temperature) were recorded.

Figure 5-6 illustrates the experimental set-up. The application area is outlined with a red border where emission measurements took place at the tower within the application area (blue triangle). Soil moisture and temperature measurements also took place in this area. Deposition towers measured ammonia fluxes using the gradient technique while particulate matter measurements using filter packs were taken upwind and downwind of the emission area. Soil respiration measurements were taken in and outside of the emission area.

Contribution to the experiment included laboratory, field work and data analysis. Laboratory work included preparation and sample extraction of the denuders and filter packs. Field work included site preparation (installation of soil moisture and temperature probes), collecting ammonia samples (placing and removing denuders), soil moisture and respiration measurements, soil sampling and manure sampling. Data analysis included assisting Agriculture and Agri-Food Canada (AAFC) with converting raw data into

spreadsheet form although most of this work was completed by Christophe Forget and Elizabeth Pattey from AAFC.

Figure 5-6: Forage Field Experimental Set-Up for Summer 2005.
Figure courtesy of Agriculture and Agri-Food Canada.

Table 5-1: Input values for Richmond Experiment

Input	Value	Source
Hourly air temperature, wind speed, precipitation, solar radiation	-	Site data from AAFC
Hourly dew point temperature, cloud cover	-	Environment Canada online climate data
Surface roughness lengths	0.001 m	Assumed
Zero plane displacement	0.0 m	Assumed
Initial temperature profile	-	Based on site data from AAFC
Initial moisture profile	0.35 cm ³ cm ⁻³	Assumed
Initial NH ₄ ⁺ and NO ₃ ⁻ soil surface concentrations	9.35E-7 and 8.1E-6 g cm ⁻³	Site data from AAFC
Initial NO ₂ ²⁻ profile	0.0 g cm ⁻³	Assumed
Initial soil surface pH	6.3	Assumed
Initial residue and soil organic carbon soil surface concentrations	0.024 and 0.019 g cm ⁻³	Grant and Pattey (2003)
Soil gradients for pH, nitrogen and carbon	-	Grant and Pattey (2003)
Soil texture class	Loam	Based on site data from AAFC
Soil bulk density	1.4 g cm ⁻³	Site data from AAFC
Slurry application rate	78600 L ha ⁻¹	Site data from AAFC
Slurry DM content	2.1%	Site data from AAFC
TAN application rate	18.3 kg-N ha ⁻¹	Site data from AAFC
Slurry NO ₃ ⁻ concentration	0.011 g L ⁻¹	Assumed that 1% of total N
Slurry organic matter content	1.7%	Site data from AAFC
Application area ^a	22 ha	Assumed based on discussions with AAFC
Application timing	11:00 to 17:00 (EST)	Assumed based on discussions with AAFC

^aArea upwind of measurement towers

Table 5-2: Input values for Forage Field Experiment

Input	Value	Source
Hourly air temperature, dew point temperature, wind speed, precipitation, solar radiation	-	Site data from AAFC
Hourly cloud cover	-	Environment Canada online climate data
Surface roughness lengths	0.001 m	Assumed
Zero plane displacement	0.0 m	Assumed
Initial temperature profile	-	Based on site data from AAFC
Initial moisture profile	0.35 cm ³ cm ⁻³	Assumed
Initial NH ₄ ⁺ and NO ₃ ⁻ soil surface concentrations	9.35E-7 and 8.1E-6 g cm ⁻³	Assumed
Initial NO ₂ ²⁻ profile	0.0 g cm ⁻³	Assumed
Initial soil surface pH	6.3	Assumed
Initial residue and soil organic carbon soil surface concentrations	0.024 and 0.019 g cm ⁻³	Grant and Pattey (2003)
Soil gradients for pH, nitrogen and carbon	-	Grant and Pattey (2003)
Soil texture class	Clay loam	Soils report for site
Soil bulk density	1.5 g cm ⁻³	Assumed
Slurry application rate	33000 L ha ⁻¹	Site data from AAFC
Slurry DM content	7%	Site data from AAFC
TAN application rate	41.0 kg-N ha ⁻¹	Site data from AAFC
Slurry NO ₃ ⁻ concentration	0.017 g L ⁻¹	Manure analysis for site
Slurry organic matter content	6.5%	Manure analysis for site
Application area ^a	3.0 ha	Assumed based on discussions with AAFC
Application timing	8:00 to 11:00 (EST)	Assumed based on discussions with AAFC

^aArea upwind of measurement towers

5.2.2 Infiltration Investigation

AGRIN's theoretical equations are based on existing models that have already completed extensive sensitivity analyses (i.e. Li et al., 1992). However, unlike other models AGRIN models the slurry layer as a separate surface layer subject to evaporation and infiltration. The slurry infiltration rate is controlled by the soil's infiltration capacity and the user-specified reduction factor due to the slurry's viscosity. Générmont and Cellier's (1997) model of slurry application to a bare soil assumes that the slurry is added to the first soil layer and reduces this layer's infiltrability to 2% of its initial value. This reduction is based on the 1-10% range observed for a wide range of soils by Fiès and Panini (1995). An investigation was conducted into how this reduction factor, μ_{visc} , influences NH_3 emission magnitudes and trends.

AGRIN was run to simulate the site conditions from Richmond Experiment data using a range of different reduction factors from no infiltration ($\mu_{visc} = 1.0$) to the lowest reduction factor of 0.01 in the observed range of Fiès and Panini (1995). The simulated ammonia fluxes are shown in

Figure 5-7. As the reduction factor decreased from 1.0 to 0.01, there was no significant effect on first day emissions because the infiltration rate is instead being constrained by the rate of application which is slower than the infiltration rates being determined by Philip's Two-Term Model. A reduction factor of 0.01 does cause emissions to be slightly higher into the evening on the day of application (Day 258) and the following day. This is due to the fact that the TAN has had less time to infiltrate the soil. However, slurry

infiltration is still fast enough that there is no slurry remaining on the surface several hours after application which is often observed in the field.

The same set of reduction factors was applied to the Forage Field data and the simulated ammonia fluxes are shown in Figure 5-8. In this experiment, slurry application was fast enough that slurry infiltration was controlled by the soil's infiltration capacity once it was reduced by a factor of 0.01. This reduction caused the slurry to remain on the soil surface into the afternoon resulting in large simulated emissions because of the enhanced emissions associated with the turbulent transfer, higher surface temperatures and water evaporation that are associated with solar radiation. These results indicate just how sensitive the first day's peak emission can be to infiltration rates: the simulated first day peak increases by over 500% when the infiltration reduction factor is decreased from 0.05 to 0.01. Emissions on subsequent days are only slightly lower compared to the higher reduction factors indicating that less amount of TAN infiltrated the soil surface.

The Richmond Experiment infiltration investigation shows that there is no significant effect on simulated emissions when slurry application is slow and occurs over the entire day. The Forage Field Experiment investigation shows that simulated emissions on the day of application can be very sensitive to infiltration rates if application occurs over a shorter time period. A shorter application period shows that infiltration rates may control whether or not the slurry is exposed at the surface during the afternoon when climatic conditions can greatly enhance surface emission rates. Both studies showed contrasting results as infiltration rates decrease: the Richmond investigation

showed a reduction factor of 0.01 resulted in higher emissions on the day after application while the Forage Field investigation showed slightly lower emissions on subsequent days. This means the reduction factor can impact subsequent day simulated emissions in two ways: (1) it increases the amount of time the TAN takes to infiltrate meaning more TAN is available at the surface for volatilization and (2) it reduces the amount of TAN that actually infiltrates such that less is available for volatilization. Which of these effects dominates would be governed by application timing and meteorological conditions.

Both investigations show that simply applying a factor within Fiès and Panini's (1995) range is not adequate. There is a need for an empirical model of slurry infiltration that can more accurately describe the multiple processes controlling infiltration rate including soil infiltration capacity, slurry dry matter content, application timing and slurry application rate.

Figure 5-7: Influence of slurry infiltration rate on NH_3 volatilization at Richmond. Soil infiltration capacity reduced by reduction factor μ_{visc} . Application of slurry occurred on Day 258. A constant pH of 7.7 in soil-slurry surface layers was assumed.

Figure 5-8: Influence of slurry infiltration rate on NH_3 volatilization at Forage Field. Soil infiltration capacity reduced by reduction factor μ_{visc} . Application of slurry occurred on Day 219. A constant pH of 7.5 in soil-slurry surface layers was assumed (model adjusted for pH in subsequent simulations).

5.2.3 *pH Investigation*

Génermont and Cellier's (1997) sensitivity analysis showed that NH_3 volatilization is most sensitive to pH. Sommer and Hutchings (2003) have stated that the factors controlling the magnitude of the increase in pH are complex and that NH_3 emissions may not be closely related to initial manure pH. Since there is no adequate scientific description of the change in slurry-soil pH, an investigation was conducted into how the magnitude of this pH influences NH_3 emissions.

If it is assumed that the dairy cattle slurry pH is 7.3 (Hengnirun et al., 1999), Génermont and Cellier's (1997) model showed that a constant pH based on an increase of the slurry pH by 0.5 units (pH = 7.8) best fit emissions data. A study measuring slurry pH following application by Vandr and Clemens (1997) showed that the pH increases by approximately 0.5 units and an increased pH can be maintained for at least 72 h. For the pH investigation constant pH values within the range 6.5 to 8.0 were used in simulation runs to investigate how NH_3 volatilization was affected. Figure 5-9 shows predicted NH_3 emissions based on different pH values for the Richmond site. Compared to subsequent emissions, the initial peak flux is the most sensitive to pH with a 0.5 increase in pH (7.5 to 8.0) resulting in an almost 300% larger initial peak emission.

Emissions are still sensitive to pH on the days following application, but the effect isn't as obvious since the peaks are small in comparison to first day emissions. Figure 5-10 shows similar results for the Forage Field site. The results for both sites demonstrate the large influence of soil-slurry surface pH and the need for an empirical or

process-based model of how soil-slurry properties and interactions determine surface pH immediately following application.

Figure 5-9: Influence of surface pH on NH₃ volatilization at Richmond. Application of slurry occurred on Day 258. Infiltration reduction factor of 0.05 assumed.

Figure 5-10: Influence of surface pH on NH₃ volatilization at Forage Field. Application of slurry occurred on Day 219. Infiltration reduction factor of 0.05 assumed.

5.2.4 Microbial Processes Investigation

The influence of microbial processes on ammonia volatilization following slurry application was another aspect considered. Process-based models of ammonia volatilization do not include all microbial processes (mineralization, immobilization, nitrification, and denitrification) that control soil nitrogen dynamics. Sommer and Hutchings (2001) state that mineralization and nitrification have negligible effect on ammonia emissions in the first 2 weeks following application. However, these generalizations were based on the assumption of northern European conditions.

The uncertainty in the contribution of microbial processes to ammonia emissions warranted a comparison of model results with and without inclusion of microbial processes. However, simulations based on the two conditions showed that microbial processes have no significant impact on ammonia emissions the week following application. This confirms Sommer and Hutching's (2001) statement that microbial processes can be neglected in the first couple of weeks following application due to the fact that microbial processes are slow and most ammonia is lost within a short period of application. Section 7.0 will present an example simulation of a longer period and how microbial processes influence emissions over this period.

6.0 MODEL RESULTS

6.1 NH₃ Emissions

6.1.1 *Richmond Results*

The inputs required to simulate the Richmond site can be found in Table 5-1. Ammonia emissions at the Richmond site were first simulated assuming a constant pH of 7.7 which is based on the 0.5 pH increase assumed by the model of Générmont and Cellier (1997). The initial slurry pH was taken to be 7.2 for dairy cattle slurry (from Hengnirun et al., 1999).

Figure 6-1 shows the predicted NH₃ fluxes compared to measurement data. While the diurnal emission trends associated with solar radiation (Figure 6-2) is simulated well, the peak simulated emissions on the application day are lagged by 1 to 2 hours compared to measurements. This may be attributed to the location of the measurement towers and the flux footprint concept. Application started directly beneath the towers at 11:00 (EST), giving an earlier emission peak since footprint measurements will give the most weight to emissions closest to the towers. In reality, application over the entire upwind field ended at 17:00 and fluxes averaged over the entire field will remain high until this time. The simulation also showed overestimation on the days following application.

A simulation was then run assuming that the pH is not constant and decreases gradually following application. Figure 6-3 shows this simulation using a decreasing pH

that best fit emissions data. The simulation assumed that the pH of the surface layers is 7.4 immediately following application and decreases linearly until the initial soil pH is reached. The best fit to emissions data resulted in the pH decreasing to initial soil pH by Day 263. Both the simulated diurnal trends and magnitudes of emissions are simulated well using a decreasing pH. Cumulative losses are lower in that losses are less than 20% by the end of Day 268 compared to 26% for the constant pH assumption (Figure 6-1). Note that these cumulative losses are due to volatilization only.

Unlike the model testing of Genermont and Cellier (1997), simulation results showed that assuming a constant pH over an ammonia volatilization event is inadequate as there are other factors (i.e. soil buffering capacity) besides slurry type controlling the pH. Some overestimation during simulations of constant pH could be attributed to the AGRIN's assumption of zero atmospheric concentration. In reality there are background concentrations and advective flows from nearby fields leading to a smaller driving force for volatilization when looking at Equation 3.85.

Figure 6-1: Comparison of predicted NH_3 fluxes to Richmond field data (constant pH). Constant surface pH of 7.7 assumed. Application of slurry occurred on Day 258. Infiltration reduction factor of 0.05 used in simulation. FG: flux gradient measurements. REA: relaxed eddy accumulation measurements.

Figure 6-2: Simulated net radiation for Richmond.

Figure 6-3: Comparison of predicted NH_3 fluxes to Richmond field data (decreasing pH). Application of slurry occurred on Day 258. Infiltration reduction factor of 0.05 used in simulation. FG: flux gradient measurements. REA: relaxed eddy accumulation measurements.

6.1.2 Forage Field Results

The inputs required to simulate the Forage Field site can be found in Table 5-2. The ammonia fluxes following slurry application were simulated assuming that the pH is not constant and decreases following application. Figure 6-4 shows this simulation using a decreasing pH that best fit emissions data. This simulation assumes that the pH of the surface layers starts at 6.6 and decreases linearly to the initial soil pH before application. Emissions data are best fit by decreasing the pH to the initial pH by Day 220. Both the simulated diurnal trends and magnitudes of emissions are simulated well using a decreasing pH.

The sudden peak in simulated emissions seen in the afternoon on Day 222 is due to an increase in turbulent transfer based on simulated aerodynamic resistance. The resistance calculation is based on site meteorological data which shows high wind speeds (almost 8 m s^{-1}). The last recorded emission measurement occurs an hour before these winds are experienced. Another contribution to the overestimation is the assumption of a zero surface resistance.

There is some overestimation on Day 221 and there could be several reasons for this: (1) changes in wind direction caused the measurement tower to no longer be downwind of the emission area; (2) the simulated surface TAN available for volatilization is overestimated as a result of TAN infiltration being underestimated; (3) an overestimated surface temperature; and (4) the simulated surface pH is too high. Site data indicated that the measurement tower is downwind of the emission area on Day 221. Testing of the soil heat and moisture module indicated that soil moisture movement was being adequately modelled; however, testing did indicate that surface temperature was overestimated by 5°C at times. The simulated surface pH is constrained by the initial soil pH before application; since the soil pH was assumed to be 6.3 based on past data from similar sites in the area it is possible that the actual pH may have been overestimated.

Figure 6-4: Comparison of predicted NH_3 fluxes to field data for Forage Field (decreasing pH). Application of slurry occurred on Day 219. Infiltration reduction factor of 0.05 used in simulation. REA: relaxed eddy accumulation measurements.

Figure 6-5: Simulated net radiation for Forage Field.

6.2 Nitrogen Species Profiles

6.2.1 *Richmond Results*

Figure 6-6 shows the predicted soil TAN concentrations near the soil surface following application while Figure 6-7 shows the predicted nitrate concentrations. The highest concentrations for TAN occur immediately following application at a soil depth less than 0.5cm. These peak concentrations are due to infiltration of the slurry which contains higher species concentrations relative to the soil prior to application. As TAN and nitrate infiltrate through the soil profile and, in the case of TAN, volatilizes through the soil surface, concentrations begin to approach a more uniform profile after 72 hours. It becomes clear that NH_3 fluxes decrease over time because of the reduced availability of TAN at the soil surface. These reduced concentrations are due to volatilization losses, adsorption and infiltration.

The concentration of nitrate infiltrating the soil from the slurry is not that high relative to nitrate concentrations throughout the soil profile. Figure 6-7 shows the concentrations are much more uniform throughout the soil profile compared to TAN. The fact that concentrations are decreasing uniformly through the profile suggests that soil water infiltration is as much a controlling factor as slurry infiltration. The steady decrease to concentrations below those experienced before slurry application indicate that the assumed initial concentration profile may be too high.

Figure 6-6: Predicted total ammoniacal nitrogen (TAN) concentration profiles for Richmond.

Figure 6-7: Predicted nitrate concentration profiles for Richmond.

6.2.2 Forage Field Results

Figure 6-8 shows the predicted soil TAN concentrations near the soil surface following application while Figure 6-9 shows the predicted nitrate concentrations up to a 1 metre depth for Forage Field. Again, the highest concentrations for TAN occur immediately following application at a soil depth less than 0.5cm and the concentration of nitrate infiltrating the soil from the slurry is not that high relative to nitrate concentrations throughout the soil profile.

Figure 6-8: Predicted total ammoniacal nitrogen (TAN) concentration profiles for Forage Field.

Figure 6-9: Predicted nitrate concentration profiles for Forage Field.

6.3 Comparison to Emission Factors

Figure 6-10 and Figure 6-11 compare simulated ammonia fluxes to emission factor (EF) predictions and demonstrate AGRIN's improvement upon empirical EF's. The straight lines are the EF prediction. The EF of 17.5% (% of TAN applied that is lost through NH_3 emissions) used was chosen based on an average of a 15% EF given by Misselbrook et al. (2000) for dairy cattle slurry spread between August and April and a 20% EF given by de Vries et al. (2002) for any slurry that is surface applied to arable land. This EF represents

how much TAN is lost in total from the slurry due to volatilization and does not incorporate any temporal resolution.

If the EF is applied on a daily scale, emissions are assumed to only occur on the day of application and the timing and magnitude of peak emissions are missed. While an EF applied on a weekly scale can account for fluxes on subsequent days, it largely underestimates emission peaks and still cannot account for any diurnal trend. However, the 17.5% total loss corresponds well to the approximate 20% cumulative losses predicted by AGRIN. The difficulty in applying the appropriate EF is that the factors were developed for UK agriculture and no EF describing emissions from manure application could be found for the United States or Canada (only factors on a cow basis were found).

Figure 6-10: Comparison of model results to emission factors for Richmond. Emission factors (EF's) represent % of TAN applied lost to NH_3 volatilization.

Figure 6-11: Comparison of model results to emission factors for Forage Field. Emission factors (EF's) represent % of TAN applied lost to NH_3 volatilization.

7.0 EXAMPLE APPLICATION

One of the objectives of developing AGRIN is to use a process-based approach to examine emission trends over different time periods (hourly to length of growing season). This section presents an example application of AGRIN over the growing season (May to October) and investigates the influence of environmental conditions and microbial processes.

7.1 Simulated Site

The site data is not based on a specific location in Ottawa, Ontario and the application scenario is not based on one specific field study but rather data from various online data and literature sources. The input values required to run the model for various conditions are listed in Table 7-1. The model was run for the duration of a typical growing season assumed to be 165 days from early May to mid-October 2005. A tillage event occurs in the fall on Julian Day 288 and is simulated by making the soil profiles uniform up to an assumed tillage depth of 10cm. The input file can be found in Appendix B (exappn.inp).

Table 7-1: Input values for example application

Input	Value	Source
Site Data		
Hourly temperatures, wind speed, cloud cover	-	Environment Canada 2005 online data (2005 data)
Hourly solar radiation and precipitation	-	Central Experimental Farm online data (2005 data)
Surface roughness lengths	0.001 m	Assumed
Zero plane displacement	0.0 m	Assumed
Type of soil	Loam	Assumed
Soil bulk density	1.4 g cm ⁻³	Assumed
Initial temperature profile	-	Central Experimental Farm online data (2005 data)
Initial moisture profile	0.35 cm ³ cm ⁻³	Assumed
Initial surface NO ₃ ⁻ and NH ₄ ⁺ concentrations	9.35E-7 and 8.1E-6 g cm ⁻³	Assumed
Initial NO ₂ ²⁻ profile	0.0 g cm ⁻³	Assumed
Initial soil surface pH	6.9	Assumed
Initial residue and soil organic carbon soil surface concentrations	0.024 and 0.019 g cm ⁻³	Grant and Pattey (2003)
Gradients for pH, nitrogen and carbon	-	Grant and Pattey (2003)
Manure data		
Type	Dairy cattle slurry	Assumed
Solids content (% weight based)	6.9	Hengnirun et al. (1999)
Total nitrogen (% weight based)	0.49	Hengnirun et al. (1999)
Nitrate content	0.036 g-N L ⁻¹	Hengnirun et al. (1999)
pH	7.2	Hengnirun et al. (1999)
C:N ratio	10.2	Hengnirun et al. (1999)
Application data		
Rate	83 340 L ha ⁻¹	Hengnirun et al. (1999)
TAN application rate	135 kg N ha ⁻¹	Hengnirun et al. (1999)
Day of application	Julian Day 135	Assumed
Area	10 ha	Assumed
Timing	8:00 to 16:00 (EST)	Assumed

7.2 NH₃ Emission Simulation Results

7.2.1 *Influence of Microbial Processes*

Previous model testing showed that microbial processes do not significantly affect ammonia volatilization in the days immediately following manure application. To determine the influence of microbial processes, the example application considers a longer term. Figure 7-1 shows modelled ammonia volatilization and TAN profiles not including microbial processes (nitrification, denitrification and decomposition are not included as source-sink terms) while Figure 7-2 shows simulation results when these processes are included. While emissions in the week following application are not significantly reduced, Figure 7-2 shows that microbial processes are depleting TAN such that less is available for volatilization at the soil surface. Immobilization will reduce the amount of TAN through conversion to organic N while nitrification will also act to reduce TAN through oxidation to nitrate.

Microbial processes are slow enough to not significantly impact emissions in the week following application, but over the growing season microbial activity will significantly reduce emission in the following months. Cumulative emissions continuously increased for the simulation not including microbial processes while cumulative emissions plateau when these processes are included due to reduced TAN. The cumulative emissions with microbial processes much better represent the emission factors present in literature (15-20%). This demonstrates that a process-based model lacking inclusion of decomposition, nitrification, and denitrification rates cannot

adequately assess ammonia volatilization losses over longer-terms (longer than 1 week after application).

(a)

(b)

Figure 7-1: Example application over growing season with no microbial processes.
 (a) Simulated ammonia volatilization. Application of dairy cattle slurry occurs on Day 125. (b)
 Predicted total ammoniacal nitrogen (TAN) concentration profiles in soil surface layers.

(a)

(b)

Figure 7-2: Example application over growing season with microbial processes.
 (a) Simulated ammonia volatilization. Application of dairy cattle slurry occurs on Day 125. (b) Predicted total ammoniacal nitrogen (TAN) concentration profiles in soil surface layers.

7.2.2 Influence of Environmental Conditions

To demonstrate the influence of environmental variables on ammonia volatilization, solar radiation and rainfall were examined. Solar radiation will affect atmospheric stability (wind speed and temperature profiles) and increasing radiation should lead to unstable conditions which should increase volatilization rates (Sommer et al., 2003). Figure 7-3 shows a 5 day period during the example simulation where a couple of cloudy and rainy days (Days 169 and 170) are followed by mainly clear days with no precipitation (Days 171 and 172) and then another cloudy day (Day 173). The rate of ammonia volatilization is increasing with increasing net radiation and then decreases on Day 173 when net radiation is reduced due to clouds.

On Day 170, when the net radiation is higher than Day 169, ammonia volatilization decreases compared to the previous day which is contrary to the proportional relationship expected between radiation and volatilization. This is likely due to the influence of high wind speeds experienced on Day 169 which would promote higher volatilization rates. Sommer et al. (2003) note that volatilization rates will increase with increasing wind speed when solar radiation is low while volatilization rates will decrease with wind speed when radiation is high. This is due to the fact that wind speed will increase turbulent transport at low radiation levels but will lower the surface temperature (and the ammonia surface concentration) at high radiation levels.

(a)

(b)

Figure 7-3: Influence of net radiation on ammonia volatilization rates. Application of dairy cattle slurry occurred on Day 125. (a) Predicted net radiation and (b) ammonia volatilization over 5 day period.

The effect of rainfall was examined by looking at ammonia volatilization, moisture and TAN profiles before, during and after a rainfall event. Figure 7-4 shows the precipitation pattern and simulated fluxes and profiles over a 4 day period. A major rainfall event occurs over Days 134 and 135 and Figure 7-4(b) shows that ammonia volatilization is reduced immediately before and during the rainfall event due to reduced turbulent transfer and diluted TAN concentrations. After the rainfall event ends on the morning of Day 135, ammonia volatilization rates increase drastically resulting from the increased solar radiation causing evaporation of the infiltrated rainwater which will contain TAN from the soil. Figure 7-4(c) demonstrates that soil moisture will increase during the rainfall event while Figure 7-4(d) shows the TAN profiles before, immediately following and 1 day after the rainfall event. The TAN profiles show that TAN concentrations are slightly reduced as a result of the rainfall event but the concentration profile is redistributed such that TAN concentrations at the surface are actually higher than before the precipitation. While emissions are significantly reduced during a rainfall event (due to diluted concentrations at the surface), emissions are enhanced immediately after as soil water evaporates through the soil surface.

(a)

(b)

(c)

(d)

Figure 7-4: Influence of precipitation on ammonia volatilization rates and TAN profiles. Application of dairy cattle slurry occurred on Day 125. (a) Precipitation, (b) ammonia volatilization, (c) soil moisture and (d) total ammoniacal nitrogen (TAN) soil surface profiles.

7.2.3 Comparison to Emission Factors

Figure 7-5 compares simulated ammonia fluxes to the emission factor (EF) prediction and once again demonstrates AGRIN's improvement upon empirical emission factors. The EF of 17.5% (% of TAN applied that is lost through NH_3 emissions) was used again as in previous comparisons. This EF represents how much TAN is lost in total from the slurry and does not incorporate any temporal resolution. On an annual basis, the 17.5% EF agrees well with the cumulative ammonia losses to volatilization simulated by AGRIN. However, this EF is not capable of capturing the diurnal trends associated with environmental conditions such as solar radiation.

Figure 7-5: Comparison of model results to emission factor for example application. Emission factor (EF) represent % of TAN applied lost to NH_3 volatilization. Note that Ammonia Flux axis has been scaled to better show EF line and maximum simulated fluxes are much higher than $1 \mu\text{g m}^{-2} \text{s}^{-1}$ such that they are not shown on graph.

7.3 Other N Trace Gas Simulations

The example application was also used to simulate nitrous oxide (N_2O) and nitric oxide (NO) soil emissions. Simulations using the bulk transfer coefficient (inverse of the sum of the resistances) for ammonia caused emissions to be too high such that N trace gases were within the soil profile were depleted within three days. Simulations shown in Figure 7-6 and Figure 7-7 are based on an upper boundary condition from the surface concentration gradient (i.e. assuming surface fluxes dominated by diffusion).

High emission peaks of N_2O are simulated immediately following manure application indicating that denitrifier activity is being stimulated by the addition of inorganic N. Higher fluxes of NO are also simulated following manure application due to enhanced nitrification and denitrification rates due to the addition of inorganic N. There are also two other periods of enhanced emissions: a period between Days 167 and 200 and the period after Day 270. An investigation into why these enhanced emissions occurred examined the influence of temperature which increases microbial activity and turbulent fluxes. These factors appear to be the cause of the increased emissions shown between Days 167 and 200 but do not explain the sudden emission increases simulated after Day 270. Microbial process rates (nitrification and denitrification) did not increase dramatically so it seems the increased surface concentrations causing the high emissions may be a result of numerical error or discretization problems although an investigation into this yielded no evidence of either of these problems.

These preliminary simulations of N₂O and NO emissions indicate that the factors controlling emissions are not only dominated by manure application in that environmental variables such as temperature and precipitation may play just as important a role. The production rates of these trace gases are controlled by microbial processes where inorganic N must be transformed through decomposition, nitrification and denitrification whereas NH₃ emissions can occur almost instantaneously from the inorganic N pool.

Figure 7-6: Simulated nitrous oxide emissions for an example application.
Application of dairy cattle slurry occurred on Day 125.

Figure 7-7: Simulated nitric oxide emissions for an example application.
Application of dairy cattle slurry occurred on Day 125.

8.0 CONCLUSIONS AND RECOMMENDATIONS

This thesis developed a temporally refined process-based model capable of predicting ammonia (and other nitrogen trace gases) soil emissions following slurry application to a bare soil. Based on the theory developed and model testing conducted, several conclusions can be drawn and recommendations can be made. These conclusions and recommendations are outlined below.

8.1 Conclusions

Based on model testing and comparison to emission factors it can be concluded that:

- A process-based model capable of predicting ammonia emissions from a bare soil following slurry application has been successfully developed. This model (AGRIN) improves upon existing models by using a temporally refined scale (hourly) and incorporating all of the biological, physical and chemical processes controlling nitrogen transformations and transport in the soil.
- In the immediate days following slurry application, ammonia volatilization is most sensitive to pH while slurry infiltration rate affects emissions to a lesser degree. The assumption of constant surface pH following application cannot adequately describe emission magnitudes while a gradually decreasing pH is more successful at capturing these magnitudes. In addition to soil-slurry characteristics, the influence of

slurry infiltration rate is also governed by timing of application and the rate of application.

- Ammonia volatilization diurnal trends are strongly related to environmental conditions. Increasing solar radiation will enhance emissions through the enhancement of turbulent transfer. Rainfall events will suppress emissions because of the reduced solar radiation associated with these events (if occurring during the daytime) and the fact that infiltrating rainfall will dilute and force aqueous TAN downward away from the soil surface.
- While AGRIN and emission factors predict similar cumulative TAN losses due to volatilization, emission factors are not capable of capturing the application day peak emissions and the diurnal emission trends associated solar radiation.
- Microbial processes (nitrification, denitrification, and decomposition) have no significant impact on soil ammonia emissions in the week following slurry application, however these processes significantly deplete soil TAN over periods longer than a week.
- Preliminary simulations of other nitrogen trace gases besides ammonia were able to demonstrate the enhanced emissions associated with manure application but showed that other factors which influence microbial activity (i.e. temperature) also play an important role. These simulations indicated that there may be issues with numerical error or discretization

schemes as sudden increases in emissions in the fall season could not be correlated with any increase in microbial activity.

8.2 Recommendations

Based on model testing and the long-term objective of developing a national ammonia emission inventory some recommendations for future work include:

- Empirical/process models describing slurry infiltration rates and changing soil surface pH after slurry application should be developed. Surface pH in particular is a major controlling factor of ammonia emissions and an empirical model would have potential to better simulate emissions versus assuming a constant pH.
- Development of more accurate default parameters that can better reflect different soil types, slurry characteristics, climate regimes and microbial kinetics.
- Increase AGRIN's applicability by the inclusion of the soil freeze/thaw cycle, a canopy layer and two-dimensional considerations.
- Use AGRIN to test what if scenarios such as testing different farm management practices which could be implemented to reduce emissions.
- Use AGRIN to develop emission inventories on larger spatial scales (local to regional to national). These emission inventories have potential to better understand emission trends and can act as input for models of short- and long-range deposition models.

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APPENDIX A: SOURCE CODES

A.1 Initialization file: agrininit.inc

```
!-----  
! File agrininit.inc  
! Program Units: ALL  
! All common blocks and constants are initialized, with the  
! exception of some constants set in agrin in.f  
!-----  
DATA DELT,DIFMAX,DELSAV,ISWDIF,DELSUB,TSUB,TSTART,IDAY,N,IGO150, &  
& RFACT,HTIME,HOUR,NHR,OUTTIM /15*0/  
DATA RTIME/25*0/,RRHA,RRHS/2*0.5/,AMOUNT/25*0/  
DATA TDWT/25*0/,TAT/25*0/,WDT/25*0/,SRT/25*0/,CLDT/25*0/,RNT/25*0/  
DATA Z/M1*0/,THETA/M1*0/,TTHETA/M1*0/,T/M1*0/,TT/M1*0/,KL/M1*0/  
DATA HSOL/M1*0/,ZY/M1*0/,KDNH4/M1*0.0/,NH3G/M1*0.0/,NNH3G/M1*0.0/  
DATA NH3L/M1*0.0/,NNH3L/M1*0.0/,KHNH3/M1*0.0/,NH4S/M1*0.0/  
DATA HION/M1*0.0/,HHION/M1*0.0/,CTOBIOR1/M1*0.0/,NTOBIOR1/M1*0.0/  
DATA KKH MID/M1*0/,CTOBIOR2/M1*0.0/,NTOBIOR2/M1*0.0/,NNH4S/M1*0.0/  
DATA RESINIT,SOCINIT,NH4INIT,NO3INIT,NO2INIT,PHINIT,CLY/7*0.0/  
DATA  
SRES,BLKDEN,CNRES,KRES0,HRES0,RESRATE,SOCRATE,NH4RATE/8*0.0/  
DATA NO3RATE,NO2RATE,PHRATE,TOTALA/4*0/  
DATA QT/M1*0/,CCH/M1*0/,THICK/M1*0/,ZZ/M1*0/,QHC/M1*0/,QHW/M1*0/, &  
& SUBQHC/M1*0/,QL/M1*0/  
DATA APPNA/366*0/,APPNSRT/366*0/,APPNEND/366*0/,APPNDEN/366*0.0/  
  
DATA APPNRATE/366*0.0/,APPNDEPTH/366*0.0/,CNAPPN/366*0.0/  
DATA NTOTAPPN/366*0.0/,OMAPPN/366*0.0/,DMAPPN/366*0.0/  
DATA PHAPPN/366*0.0/,APDAY/366*0/,SUBQHW/M1*0/,IDENITBIO/M1*0.0/  
DATA CRES/M1*0.0/,CBIO/M1*0.0/,CHUM/M1*0.0/,CPASS/M1*0.0/  
DATA CCRES/M1*0/,CCBIO/M1*0/,CCHUM/M1*0/,CCPASS/M1*0/,N2/M1*0/  
DATA SOC/M1*0/,NH4/M1*0/,NO3/M1*0/,NO2/M1*0/,NN2/M1*0/,SSOC/M1*0/  
DATA NNH4/M1*0/,NNO3/M1*0/,RNH4MIN/M1*0.0/,RNH4DISS/M1*0.0/  
DATA RNH3PROD/M1*0.0/,NNO2/M1*0/,PH/M1*0/,INITBIO/M1*0/,PPH/M1*0/  
DATA BIONIT/M1*0.0/,BBIONIT/M1*0.0/,BIODENIT/M1*0.0/  
DATA BBIODENIT/M1*0.0/  
DATA  
DMAXBA,DMAXHE,DELMAX,DELMIN,TMOIST,LOG10E,MGR,SSFLUX,QHLAST, &  
& TGRAD,RKMOD,VAPDIF,HSTORE,OSMPOT/14*0.0/  
DATA IPLANT,LOWER,NDAYS,NDAY,KOPT,IVAPOR,MATN,NPT,NGRAV,IEVOPT,  
&  
& INC,NWATER,NPRINT,IETOPT,ISHOPT,IHEAT,IRAD,ISOL,LOWERH,UPPERH, &  
& ICLOUD,ICONVH,IDBEG,IDEND,NODEIN,ITRACE,IAPPN,IRES,NAPPN/29*0/  
DATA START,FINISH /2*.TRUE./  
DATA MAT /M1*0/,CHS/M2*0/
```

```

DATA CHSOIL/M1*0/,CH/M1*0/,KH/M1*0/
DATA DAYMET,LAT,ALBEDO,ZH,ZM,ZT,ZU,D,HOURSEXT,TAQ,SINDEC,COSDEC,
&
& SINLAT,COSLAT,TANLAT,TPIY,SLALT,RN,SUBSEN,SUBSHF,SUBRN,      &
&
SUBLE,SUBHBE,VD_A,SR_FRAC,SHFLUX,USTAR,TMAX,TMIN,TMEAN,SR_MEAS, &
& WIND,CLOUD,EMISS_A,EMISS_S,TSMEAN,KKHNP,ILEAP,RHMEAN,METDAY,
&
& QHCTOP,SENFLX,LE/43*0.0/
DATA DAYSTP,TSTP,LOUT,QHW0,SUBQHW0,NTOTAL,MAXREC,IREF,IERROR,
&
& NCHR,REC,UPPER,STOPHR,NDEPTH /14*0/
DATA PI/3.14159265358979/

```

! Soil module parameters

```

! CHA = Volumetric specific heat of air [J/m3/K]
! CHV = Volumetric specific heat of vapor [J/cm3/K]
! CHW = Volumetric specific heat of water [J/cm3/K]
! GASCON = Gas constant [erg/mole/K]
! GRAV = Gravity constant [m/s2]
! MOLAR = Molar mass of water [g/mole]
! LHV0 = Latent heat of vaporization at [J/g]
! reference temperature T0
! SB = Stephan-Boltzman constant [W/m2/K4]
! SEXT = Solar constant [W/m2]
! T0 = Reference temperature [K]
! VK = von Karmens constant [-]
! WATDEN = Density of water [g/cm3]

```

```

DATA CHA /1200.0/
DATA CHV /1.8/
DATA CHW /4.18/
DATA GASCON /8.3143E7/
DATA GRAV /9.807/
DATA MOLAR /18.0/
DATA LHV0 /2500./
DATA SB /5.67E-8/
DATA SEXT /1360.0/
DATA T0 /273.16/
DATA VK /0.4/
DATA WATDEN /1.0/

```

! Decomposition parameters

```

! SBIO = labile fraction of biomass pool [-]
! SHUM = labile fraction of humads pool [-]
! KBIO0 = SDR for labile fraction of biomass pool [1/d]
! KHUM0 = SDR for labile fraction of humads pool [1/d]
! HBIO0 = SDR for resistant fraciton of biomass pool [1/d]
! HHUM0 = SDR for resistant fraciton of humads pool [1/d]
! CNBIO = C/N ratio of biomass pool [kg C/kg N]
! CNHUM = C/N ratio of humads pool [kg C/kg N]

```



```

!      FBIO = fraction of initial SOC (exluding residues) that resides in biomass pool
!      FHUM = fraction of initial SOC (exluding residues) that resides in humads pool
!      FPASS = fraction of initial SOC (exluding residues) that resides in passive pool
!      FNBIO = efficiency of microbial biomass or fraction of C flow
!              out of residue pool in biomass pool      [-]
!      FNBIOR1 = fraction of C flow out of biomass pool recycled
!              in biomass pool [-]
!      FNHUM = fraction of C flow out of biomass pool into humads
!              pool [-]
!      FNBIOR2 = fraction of C flow out of humads pool recycled
!              into biomass pool [-]
!      FNPASS = fraction of C flow out of humads pool into passive
!              pool [-]
!      Note that residue parameters are defined in agrin in.f or by the user

```

```

DATA SBIO /0.9/
DATA SHUM /0.16/
DATA KBIO0 /0.00825/
DATA KHUM0 /0.004/
DATA HBIO0 /0.001/
DATA HHUM0 /0.00015/
DATA CNBIO /8.0/
DATA CNHUM /8.0/
DATA FBIO /0.03/
DATA FHUM /0.47/
DATA FPASS /0.5/
DATA FNBIO /0.2/
DATA FNBIOR1 /0.6/
DATA FNHUM /0.2/
DATA FNBIOR2 /0.2/
DATA FNPASS /0.4/

```

! Nitrification Parameters

```

!      DO2A = diffusion constant of oxygen in air [cm2/hr]
!      O2ATM = atmospheric oxygen concentration [mol/cm3 air]
!      FINITBIO = fraction of initial biomass that consists of nitrifiers [-]
!      FDENITBIO = fraction of initial biomass that are denitrifiers [-]
!      GMAXNIT = maximum growth rate for nitrifiers [1/hr]
!      DMAXNIT = maximum death rate for nitrifiers [1/hr]
!      RMAXNIT = maximum nitrification rate [cm3water/g/hr]
!      VO2 = potential O2 reaction potential [mol m-3 s-1]

```

```

DATA DO2A /655.2/
DATA O2ATM /0.00000886/
DATA FINITBIO /0.1/
DATA FDENITBIO /0.02/
DATA GMAXNIT /0.2/
DATA DMAXNIT /0.008/
DATA RMAXNIT /0.00021/
DATA VO2 /20.0e-6/

```

! Equilibrium parameters

! DIFFH = diffusivity of [H+] in soil water [cm²/hr]
 ! KADS = Freundlich isotherm parameter [g soil solution / g soil or cm³/g]
 ! BADS = Freundlich isotherm parameter [-]
 ! KDDOC = liquid-solid partitioning coefficient for carbon [g soil solution/ g soil or cm³ H₂O/ g soil]
 ! KHNO = Henry's Law constant for nitric oxide [cm³ H₂O/ cm³ air]
 ! KHN₂O = Henry's Law constant for nitrous oxide [cm³ H₂O/ cm³ air]
 ! KHN₂ = Henry's Law constant for dinitrogen gas [cm³ H₂O/ cm³ air]
 ! KHO₂ = Henry's Law constant for oxygen [cm³ H₂O/ cm³ air]
 ! KDNO₃ = solid-liquid partitioning coefficient for nitrate [cm³ water/g soil]
 ! KDHION = solid-liquid partitioning coefficient for hydrogen ion [cm³ water/g soil]
 ! BUFFCAP = buffering capacity of soil [mol/kg/pH]

DATA DIFFH /0.00057/
 DATA KADS /50000.0000000/
 DATA BADS /1.0/
 DATA KDDOC /0.0011/
 DATA KHNO /21.52/
 DATA KHN₂O /1.635/
 DATA KHN₂ /67.01/
 DATA KHO₂ /31.44/
 DATA KDNO₃ /0.0/
 DATA KDHION /0.0/
 DATA BUFFCAP /0.07/

! Denitrification parameters

! MCD = maintenance coefficient with respect to carbon [g g⁻¹ h⁻¹]
 ! MNO₃ = maintenance coefficient with respect to nitrate [g g⁻¹ h⁻¹]
 ! MNO₂ = maintenance coefficient with respect to nitrite [g g⁻¹ h⁻¹]
 ! MNO = maintenance coefficient with respect to nitric oxide [g g⁻¹ h⁻¹]
 ! MN₂O = maintenance coefficient with respect to nitrous oxide [g g⁻¹ h⁻¹]
 ! YCD = maximum growth yield on carbon [g g⁻¹]
 ! YNO₃ = maximum growth yield on nitrate [g g⁻¹]
 ! YNO₂ = maximum growth yield on nitrite [g g⁻¹]
 ! YNO = maximum growth yield on nitric oxide [g g⁻¹]
 ! YN₂O = maximum growth yield on nitrous oxide [g g⁻¹]
 ! UNO₃MAX = maximum relative growth rate on nitrate denitrifier [h⁻¹]
 ! UNO₂MAX = maximum relative growth rate on nitrite denitrifier [h⁻¹]
 ! UNOMAX = maximum relative growth rate on nitric oxide denitrifier [h⁻¹]
 ! UN₂O MAX = maximum relative growth rate on nitrous oxide denitrifier [h⁻¹]
 ! KCD = half-saturation value with respect to carbon [g cm⁻³]
 ! KND = half-saturation value with respect to N oxides [g cm⁻³]
 ! CNDEN = C/N ratio of denitrifier biomass [g g⁻¹]
 ! FDEN = initial fraction of biomass that are denitrifiers

DATA MCD /0.0076/
 DATA MNO₃ /0.09/
 DATA MNO₂ /0.035/
 DATA MNO /0.079/
 DATA MN₂O /0.079/

DATA YCD /0.503/
 DATA YNO3 /0.401/
 DATA YNO2 /0.428/
 DATA YNO /0.151/
 DATA YN2O /0.151/
 DATA UNO3MAX /0.67/
 DATA UNO2MAX /0.67/
 DATA UNOMAX /0.34/
 DATA UN2OMAX /0.34/
 DATA KCD /0.000017/
 DATA KND /0.000083/
 DATA CNDEN /3.45/
 DATA FDEN /0.02/

!
 ! Transport module parameters
 ! DNO3L = nitrate molecular diffusivity in water [cm² h⁻¹]
 ! DNO2L = nitrite molecular diffusivity in water [cm² h⁻¹]
 ! DDOCL = DOC molecular diffusivity in water [cm² h⁻¹]
 ! DHL = H ion molecular diffusivity in water [cm² h⁻¹]
 ! DNH3A = ammonia molecular diffusivity in air [cm² h⁻¹]
 ! DN2OA = nitrous oxide molecular diffusivity in air [cm² h⁻¹]
 ! DNOA = nitric oxide molecular diffusivity in air [cm² h⁻¹]
 ! DN2A = dinitrogen molecular diffusivity in air [cm² h⁻¹]
 ! DCO2A = carbon dioxide molecular diffusivity in air [cm² h⁻¹]
 ! DCO2L = carbon dioxide molecular diffusivity in water [cm² h⁻¹]
 ! KHCO2 = Henry's Law constant for carbon dioxide [cm³ H₂O/cm³ air]
 ! UAIR = molecular viscosity of air [g/cm/s]
 ! KAIR = thermal conductivity of air [W/cm/K]
 ! CPAIR = heat capacity of air [J/g/K]
 ! NH4RAIN = concentration of NH₄⁺ in precipitation [g N/cm³]
 ! NO3RAIN = concentration of NO₃⁻ in precipitation [g N/cm³]
 ! HIONRAIN = concentration of H ions in precipitation [mol/cm³]
 ! CO2AIR = atmospheric CO₂ concentration [g/cm³ air]
 ! XAIR = atmospheric concentrations [mol or g/cm³ air]

DATA DNO3L /0.068/
 DATA DNO2L /0.069/
 DATA DDOCL /0.00684/
 DATA DHL /0.0342/
 DATA DN2OA /520.0/
 DATA DNOA /850.0/
 DATA DN2A /643.7/
 DATA DCO2A /576.0/
 DATA DCO2L /0.0576/
 DATA KHCO2 /1.2/
 DATA UAIR /0.000185/
 DATA KAIR /0.000257/
 DATA CPAIR /1.005/
 DATA NH4RAIN /0.0/
 DATA NO3RAIN /0.0/

```

DATA HIONRAIN /0.0/
DATA CO2AIR /5.72E-7/
DATA O2AIR /9.047e-6/
DATA NH3AIR /0.0/
DATA NOAIR /0.0/
DATA N2OAIR /0.0/
DATA N2AIR /4.76E-4/
!
!
! WCOMPR is the compressibility of water, 1/cm
!
DATA WCOMPR /4.58D-08/
!
! Minimum time resolution (hour)
!
DATA TIMRES /1.0D-4/
!
! Output logical - if user writes to file, warning messages sent to
! screen and file
!
LUSLUW = .FALSE.
!-----

! End of file agrininit.inc
!-----

```

A.2 Globalization file: agringlob.inc

```

!-----
! File AGRINGLOB.INC
! Dimensions
! Logical unit parameters
! Record length specification
! Common blocks
! Equivalences
! Program Units: all
!-----
IMPLICIT REAL*8 (A-H,O-Z)
IMPLICIT INTEGER (I-N)
!-----
! PARAMETER assignments
!-----
!
! M1 is the maximum dimension for nodal arrays
!
PARAMETER (M1 = 1000)
!

```

```

! M2 is the maximum number of soil types
!
PARAMETER (M2 = 10)
!
! IRLMOD modifies the output file record length.
! IRLMOD = 1 VAX and PC single precision
! IRLMOD = 2 VAX and PC double precision
!
PARAMETER (IRLMOD = 2)
!
! Logical unit assignments
! LUI = binary input file unit, input to main program
! LUB = binary output file unit from input program
!       binary output file unit from main program
! LUR = read (interactive input unit)
! LUS = screen (interactive and additional output unit)
! LUW = output files from DATAOUT
! LUH = output file containing hysteresis restart information
! LUX = scratch file
!
PARAMETER (LUI = 1, LUB = 2, LUR = 5, LUS = 6, LUW = 7, LUH = 8)
PARAMETER (LUX = 3)
!
! Internally calculated parameters (used in equivalence statements)
!
! M9 = total number of PET/MET and PRECIP input file names
!
PARAMETER (M9 = 100)
!-----
! End of PARAMETER assignments
!
! Begin data type assignments
!-----
CHARACTER*80 IFILE,OFIL,FILE,BIFILE,RFILE,TMFILE,PMFN(M9),      &
& PRFN(M9),TITLE,DUMMY,STIME*11,SDATE*11
DIMENSION RATE(50),CHS(M2),CHSOIL(M1),AMOUNT(25),RTIME(25)
REAL*8 LOG10E,MGR,LAT,LHV0,LE,KKLMID,KKLNPT,KL,KKHNP,KH(M1),KH1,
&
& KH2,KHMID(M1),KKHMID(M1),KLMID,KKL,KKH(M1),KDNH4,KAIR
REAL*8
NH4INIT,NO3INIT,NO2INIT,NH4RATE,NO3RATE,NO2RATE,NNH3,NH3
REAL*8 NH3L,NNH3L,NNOL(M1),NOL(M1),NH3FLUXMAX,TANFLUXBOT
REAL*8 NO3(M1),NO2(M1),NO(M1),N2O(M1),N2(M1),NH4(M1),NNH4(M1)
REAL*8 NNO3(M1),NNO2(M1),NNO(M1),NN2O(M1),NN2(M1),NNH4S(M1)
REAL*8 NH4S(M1),NO3L(M1),NNO3L(M1),NO2L(M1),NNO2L(M1),NNH4L(M1)

REAL*8 KRES0,INITBIO,IDENITBIO(M1),NH4APPN,NTOTAPPN,NH4L(M1)
REAL*8 NMINBIO1(M1),NINBIO(M1),NNTOBIO,NMINRES,NINBIO1(M1),KHO2
REAL*8
KBIO0,KHUM0,KADS,KHNNH3,NTOBIOR1,NTOBIOR2,GRAV,KHH,KDDOC

```

```

      REAL*8
N4TOTAL,NN4TOTAL,NH3FREE,NNH3FREE,NH3G,NNH3G,NH3GP,NNH3GP
      REAL*8
KHCO2,NH4FLUX,NNTOHUM,NH3FLUX,NH4RAIN,NH3AIR,NH4FLUXBOT
      REAL*8
NH4SOIL1,NH4SOIL2,NH4BAL,MINTOT,NH3SOIL1,NH3SOIL2,NH3BAL
      REAL*8
NONIT(M1),N2ONIT(M1),NO3RAIN,KDNO3,NO3FLUXBOT,NO3FLUX,MN2O
      REAL*8 KDHION,HIONRAIN
      REAL*8
N2OL(M1),NN2OL(M1),KHN2O,KHNO,KCD,KND,MCD,MNO3,MNO2,MNO
      REAL*8
NRES,NNRES,NOAIR,NOFLUX,NOG(M1),NNOG(M1),N2OG(M1),NN2OG(M1)
      REAL*8
N2G(M1),NN2G(M1),N2OFLUX,N2FLUX,N2OAIR,N2AIR,KHN2,NO3BAL
      REAL*8 NO3SOIL1,NO3SOIL2,NNBIO(M1),NNRES1(M1),NMINRES1(M1)
      REAL*8
NO3APINIT,INITMOIST(366),NO3APPN(366),NH3FLUX1,NH4APPNRATE
      REAL*8
NMINBIO2(M1),NMINHUM1(M1),NMINHUM2(M1),NH4APINIT,NH3GSURF
      INTEGER
UPPER,UPPERH,NODEIN,KEST,APDAY,APPNSRT,APPNEND,TILLDAY
      INTEGER TFLAG
      LOGICAL LUSLUW
!-----
!   End data type assignments
!
!   Begin COMMON and EQUIVALENCE assignments
!-----
!
!   Character variables
!
      COMMON /CHAR/ IFILE,OFIL,FILE,BIFILE,RFILE,TMFILE,HYFILE,PMFN,PRFN, &
& TITLE,DUMMY,STIME,SDATE
!
!   Meteorological and surface variables
!
      COMMON /CMET/RMDATA(8,366),TDDATA(25,366),TADATA(25,366)
      COMMON /CMET/WDDATA(25,366),SRDATA(25,366)
      COMMON /CMET/CLDATA(25,366),RNDATA(25,366),WND
      COMMON /CMET/ TDWT(25),TAT(25),WDT(25),SRT(25),CLDT(25),RNT(25)
      COMMON /CMET/ TDEWT(25),TAIR(25),TTAIR(25),VD_AT
      COMMON /CMET/ ALBEDO,VK

      COMMON /CMET/LHV0,PI,CHW,ZH,ZM,ZT,ZU,D,CHA,SB,SEXT,      &
& GRAV,HPR,SINDEC,COSDEC,LAT,SINLAT,COSLAT,TANLAT,TPIY,SLALT, &
& HOURSEXT,TAQ,RN,VD_A,SR_FRAC,SHFLUX,USTAR,TMAX,TMIN,TMEAN,TA,
&
& TTA,SR_MEAS,WIND,CLOUD,EMISS_A,WATDEN,TSMEAN,RHMEAN,SENFLX,
&
& EMISS_S,T0,CHV,LE,RLNZU,RLNZT,ICLOUD,NWATER,IRAIN,IETOPT,UPPER, &

```

```

& UPPERH,ISHOPT,ITOPBC,SA,ST,RNET,RH,TSQ
EQUIVALENCE (T(1),TS)
!
! Soil property variables
!
COMMON
/CSOIL/B(M2),SATMA(M2),THET(M2),SK(M2),VAPDIF,CHSOIL,WCOMPR
COMMON /CSOIL/ INC,IVAPOR,MAT(M1)

!
! Time parameters
!
COMMON
/CTIM/AMOUNT,RTIME,DELT,DIFMAX,DELSAV,DELSUB,TSUB,TSTART, &
&
& DMAXBA,DMAXHE,DELMAX,DELMIN,RFACT,HTIME,HOUR,OUTTIM,HEATBAL, &
& DAYTIM,STOPHR,TIMRES,TSTEPB,TSTPEM,TSTEPE,NDAYS,NDAY,DAYSTP,
&
& TSTP,IDAY,IDBEG,IDEND,METDAY,N,ISWDIF,IGO150,IN,NTOTAL,NYEARS, &
& IYS,NHR,RATE
!
! Water variables
!
COMMON /CWATER/THETA(M1),HSOL(M1),TTHETA(M1),T(M1),TT(M1),QT(M1), &
& ZY(M1),THICK(M1),ZZ(M1),QL(M1),QQL(M1),THETADIFF(M1),DIFFTOT(M1)
COMMON /CWATER/ KL(M1),KKL(M1),KLMID(M1),KKLMID(M1),DIFFY(M1)
COMMON /CWATER/ DDIFFY(M1),RHUMID,HEAD,SFLUX
SSFLUX,SSFLUXEXTRA
COMMON /CWATER/ TPREV,TMOIST,SMOIST,EXCESS,HPOND,PRAIN,PIRRI
COMMON /CWATER/ INMAX,IRTYPE,DHMAX,DHTOL,DHFACT,RAINIF

! Heat variables
!
COMMON /CHEAT/KH,KHMID,KKHMID,CH(M1),CCH(M1),QHC(M1), &
& SUBQHC(M1),QHW(M1),SUBQHW(M1),KKHNPT,KH1,KH2,KKLNPT,DHPREV,
&
& HSTORE,THPREV,SHSTORE,QHW0,KKH
COMMON /CHEAT/IHEAT,IRAD,ISOL

!
! Plant variables
!
COMMON /CPLANT/ IPLANT

!
! Decomposition, nitrification, denitrification variables
!
COMMON /CTRACE/ NINBIO,N2G,NO3RATE,NO2RATE,KDNH4(M1),NH3L(M1)
COMMON /CTRACE/
NNH3L(M1),NH4INIT,NO3INIT,NH3GSURF,NH4APPN(366)
COMMON /CTRACE/ NO2INIT,INITBIO(M1),KHNH3(M1),NH3(M1),NMINBIO1
COMMON /CTRACE/ KBIO0,KHUM0,IDENITBIO,NH4S,NNH4S,NH4L,NNH4L

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COMMON /CTRACE/
N4TOTAL(M1),NN4TOTAL(M1),NNH3G(M1),NH3FREE(M1)
COMMON /CTRACE/ NNH3FREE(M1),NH3GP(M1),NNH3GP(M1),NH3G(M1)
COMMON /CTRACE/
NH4FLUX,NH3FLUX,NH4FLUXBOT,NH4SOIL1,NH4SOIL2
COMMON /CTRACE/ NH4BAL,MINTOT,NH3SOIL1,NH3SOIL2,NH3BAL,N2OG
COMMON /CTRACE/
NONIT,N2ONIT,NO3FLUXBOT,NO3FLUX,NNOL,NOL,NO3L
COMMON /CTRACE/ N2OL,NN2OL,NRES(M1),NNRES(M1),NOG,NNOG,NN2OG
COMMON /CTRACE/ NO3,NO2,NO,N2O,N2,NNO3,NNO2,NNO,NN2O,NN2,NH4
COMMON /CTRACE/ NNTOBIO(M1),NNTOHUM(M1),NMINRES(M1),NINBIO1
COMMON /CTRACE/
N2OFLUX,N2FLUX,NO3BAL,NO3SOIL1,NO3SOIL2,NNBIO
COMMON /CTRACE/
NNRES1,NMINRES1,NMINBIO2,NMINHUM1,NMINHUM2,NN2G
COMMON /CTRACE/
NNH4,NH4RATE,M(M1),NH4APINIT(366),NO3APINIT(366)
COMMON /CTRACE/
NO3APPN,NTOBIOR1(M1),NTOBIOR2(M1),NH4APPNRATE(366)
COMMON /CTRACE/ CCRES(M1),CCBIO(M1),CCHUM(M1),SOC(M1),SSOC(M1)
COMMON /CTRACE/ CCRES1(M1),CRES1(M1),C2PRES1(M1),COUTRES(M1)
COMMON /CTRACE/ CRESPT(M1),crespt1(m1),BUFFCAP,PHPRE(M1)
COMMON /CTRACE/ iNITMOIST, CPASS(M1),CCPASS(M1)
COMMON /CTRACE/ DOC(M1),DDOC(M1),CO2(M1),O2(M1),OO2(M1),RO2(M1)
COMMON /CTRACE/ CCO2(M1),HION(M1),HHION(M1),CRES(M1),CBIO(M1)
COMMON /CTRACE/ RRO2(M1),DO2S(M1),DDO2S(M1),DO2SMID(M1)
COMMON /CTRACE/ DDO2SMID(M1),PHRATE,TOTALA,CHUM(M1),NNH3(M1)
COMMON /CTRACE/ ANVF(M1),AVF(M1),BIONIT(M1),BBIONIT(M1)
COMMON /CTRACE/ DBIONITDT(M1),RNIT(M1),DDDOCL1(M1),DDOCL1(M1)
COMMON /CTRACE
/SRES,CNRES,CLY,BLKDEN,RNH4DISS(M1),RNH3PROD(M1)
COMMON /CTRACE/ HRES0,HBIO0,HHUM0,EBIO,EBIOR1,EBIOR2,EHUM,SRESVL,
&
& EPASS,SOCINIT,RESINIT,PHINIT,CTOBIOR1(M1),CTOBIOR2(M1),CNRESVL
COMMON /CTRACE/ SOCRATE,RESRATE,FBIO,FHUM,FPASS,FINITBIO
COMMON /CTRACE/ PH(M1),PPH(M1),FDENITBIO,RNH4MIN(M1),DOCL(M1)
COMMON /CTRACE/
DDOCL(M1),DOCS(M1),DDOCS(M1),DNH3G(M1),DDNH3G(M1)
COMMON /CTRACE/
DNO3DTD(M1),DNO2DTD(M1),DNODTD(M1),DN2ODTD(M1)
COMMON /CTRACE/ DN2DTD(M1),BIODENIT(M1),BBIODENIT(M1),KRES0
COMMON /CTRACE/
SSRCENH4(M1),SRCENH4(M1),SRCENO3(M1),SSRCENO3(M1)
COMMON /CTRACE/ SRCETAN(M1),SSRCETAN(M1),TANSLURR,RVOL(M1)
COMMON /CTRACE/ SRCENO2(M1),SSRCENO2(M1),DDNH4(M1),DNH4(M1)
COMMON /CTRACE/
DNH3(M1),DDNO2(M1),DNO2(M1),DDNH3(M1),DDCO2(M1)
COMMON /CTRACE/
DCO2(M1),DDDOC1(M1),DDOC1(M1),SSRCEDOC(M1),DNO3(M1)
COMMON /CTRACE/
SRCEDOC(M1),SSRCEDO2(M1),SRCECO2(M1),DDNO3(M1)

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COMMON /CTRACE/
SRCEO2(M1),SSRCEO2(M1),DO2(M1),DDO2(M1),BLKCNH3
COMMON /CTRACE/ RDOCENIT(M1),RCO2DENIT(M1),RNASSDENIT(M1)
COMMON /CTRACE/
O2G(M1),OO2G(M1),SRCEH(M1),SSRCEH(M1),DH(M1),DDH(M1)
COMMON /CTRACE/
SSRCENH3(M1),SSRCECO2(M1),SRCENH3(M1),RCO2P(M1)
COMMON /CTRACE/
CCTOBIO(M1),CCTOHUM(M1),AFPS(M1),AAFPS(M1),RRB,RRC
COMMON /CTRACE/ CCTOPASS(M1),CINBIO(M1),C2PRES(M1),C2PBIO(M1)
COMMON /CTRACE/ C2PHUM(M1),CCO2G(M1),CO2G(M1),DISSTOT,PRODTOT
COMMON /CTRACE/ RH2OSLURR(366),RHSLURR(366),RNH4SLURR(366)
COMMON /CTRACE/ RNH3SLURR(366),TANINIT,HINIT(366),H2OINIT(366)
COMMON /CTRACE/ RCRESLURR(366),RNO3SLURR(366),RNRESLURR(366)
COMMON /CTRACE/
HIONL(M1),HHIONL(M1),HFLUX,HFLUXBOT,RNO3DENIT(M1)
COMMON /CTRACE/
RNO2DENIT(M1),RNODENIT(M1),RN2ODENIT(M1),SRCENO(M1)
COMMON /CTRACE/
RN2DENIT(M1),SSRCENO(M1),DNO(M1),DDNO(M1),DN2O(M1)
COMMON /CTRACE/
SRCEN2O(M1),SSRCEN2O(M1),SRCEN2(M1),SSRCEN2(M1)
COMMON /CTRACE/
DDN2O(M1),DN2(M1),DDN2(M1),CNRES1(M1),SLURRNH4TOT
COMMON /CTRACE/
CRESAPINIT(366),SLURRMAS(366),SLURRMAS1,SFLUX1
COMMON /CTRACE/ THICKNEW,SLFLUX1,DMNEW,dminit(366),THICKLOST
COMMON /CTRACE/
SQL1,SQL2,RHLE,CRESINPUT(M1),SLURRNH3FLUX,dnh4l(M1)
COMMON /CTRACE/
COUTRES1(M1),UCN(M1),SLURRNH4FLUX,SLURRNO3FLUX
COMMON /CTRACE/ TANAPINIT(366),TANL(M1),TTANL(M1),TTANTOT(M1)
COMMON /CTRACE/ TANCONC(M1),NH3FLUX1,RED,THICKADDED
COMMON /CTRACE/ SLURRTANfLUX1,h2olost,PHSOIL(M1),surfflux1
COMMON /CTRACE/
TANTOT(M1),AREATIME(366),H2OMASS(366),AREACOVERED
COMMON /CTRACE/
THICKEND,VOLH2O,SLURRTANFLUX,H2OLEFT,SFLUX21
COMMON /CTRACE/ RBNH3,APDAY1,TANFLUXBOT,TANFLUXTOP
COMMON /CTRACE/
TANSOIL1,TANSOIL2,O2L(M1),OO2L(M1),SFLUX3,SFLUX2
COMMON /CTRACE/ NODEIN,ITRACE,IAPPN,IRES,ITLL
!
! Application variables
!
COMMON /CAPPN/
APPNSRT(366),APPNEND(366),APPNRATE(366),APDAY(366)
COMMON /CAPPN/ APPNDEPTH(366),APPNDEN(366),CNAPPN(366)
COMMON /CAPPN/
TANAPPN(366),NTOTAPPN(366),PHAPPN(366),OMAPPN(366)
COMMON /CAPPN/ DMAPPN(366)

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```

COMMON /CAPPN/ APPNA(366),NAPPN,ITILL,TILLDAY
!
! Real variables
!
COMMON /CREAL/LOG10E,MGR,QHLAST,TGRAD,QLAST,PESUB,EEFLUX,EFLUX,
&
& RHA,VVD_S,VD_S,SVD_S,OSMPOT,PE,PT,DOV,SUBQHW0
!
! Geometry variables
!
COMMON /CGEOM/Z(M1),G,NPT
!
! Integer variables
!
COMMON /CINTEG/LOWER,ISAVUP,ISATUK,IEVOPT,LOWERH,ILEAP
!
! Output processing variables
!
COMMON /COUT/NODE(7),LOUT,NPRINT,MAXREC,IREC,NDEPTH,NCHR,IERROR
COMMON /COUT/REC,IPRINT
!-----
! End of file AGRINGLOB.INC
!-----

```

A.3 AGRIN IN source code

```

PROGRAM AGRIN IN
!-----
!
! Reads the data file *.INP, check the data and writes to
! the binary output file *.BIN, which serves as the input
! file to AGRIN MAIN
!-----
!
INCLUDE 'agringlob.inc'
INCLUDE 'agrininit.inc'
DATA DV/1.0/
LHV0 = LHV0*WATDEN !J/cm3
LOG10E = LOG10(EXP(1.D0))
CALL TIMEX
!
! IFILE = Input filename
!
CALL WELCOME('AGRIN')
20 WRITE(LUS,1010)
READ(LUR,'(A)') TMFILE
IF (INDEX(TMFILE(1:1),'0') .GT. 0) GOTO 999
NCHR = INDEX(TMFILE,' ')
TMFILE(NCHR:NCHR+3) = '.inp'
OPEN(UNIT=LUI,FILE=TMFILE,STATUS='OLD',IOSTAT=INERR)
IF (INERR .GT. 0) THEN

```

```

        WRITE(LUS,6005) IFILE
        GOTO 20
    ENDIF
6005  FORMAT(/,' No record of file ',A50,/, ' Try again...',/)
    INQUIRE(UNIT=LUI,NAME=IFILE)
    LOUT = LUW
    LUSLUW = .TRUE.
    TMFILE(NCHR:NCHR+3) = '.lis'
    OPEN (UNIT=LOUT,FILE=TMFILE,STATUS='UNKNOWN')
    CLOSE(UNIT=LOUT,STATUS='DELETE')
    OPEN(UNIT=LOUT,FILE=TMFILE,STATUS='NEW')
    INQUIRE(UNIT=LOUT,NAME=OFILE)
    WRITE(LUS,1040) OFILE
    WRITE(LOUT,1050) DV,IFILE,SDATE,STIME
1010  FORMAT(/,
    &' Enter input filename without the ".INP" extension',/,
    &
    &' (a "0" terminates the program) ==> ', $)
1020  FORMAT(/,
    &
    &' Output options in addition to creating < >.bin:',/,
    &
    &' (0) = no output',/,
    &
    &' (1) = options, nodes, soil properties,initial',/,
    &
    &' conditions, rain, meteorological conditions',/,
    &
    &' Enter choice ==> ', $)
1040  FORMAT(/,' The input summary filename is:',/,1X,A79)
1050  FORMAT(80('-',/, "!",T30,' Program AGRIN',T80,"!",/,
    &
    &"!",T32,' Version ',F4.2,T80,"!",/,80('-',/,
    &
    &' Input Filename: ',A60,/,
    &
    &' Date Processed: ',A11,/, ' Time Processed: ',A11)
!*****
!
!   OPTIONS, CONSTANTS, AND LIMITS
!*****
!
!   Read TITLE
!
    READ(LUI,'(A)') TITLE
    IPRINT = 1
    IF (IPRINT .GT. 0) THEN
        WRITE(LOUT,'(A,/,1X,A79)') ' Title:',TITLE
        WRITE(LOUT,'(/,A,/)') ' General options:'
    ENDIF
!
!   Read IPLANT,ITRACE,IAPPN,IRES,ITLL
!
    READ(LUI,'(5I)') IPLANT,ITRACE,IAPPN,IRES,ITILL
    IF (IPRINT .GT. 0) WRITE(LOUT,2010) IPLANT,ITRACE,IAPPN,ITILL

```

```

2010  FORMAT(T2,'IPLANT =',I5,T22,'ITRACE =',I5,T42,'IAPPN =',I5,T62,
&
&      'ITILL =',I5)
      G = 1 !Domain orientation always vertical
!
!      Read IFDEND,IDTBEG
!
      READ(LUI,'(2I)') IFDEND,IDTBEG
      IF (IPRINT .GT. 0) WRITE(LOUT,2020) IFDEND,IDTBEG
      IDTEND = IFDEND
      IF (IDTBEG .GT. IDTEND .OR. IDTBEG .LT. 1 .OR.
&
&      IDTEND .GT. 366) THEN
        WRITE(*,'(A)') ' IDTBEG and IDTEND must be between 1 and 366'
        WRITE(*,'(A)') ' and IDTBEG must be < or = than IDTEND.'
        GOTO 999
      ENDIF
2020  FORMAT(T2,'IFDEND =',I5,T22,'IDTBEG =',I5)

      IFLIST = 0 !Maintains that only option for entering met info is
single input file
      ISTEAD = 0 !Maintains that only transient solution available
      IYS = 1 !Maintains option of 1 year simulation
      NYEARS = 1 !Maintains options of 1 year simulation
!
!      Check if IDTEND and IFDEND within a calendar year
!
      IF (IDTEND .GT. 365 .OR. IFDEND .GT. 365) THEN
        WRITE(*,'(A)')
&
&      ' IDTEND and/or IFDEND exceeds no. of days in last year'
        GOTO 999
      ENDIF

      IF ((NYEARS .EQ. 1 .AND. IFDEND .LT. IDTBEG) .OR.
&
&      IFDEND .GT. IDTEND) THEN
        WRITE(*,'(A)')
&
&      ' IFDEND is not within range of IDTBEG and IDTEND.'
        GOTO 999
      ENDIF
!
!      Check if IFDEND between IDTBEG and IDTEND
!
      IF (NYEARS .EQ. 1) THEN
        NDAYS = IDTEND - IDTBEG+1
        IDEND = IFDEND
      ELSE
        NDAYS = (365+ILEAP)-IDTBEG+1
        IDEND = 365+ILEAP
      ENDIF
      NPRINT = 1 !Maintain option of delsub output level
      STOPHR = 24.0 !Maintain option of stopping simulation at end of
day
!
!      Read INMAX,DMAXBA

```

```

!
  READ(LUI,'(I,3D)') INMAX,DMAXBA,DELMAX,DELMIN
  ISWDIF = 1 !Maintain option that mass balance is based on entire
profile
  IF (INMAX .LT. 2) INMAX = 2
  IF (IPRINT .GT. 0) WRITE(LOUT,2071) INMAX,DMAXBA,DELMAX,DELMIN
  OUTTIM = 1.0 !size of delsub period set at 1.0 h
2071  FORMAT(T2,'INMAX  =',I5,T22,'DMAXBA =',E10.3,T42,'DELMAX
=' ,E10.3,&
    & T62,'DELMIN =',E10.3)
  RFACT = 1.0 !maintain option that time step cannot be increased
  RAINIF = 0.5 !maintain option that time step decreased by 0.5
when rain occurs
  KEST = 1 !maintain option that hydraulic conductivities are an
arithmetic mean
  WTF = 0.5 !weighs nodes equally
  UP   = WTF
  DOWN = 1.0-UP
  ITOPBC = 0 !Maintain UNSATH option of flux surface boundary
condition
  IEVOPT = 1 !Maintain UNSATH option to allow evaporation
!
!   Read ICLOUD,IRAD,ISOL,DMAXHE
!
  READ(LUI,'(3I,d)') ICLOUD,IRAD,ISOL,DMAXHE
  IF (IPRINT .GT. 0) WRITE(LOUT,2030) ICLOUD,IRAD,ISOL, DMAXHE
2030  FORMAT(T2,'ICLOUD =',I5,T22,'IRAD =',I5,T40,'ISOL
='I5,T55,'DMAXHE&
    &      =' ,E10.3)
  IETOPT = 1 !Maintain UNSATH option that met data provided in
input file
  LOWER = 1 !Maintain option of unit gradient lower boundary
condition
  UPPERH = 0 !Maintain UNSATH option of upper boundary condition of
flux based on met data
  IVAPOR = 0 !Maintain UNSATH option of no vapor flow
  VAPDIF = 0.24 !Diffusion coefficient of vapor in air, cm2/s
  MGR = 1.E2*MOLAR*GRAV/GASCON
!-----
!   NODE INFORMATION:  Define geometric details of the problem
!-----
!
!   Read NPT
!
  IF (IPRINT .GT. 0) WRITE(LOUT,'(/,A,/)' ) ' Grid options:'
  READ(LUI,'(I)') NPT
  MATN = 1 !maintain UNSATH option of one soil type
  IF (IPRINT .GT. 0) WRITE(LOUT,3000) NPT
3000  FORMAT(T2,'   NPT =',I5)
!
!   Ensure number of nodes and materials don'ts exceed defined array
dimensions
!
  IF (NPT .GT. M1) THEN
    WRITE(LUS,'(A)') ' NPT exceeds node dimensions M1'

```

```

        GOTO 999
    ENDIF
!
!   Read Z:  Depth below the surface
!
    READ(LUI,'(4(D))') (Z(I),I=1,NPT)
    DO I=1,NPT-1
        ZZ(I) = Z(I+1)-Z(I)
        MAT(I) = MATN
        IF (ZZ(I) .LE. 0.0) THEN
            WRITE(LUS,'(A,I)') ' Z does not increase at node ',I+1
            GOTO 999
        ENDIF
    ENDDO
    ZZ(NPT) = 0.0
!-----
!   SOIL PROPERTY DESCRIPTION
!-----
!
!   Read soil property parameters
!
    CALL SOILPROP(LUSLUW,MATN)
!
!   Read in soil parameters for decomposition simulation
!   User can specify residue values or use default values.  If there
is manure
!   application then residue values (during and following
application) are based
!   on manure parameters specified in the manure property section of
input file.
!
    IF (ITRACE .GT. 0) THEN
        IF (IRES .EQ. 1) THEN !If residue values specified in file
            READ(LUI,'(6D)',ERR=999)
            CNRES,KRES0,HRES0,SRES,SRESVL,CNRESVL
            IF (IPRINT .GT. 0) THEN
                WRITE(LOUT,4001)
                WRITE(LOUT,4002) CNRES,KRES0,HRES0,SRES
            END IF
        ELSE !Set residue parameters to default values
            CNRES = 20.0
            KRES0 = 0.00185 !d-1
            HRES0 = 0.0005 !d-1
            SRES = 0.32
            SRESVL = 0.08
            CNRESVL = 2.35
        END IF
4001  FORMAT('Option to include user-defined residue data')
4002  FORMAT(1X,'CNRES = ',F10.1,1X,T24,'KRES0 = ',E12.3,T65,
&
&      'HRES0 = ',E12.3,T75,'SRES = ',F5.2/)
    END IF
!-----
!   INITIAL CONDITIONS

```



```

      CBIO(I) = CBIO(I)-IDENITBIO(I)
      CHUM(I) = SOC(I)*FHUM
      CPASS(I) = SOC(I)*FPASS
      END DO
    END IF

    IF (IPRINT .GT. 0) THEN
      WRITE(LOUT,5010) NDAY
      WRITE(LOUT,5020) (I,Z(I),THETA(I),KL(I),DIFFY(I),I=1,NPT)
    IF (ITRACE .GT. 0) THEN
      WRITE(LOUT,5011) NDAY
      WRITE(LOUT,5021) (I,Z(I),CRES(I),CBIO(I),CHUM(I),I=1,NPT)
      WRITE(LOUT,5012) NDAY
      WRITE(LOUT,5021) (I,Z(I),NH4(I),NO3(I),NO2(I),I=1,NPT)
    END IF
  ENDIF

5010  FORMAT(/,' NDAY = ',I3,/,T2,'NODE',T11,'Z',T16,'THETA',
&
& T36,'CONDUCTIVITY',T53,'DIFFUSIVITY',/,T9,'(cm)'
&
& T18,'(vol.)',T38,'(cm/h)',T53,'(cm2/h)',/,T2,
&
& '----',T9,'-----',T16,'-----',T22,'-----',T36,
&
& '-----',T52,'-----')
5011  FORMAT(/,' NDAY = ',I3,/,T2,'NODE',T11,'Z',T16,
&
& 'CRES',T36,'CBIO',T53,'CHUM',/,T9,'(cm)'
&
& T18,'(g/cm3)',T38,'(g/cm3)',T53,'(g/cm3)',/,T2,
&
& '----',T9,'-----',T16,'-----',T36,
&
& '-----',T52,'-----')
5012  FORMAT(/,' NDAY = ',I3,/,T2,'NODE',T11,'Z',T16,
&
& 'NH4',T36,'NO3',T53,'NO2',/,T9,'(cm)'
&
& T18,'(g/cm3)',T38,'(g/cm3)',T53,'(g/cm3)',/,T2,
&
& '----',T9,'-----',T16,'-----',T36,
&
& '-----',T52,'-----')
5020  FORMAT(I4,F9.2,1P,T20,E12.4,2E15.4,0P)
5021  FORMAT(I4,F9.2,1P,T20,E12.4,2E15.4,0P)
      THICK(1) = 0.5*(Z(2)-Z(1))
      THICK(NPT) = 0.5*(Z(NPT)-Z(NPT-1))
      DO I=2,NPT-1
        THICK(I) = 0.5*(Z(I+1)-Z(I-1))
      ENDDO

!
! Calculate initial moisture storage
!

TMOIST = THETA(1)*THICK(1)+THETA(NPT)*THICK(NPT) !cm
DO I=2,NPT-1
  TMOIST = TMOIST+THETA(I)*THICK(I) !cm
ENDDO

```



```

      IF (IPRINT .GT. 0) WRITE(LOUT,5030) TMOIST
5030  FORMAT(/,' Total Initial Storage (cm) = ',1PE13.6)
      !
      ! Calculate initial heat storage
      !
      CALL THERMK(1,NPT)
      HSTORE = 0.0
      DO I=1,NPT
        HSTORE = HSTORE+CH(I)*(T(I)-T0)*THICK(I) !J/cm2
      ENDDO
      !
      ! convert J/cm2 to J/m2
      !
      HSTORE = HSTORE*10000. !J/m2
      IF (IPRINT .GT. 0) THEN
        DO I=1,NPT
          TTHETA(I) = THETA(I)
        ENDDO
        WRITE(LOUT,5024) NDAY
        WRITE(LOUT,5025) (I,Z(I),T(I),KH(I),CHSOIL(I),CH(I),I=1,NPT)
        ENDIF
        IF (IPRINT .GT. 0) WRITE(LOUT,5031) HSTORE,T0
5024  FORMAT(/,' NDAY = ',I3,/,T2,'NODE',T11,'Z',T16,'TEMP',
      &
      &T36,'CONDUCTIVITY',T53,'CHSOIL',T68,'CH',/,T9,'(cm)',T18,
      &
      & '(K)',T37,'(J/cm/hr/K)',T53,'(J/cm3/K)',T67,'(J/cm3/K)',/,T2,
      &
      & '-----',T9,'-----',T16,'-----',T36,
      &
      & '-----',T52,'-----',T67,'-----')
5025  FORMAT(I4,F9.2,1P,T20,E12.4,3E15.4,0P)
5031  FORMAT(/,' Total Initial Heat Storage = ',1PE13.7,' J/m2',
      &
      &' for T0 = '3PE11.5,' K')
      !
      ! APPLICATION INFORMATION
      !
      IF (IAPPN .GT. 0) THEN
        IF (IPRINT .GT. 0) WRITE(LOUT,'(80("-"),/,A)')
      &
      &' Application details:'
        IF (ITILL .GT. 0) THEN
          READ(LUI,'(I,d,I)') NAPPN,red,TILLDAY
        ELSE
          READ(LUI,'(I,d)') NAPPN,red
        END IF
        DO I=1,NAPPN
          READ(LUI,'(I,D,2I,2D)') APDAY(I),APPNA(I),APPNSRT(I),APPNEND(I),
      &
      & APPNRATE(I),NH4APPNRATE(I) !day,ha,hr,L/ha,kg-N/ha
          READ(LUI,'(7D)') APPNDEN(I),CNAPPN(I),NO3APPN(I),
      &
      & NTOTAPPN(I),PHAPPN(I),OMAPPN(I),DMAPPN(I)
!g/l,g/g,g/L,G/l,pH,fraction,fraction
        END DO

```

```

      IF (IPRINT .GT. 0) WRITE(LOUT,5032) NAPPN
      DO I =1,NAPPN
        IF (IPRINT .GT. 0) WRITE(LOUT,5033)APDAY(I),APPNA(I),
&
& APPNSRT(I),APPNEND(I),APPNDEN(I),CNAPPN(I),NTOTAPPN(I),
&
& PHAPPN(I),OMAPPN(I),DMAPPN(I)
      END DO
    END IF

5032 FORMAT(/,'NAPPN = ',I3)
5033 FORMAT(/,'APDAY = ',I,T30,'APPNA = ',F5.2,T50,'APPNSRT = ',I,T50,/,
&
& 'APPNEND = ',I,T30,'APPNDEN(g/L)=' ,F8.2,T55,'CNAPPN
=' ,F5.2,/,
&
& 'NTOTAPPN(g/L)=' ,F8.4,T50,'PHAPPN = ' ,F5.2, /,
&
& 'OMAPPN(%)=' ,F5.2,T30,'DMAPPN(%)=' ,F5.2)
!-----
!
! BOUNDARY CONDITIONS
!-----
!
! Read parameters for meteorological calculations
!
CALL ETPAR(LUSLUW,NFHOURL)
LOWERH = 2 !CONSTANT TEMP option maintained for lower boundary
condition
!
! Read met data
!
CALL ETBC(LUSLUW,LUI)

!
! Write binary file (*.BIN) for input to AGRIN main
BIFILE = TMFILE
BIFILE(NCHR:NCHR+3) = '.bin'
OPEN (UNIT=LUB,FILE=BIFILE,STATUS='UNKNOWN')
CLOSE (UNIT=LUB,STATUS='DELETE')
OPEN (UNIT=LUB,FILE=BIFILE,STATUS='NEW',FORM='UNFORMATTED')
WRITE(LUB) DV,IPLANT,ITRACE,IAPPN,ITILL,LOWER,NDAYS,NDAY,NPRINT,
&
&
ITOPBC,ICONVH,IRAD,MAT,KEST,IVAPOR,IDEND,IFDEND,NYEARS, &
&
IYS,ISWDIF,ICLOUD,NPT,G,IEVOPT,IDTEND,INC,IETOPT,INMAX, &
& ISTEAD,ILEAP,UPPERH,LOWERH,IFILE,TITLE,ISOL
WRITE(LUB) DMAXBA,DELMAX,DELMIN,RAINIF,RFACT,TMOIST,LOG10E,DHMAX,
&
& DHFACT,OUTTIM,DMAXHE,UP,DOWN,STOPHR,GRAV
WRITE(LUB) (Z(I),THETA(I),KL(I),T(I),KH(I),
&
& CHSOIL(I),DIFFY(I),I=1,NPT),MGR,VAPDIF
WRITE(LUB) SINLAT,COSLAT,TANLAT,TPIY,HOUREXT,SB,CHW,THET(1),SK(1), &

```

```

&          ALBEDO, ZU, ZH, ZM, ZT, D, VK, SEXT, CHA, B(1), SATMA(1),
&
&          CHS, WATDEN, LHV0, CHV, T0, HSTORE, DHTOL, BLKDEN
IF (ITRACE .GT. 0) THEN
    WRITE(LUB) CLY, BLKDEN, NODEIN, TOTALA, CNRES, KRES0, HRES0, SRES,
&
&          SRESVL, CNRESVL, (NH4(I), NO3(I), NO2(I), PH(I), CRES(I), CBIO(I),
&
&          CHUM(I), CPASS(I), INITBIO(I), IDENITBIO(I), I=1, NPT)
IF (IAPPN .GT. 0) THEN
    WRITE(LUB) NAPPN, RED, TILLDAY, (APDAY(I), APPNA(I), APPNSRT(I),
&
&          APPNEND(I), APPNRATE(I), NH4APPNRATE(I), APPNDEPTH(I), APPNDEN(I),
&
&          CNAPPN(I), NO3APPN(I), NTOTAPPN(I), PHAPPN(I), OMAPPN(I), DMAPPN(I),
&
&          I=1, NAPPN)
    END IF
    END IF
!
!   Read precipitation data; write PET/MET and precipitation data to
LUB
!
    CALL PRECIPBC(LUSLUW, LUI, LUB)
    CLOSE (UNIT=LUI)
    CLOSE (UNIT=LUB)
    WRITE(LUS, '(80("-"),/,A)') ' Program terminated normally.'
    IF (LUSLUW) WRITE(LOUT, '(80("-"),/,A)')
&
& ' Program terminated normally.'
    STOP
999  WRITE(LUS, '(80("-"),/,A)')
&
& ' Program terminated prematurely.'
    STOP
!-----
-
!   End of program AGRIN IN
!-----
-
    END

    SUBROUTINE THERMK(IBEGIN, IEND)
!-----
-
!   Called by AGRIN IN, AGRIN MAIN
!
!   Calculates soil vol. heat capacity
!-----
-
    INCLUDE 'agringlob.inc'
    DO I=IBEGIN, IEND
        MATI = MAT(I)
        THI = THETA(I)
        KH(I) = KH(I)
        CH(I) = CHW*THI+CHSOIL(I) !*BLKDEN/1000.0 !J/cm3SOIL/K
    ENDDO

```

```

      RETURN
!-----
!
!      End of subroutine THERMK
!-----
-
      END

      SUBROUTINE TIMEX
!-----
!
!      Called by AGRIN IN, AGRIN MAIN
!
!      Queries the operating system and returns the time and date
!      SDATE = Date in format 01 Jan 1993 (dd mmm yyyy)
!      STIME = Time in format 01:02:03.42 (hh:mm:ss.ss)
!-----
-
      INCLUDE 'agringlob.inc'
      CHARACTER*3 MON(12)*3,REAL_CLOCK(3)*12
      INTEGER DATE_TIME(8)
      DATA MON /'Jan','Feb','Mar','Apr','May','Jun','Jul',
&
& 'Aug','Sep','Oct','Nov','Dec'/
      CALL DATE_AND_TIME(REAL_CLOCK(1),REAL_CLOCK(2),
&
& REAL_CLOCK(3),DATE_TIME)
      SDATE(1:2) = REAL_CLOCK(1)(7:8)
      SDATE(3:3) = CHAR(32)
      SDATE(4:6) = MON(DATE_TIME(2))
      SDATE(7:7) = CHAR(32)
      SDATE(8:11) = REAL_CLOCK(1)(1:4)
      STIME(1:2) = REAL_CLOCK(2)(1:2)
      STIME(3:3) = CHAR(58)
      STIME(4:5) = REAL_CLOCK(2)(3:4)
      STIME(6:6) = CHAR(58)
      STIME(7:11) = REAL_CLOCK(2)(5:9)
      RETURN
!-----
!
!      End of subroutine TIMEX
!-----
-
      END

      SUBROUTINE POLYKH(IBEGIN,IEND,rKL,RSATMA,RTHETM,RKH)
!-----
!
!      Called by AGRIN IN, AGRIN MAIN
!
!      Calculates the conductivity (RKL) of each node as a function of
!      the moisture content for that node
!      Calculates thermal conductivity as a function of vol. moisture
!      content
!
!-----
-

```

```

INCLUDE 'agringlob.inc'
DIMENSION RKL(*), RKH(*)
DO I=IBEGIN, IEND
  RSATMA = SATMA(1) !m
  RTHETM = THET(1)
  SKM = SK(1) !cm/hr
  BM = B(1)

!
!   Calculate hydraulic conductivity
!
  RKL(I) = SKM*((THETA(I)/RTHETM)**(2.0*BM + 3.0)) !CM/H

!
!   Calculate thermal conductivity
!
  D12 = 0.03+0.1*(BLKDEN**2.)
  BB = 1.06*BLKDEN*THETA(I)
  A12 = 0.65 - 0.78*BLKDEN + 0.6*(BLKDEN**2.)
  C12 = 1. +2.6*(CLY**(-0.5))
  RKH(I) = (A12 + 1.06*BLKDEN*THETA(I)*THETA(I) - (A12-D12)*EXP(-
&
&      (C12*THETA(I))**4.))*36. !J/S/M/K TO J/h/cm/K
  IF (RKL(I) .LT. 0.0) THEN
    WRITE(*,6000) IN,I,IDAY,TSTEPB,TTHETA(I),THETA(I),RKL(I)
    STOP
  ENDIF
ENDDO
RETURN
6000  FORMAT(/,
&      ' Subroutine POLYKH detected an invalid conductivity value',/,
&
&      &I13,' = Iteration number (IN)',/,
&
&      &I13,' = Node number (N)',/,
&
&      &I13,' = Simulation day (IDAY)',/,
&
&      &1PE13.5,' = Completed time of day (TSTEPB)',/,
&
&      &E13.5,' = Previous theta THTH(I)',/,
&
&      &E13.5,' = Current theta TH(I)',/,
&
&      &E13.5,' = Calculated conductivity RKL(I)',/)
!-----
!   End of subroutine POLYKH
!-----
-
END

SUBROUTINE DIFFUSIVITY(IBEGIN,IEND,RTHETA,RDIFFY)
!-----
!
!   Called by AGRIN IN, AGRIN MAIN
!
!   Calculates the liquid water diffusivity (D)
!   of each node as a function of the theta value for that node

```

```

!-----
-
      INCLUDE 'agringlob.inc'
      DIMENSION RTHETA(*),RDIFFY(*)

      LOGICAL LMDIFF
      INCLUDE 'agrininit.inc'

      DO I=IBEGIN,IEND

          SATM = SATMA(1) !m
          BM    = B(1)
          SKM   = SK(1) !cm/h
          THETM = THET(1)
          RDIFFY(I)=(BM*SKM*(SATM*100.0)/THETM)*(RTHETA(I)/THETM)**(BM+3.0)
!cm2/h
      END DO

      RETURN
!-----
-
      !      Format Statements
!-----
-
6000  FORMAT(
&
      &' ERROR: Liquid water diffusivity must be positive, MAT
No.',I3,/,&
      &'          Node = ',I4,', RC = ',1PE15.7,', WATCONT = ',E15.7)
6010  FORMAT(/,
&
      &' Program execution stopped in subroutine RETENT ',/,
&
      &' because of negative moisture capacity(s) for',I4,' nodes')
!-----
-
      !      End of Subroutine DIFFUSIVITY
!-----
-
      END

      SUBROUTINE WELCOME(name)
!-----
-
      !      Called by AGRIN IN, AGRIN MAIN, AGRIN OUT
      !
      !      Writes program header with version number and contact person
!-----
-
      INCLUDE 'agringlob.inc'
      CHARACTER name*7
      ver = 1.0
      WRITE(LUS,10) name,ver
10    FORMAT(/,
&

```

```

&      ' ,A7,/,
&
&      '      Version ',F4.2,/,/,
&
&      '      Contact:',/,/,
&
&      '      J Beuning',/,/,
&
&      '      University of Guelph',/,/,
&
&      '      Guelph, ON',/,/,
&
&      '      email jbeuning@uoguelph.ca',/)
      RETURN
!-----
-
!      End of subroutine WELCOME
!-----
-
      END

      SUBROUTINE ETPAR(LUSLUW,NFHOURL)
!-----
-
!      Called by AGRIN IN
!
!
!      Reads in PET/MET parameters
!-----
-
      INCLUDE 'agringlob.inc'
      IF (IPRINT.GT. 0) THEN
        WRITE(LOUT,'(80("-"),/,A,/)') ' MET parameters:'
        IF (IEVOPT.EQ. 0 .AND. IPLANT.EQ. 0) THEN
          WRITE(LOUT,'(A)') '      IEVOPT = 0 and IPLANT = 0 (no ET)'
          WRITE(LOUT,'(A)') '      Thus, no ET parameters required'
          GOTO 998
        ENDIF
      ENDIF

!
!      Read MET parameters for heat flow
!
      READ(LUI,'(6D)',ERR=999) ZH,ZM,ZT,ZU,D,LAT
      IF (IPRINT.GT. 0) WRITE(LOUT,7167) ZH,ZM,ZT,ZU,D,LAT
      HOURSEXT = SEXT*3600.0 !J/m2/h
      TPIY     = 2.0*PI/365.0
      LAT      = LAT*2.0*PI/360.0
      SINLAT   = SIN(LAT)
      COSLAT   = COS(LAT)
      TANLAT   = TAN(LAT)
7167  FORMAT(' ',/,
&
&      ' Evaporation calculated from meterological data and heat',/,
&
&      ' flow calculations',/,1P,
&

```

```

& ' ZH = ',E10.3,' (m)',/,
&
& ' ZM = ',E10.3,' (m)',/,
&
& ' ZT = ',E10.3,' (m)',/,
&
& ' ZU = ',E10.3,' (m)',/,
&
& ' D = ',E10.3,' (m)',/,
&
& ' LAT = ',E10.3,' (deg)',/)
998 RETURN
999 WRITE(LUS,'(A)') ' Program terminated prematurely in ETPAR'
    IF (LUSLUW) WRITE(LOUT,'(A)')
&
& ' Program terminated prematurely in ETPAR'
    STOP
!-----
-
! End of subroutine ETPAR
!-----
-
END

SUBROUTINE ETBC(LUSLUW,LULI)
!-----
-
! Called by AGRIN IN
!
! Reads in the MET data
!-----
-
    INCLUDE 'agringlob.inc'
    READ(LULI,*,ERR=999) ((TDDATA(I,J),I=1,25),J=1,NDAYS) !K, dew
point temp
    READ(LULI,*,ERR=999) ((TADATA(I,J),I=1,25),J=1,NDAYS) !K air temp
    READ(LULI,*,ERR=999) ((WDDATA(I,J),I=1,25),J=1,NDAYS) !m/s, wind
speed
    IF (ISOL .EQ. 1) THEN
        READ(LULI,*,ERR=999) ((SRDATA(I,J),I=1,25),J=1,NDAYS) !W/m2,
solar radiation
    END IF
    IF (ICLOUD .EQ. 1) THEN
        READ(LULI,*,ERR=999) ((CLDATA(I,J),I=1,25),J=1,NDAYS) !fraction
cloud cover
    END IF
    IF (IRAD .EQ. 1) THEN
        READ(LULI,*,ERR=999) ((RNDATA(I,J),I=1,25),J=1,NDAYS) !RN
measured, W/m2
    END IF
    READ (LULI,'(I)') NWATER
    RETURN
999 WRITE(LUS,'(A)') ' Program terminated prematurely in ETBC'
    IF (LUSLUW) WRITE(LOUT,'(A)')
&
& ' Program terminated prematurely in ETBC'
    STOP

```



```

!-----
-
!      Format Statements
!-----
-
7168  FORMAT(/,' IETOPT = 1:  Average Daily Meteorological Data',/,
&
&      '          Temperature   Wind   Cloud',/,
&
&      '  IDAY  Max  Min   Dew  Speed  Cover  Prec.',/,
&
&      '          K    K    K    m/s   tenth   cm   ',/,
&
&      '  ----  ---  ---  ----  -----  -----',/,
&
&      (F6.0,F5.0,F5.0,F6.1,F7.1,F7.1,F7.2))
7180  FORMAT(5(I4,F8.4,3X))
!-----
-
!      End of subroutine ETBC
!-----
-
      END

      SUBROUTINE PRECIPBC(LUSLUW,LULI,LULO)
!-----
-
!      Called by AGRIN IN, AGRIN MAIN
!
!      Read in precipitation data and write MET and precipitation data
!      to binary input file (LULO)
!-----
-
      INCLUDE 'agringlob.inc'
      IF(IPRINT .GT. 0)
&
&      &WRITE(LOUT,'(80("-"),/,A)') ' Precipitation parameters:'
&      &WRITE(LULO) NWATER
&      &IF (NWATER .EQ. 0) THEN
&      &IF (IPRINT .GT. 0)
&
&      &WRITE(LOUT,'(/,A)') '   NWATER = 0:  No rain'
&      &ENDIF
!
!      Water input:  IRDAY,NP,TIME,AMOUNT
!
      IF (IPRINT .GT. 0) THEN
&      &WRITE(LOUT,7410) NWATER
&      &WRITE(LOUT,7411)
&      &ENDIF
&      &IRDAY = IDEND - NDAYS
&      &LIRDAY = IRDAY
&      &IRTYPE = 1
&      &EFICEN = 1.0
&      &K = IDEND - NDAYS + 1
&      &DO I=K, IDEND
&      &W = I - K + 1

```

```

      IF (IRDAY .LT. I) THEN
      READ(LULI,'(2I)',END=775) IRDAY,NPP
      IRTYPE = 1
      EFICIEN = 1.000
      READ(LULI,'(2D)',END=775) (RTIME(J),AMOUNT(J),J=1,NPP)
    ENDIF
    IF (IRDAY .LE. I) GO TO 777
775  NP = 0
      GO TO 769
777  NP = NPP
      IF (EFICEN .EQ. 0.0) EFICEN = 1.0
      DO J=1,NP-1
        TOTALR = TOTALR+AMOUNT(J)
        IF (RTIME(J+1) .LE. RTIME(J) .AND. IRTYPE .NE. 4) THEN
          WRITE(LUS,7430) IRDAY
          IF (LUSLUW) WRITE(LOUT,7430) IRDAY
          GO TO 999
        ENDIF
      ENDDO
      IF (IRDAY .LE. -1.0) THEN
        WRITE(LUS,7440) IRDAY,NPP
        IF (LUSLUW) WRITE(LOUT,7440) IRDAY,NPP
        GO TO 999
      ENDIF
      LIRDAY = IRDAY
      IF (IPRINT .GT. 0) THEN
        WRITE(LOUT,7450) IRDAY,RTIME(1),AMOUNT(1),NP
        WRITE(LOUT,7460) (RTIME(J),AMOUNT(J),J=2,NP)
      ENDIF
769  IF (IETOPT .EQ. 0) THEN
      IF (I .EQ. IRDAY) WRITE(LULO) IRDAY,NP,(RTIME(J),AMOUNT(J)
      &
      & ,J=1,NP)
      ELSE
      METDAY = I
      ! NP = NPP
      ! IF (NP .EQ. 0) NPP = 0
      WRITE(LULO) METDAY,IRTYPE,EFICEN,NP,
      &
      & NPP,(RTIME(J),AMOUNT(J),J=1,NP),(TDDATA(J,W),J=2,25),
      &
      & (TADATA(J,W),J=2,25),(WDDATA(J,W),J=2,25)
      IF (ISOL .EQ. 1) WRITE(LULO) (SRDATA(J,W),J=2,25)
      IF (ICLOUD .EQ. 1) WRITE(LULO) (CLDATA(J,W),J=2,25)
      IF (IRAD .EQ. 1) WRITE(LULO) (RNDATA(J,W),J=2,25)

      ENDIF
    ENDDO
    IF (IPRINT .GT. 0) THEN
      WRITE(LOUT,7480) TOTALR
    ENDIF
998  RETURN
999  WRITE(LUS,'(A)') ' Program terminated prematurely in PRECIPBC'
      IF (LUSLUW) WRITE(LOUT,'(A)')
      &
      & ' Program terminated prematurely in PRECIPBC'
      STOP

```

```

!-----
-
!       Format Statements
!-----
-
7410  FORMAT(/,T4,'NWATER (number of days of rain) =',I3)
7411  FORMAT(/,T17,'Rainfall Details',/,
&
      &T4,'Day',T11,'Time',T18,'Amount',T27,'Changes In
Rate',/,T11,'(hr)&
      &',T19,'(cm)',/,T4,'---',T11,'----',T18,'-----',T29,'-----')
7430  FORMAT(' ERROR:  Time of rain not in ascending',
&
      &' order on day',I4)
7440  FORMAT(' ERROR:  Day of rain not in ascending',
&
      &' order on day',I4)
7485  FORMAT(' ERROR:  IRTYPE cannot equal 4 while IETOPT',
&
      &' is greater than zero')
7450  FORMAT(T4,I3,T9,F6.3,T17,F7.4,T32,I2)
7460  FORMAT(T9,F6.3,T17,F7.4)
7480  FORMAT(/,T4,'Total Water Applied (cm) = ',1PE13.6)
!-----
-
!       End of subroutine PRECIPBC
!-----
-
      END

      SUBROUTINE SOILPROP(LUSLUW,MATN)
!-----
-
!       Called by AGRIN IN
!
!       Read in soil hydraulic property parameters
!-----
-
      INCLUDE 'agringlob.inc'
      IF (IPRINT .GT. 0) THEN
        WRITE(LOUT,'(/,A,/)' ) ' Soil hydraulic and thermal properties:'
      ENDIF
      DO I=1 ,MATN
        READ(LUI,'(A)',ERR=999) DUMMY
        READ (LUI,'(5D)',ERR=999) SK(I),THET(I),SATMA(I),CHS(I),B(I)
!MJ/m3/K
        WRITE(LOUT,4020) SK(I),THET(I)
        WRITE(LOUT,4001) SATMA(I),CHS(I),B(I)
      ENDDO
      DO I=1,NPT
        MATI = 1 !Maintain option of one material type
        CHSOIL(I) = CHS(MATI)*(1-THET(MATI)) !J/CM3/K
      ENDDO
      READ(LUI,'(2D)' ) CLY,BLKDEN
      WRITE(LOUT,'(80("-"))')
      WRITE(LOUT,4000)CLY,BLKDEN !fraction, g/cm3
4000  FORMAT(1X,/, ' CLY(fracn)=' ,F6.3,T20,'BLKDEN(g/cm3)=' ,F6.3)

```

```

4020  FORMAT(T5,' SK(cm/h) =',E12.3,T36,' THET(vol.) =',E12.4)
4001  FORMAT(1X,T5,'SATMA (cm)=' ,E10.3,T34,'HEAT CAP (MJ/m3/K)=' ,f9.3
&
&          ,T64,'B =' ,f9.3)
440   RETURN
999   WRITE(LUS,'(A)') ' Program terminated prematurely in SOILPROP'
      IF (LUSLUW) WRITE(LOUT,'(A)')
&
& ' Program terminated prematurely in SOILPROP'
      STOP
!-----
-
!      End of subroutine SOILPROP
!-----
-
      END

```

A.4 AGRIN MAIN source code

```

      PROGRAM AGRIN MAIN
!-----
-
!
!      Determines soil heat, moisture, carbon and nitrogen profiles
!      Determines N trace gas emissions
!-----
-
      INCLUDE 'agringlob.inc'
      CHARACTER*80 AYEAR
      LOGICAL FINISH
      DIMENSION SUBQL(M1),A1(M1),A2(M1),A3(M1)

      INCLUDE 'agrininit.inc'
!
      WRITE(LUS,9000)
9000  FORMAT(/' Results are based on the use of unverified software.',/,
&
&      ' No assurance is expressed or implied as to the accuracy.',/,
&
&      ' completeness or usefulness of this information.'/)
      FINISH = .FALSE.
      CALL TIMEX
!
!      BIFILE = Binary input filename
!
      CALL WELCOME('AGRIN 1.0')
      WRITE(LUS,8)
8     FORMAT(/,' Enter input filename without the "*.BIN" extension',/,
&

```

```

&' (a "0" terminates the program) ==> ', $)
READ(LUR, ' (A80)', END=999) TMFILE
IF (INDEX(TMFILE(1:1), '0') .GT. 0) GO TO 999
RFILE = TMFILE
NCHR = INDEX(TMFILE, ' ')
TMFILE(NCHR:NCHR+3) = '.bin'
OPEN(UNIT=LUI, FILE=TMFILE, STATUS='OLD', FORM='UNFORMATTED')
INQUIRE(UNIT=LUI, NAME=BIFILE)
WRITE(LUS, 10) SDATE, STIME, BIFILE
10  FORMAT(/,
&' Date: ', A11, /,
&' Time: ', A11, /,
&' Binary Input Filename: ', /, 1X, A79, /)
ISCR = 0 !Maintain option of no screen output
! Read in the processed input file
!
READ(LUI) DV
REWIND (UNIT=LUI)
READ(LUI) DV, IPLANT, ITRACE, IAPPN, ITILL, LOWER, NDAYS, NDAY, NPRINT,
&
& ITOPBC, ICONVH, IRAD, MAT, KEST, IVAPOR, IDEND, IFDEND, NYEARS, IYS,
&
& ISWDIF, ICLOUD, NPT, G, IEVOPT, IDTEND, INC, IETOPT, INMAX,
&
& ISTEAD, ILEAP, UPPERH, LOWERH, IFILE, TITLE, ISOL
READ(LUI) DMAXBA, DELMAX, DELMIN, RAINIF, RFACT, TMOIST, LOG10E, DHMAX,
&
& DHFACT, OUTTIM, DMAXHE, UP, DOWN, STOPHR, GRAV
READ(LUI) (Z(I), THETA(I), KL(I), T(I), KH(I), CHSOIL(I),
&
& DIFFY(I), I=1, NPT), MGR, VAPDIF
READ(LUI)
SINLAT, COSLAT, TANLAT, TPIY, HOURSEXT, SB, CHW, THET(1), SK(1), &
& ALBEDO, ZU, ZH, ZM, ZT, D, VK, SEXT, CHA, B(1), SATMA(1),
&
& CHS, WATDEN, LHV0, CHV, T0, HSTORE, DHTOL, BLKDEN
IF (ITRACE .GT. 0) THEN
READ(LUI) CLY, BLKDEN, NODEIN, TOTALA, CNRES, KRES0, HRES0, SRES,
&
& SRESVL, CNRESVL, (NH4(I), NO3(I), NO2(I), PH(I), CRES(I), CBIO(I),
&
& CHUM(I), CPASS(I), INITBIO(I), IDENITBIO(I), I=1, NPT)
IF (IAPPN .GT. 0) THEN
READ(LUI) NAPPN, red, TILLDAY, (APDAY(I), APPNA(I), APPNSRT(I),
&
& APPNEND(I), APPNRATE(I), nh4appnrate(i), APPNDEPTH(I), APPNDEN(I),
&
& CNAPPN(I), NO3APPN(I), NTOTAPPN(I), PHAPPN(I), OMAPPN(I), DMAPPN(I), &
& I=1, NAPPN)
END IF
END IF
READ(LUI) NWATER
IDBEG = NDAY+1
DELT = DELMIN
NPPT = NPT-1

```

```

NTOTAL = NINT(24.D0/OUTTIM)
NSTOP  = NINT(NTOTAL*STOPHR/24.D0)
DELSUB = 24.D0/NTOTAL

!
! Calculate internodal distances (ZZ) and node thicknesses (THICK)
!
ZZ(1) = Z(2)-Z(1) !cm
THICK(1) = 0.5*ZZ(1) !cm
THICK(NPT) = 0.5*(Z(NPT)-Z(NPT-1)) !cm
DO I=2,NPT-1
    ZZ(I) = Z(I+1)-Z(I) !cm
    THICK(I) = 0.5*(ZZ(I-1)+ZZ(I)) !cm
ENDDO

!
! Initialize the met data
METLES = 0
187 READ(LUI) METDAY,IRTYPE,EFICEN,NP,NPP,(RTIME(J),AMOUNT(J),J=1,
&
& NP),(TDWT(J),J=1,24),(TAT(J),J=1,24),(WDT(J),J=1,24)
IF (ISOL.EQ. 1) READ(LUI) (SRT(J),J=1,24)
IF (ICLOUD.EQ. 1) READ(LUI) (CLDT(J),J=1,24)
IF (IRAD.EQ. 1) READ(LUI) (RNT(J),J=1,24)

!
! Ensure met data read from first day of simulation
!
IF (METDAY.LT. IDBEG) THEN
    METLES = 1
    GOTO 187
ENDIF
IF (NP.GT. 0) IRDAY = METDAY
HOUR = NTOTAL*OUTTIM

CALL ZEROA(NP+1,25,RTIME)
CALL ZEROA(NP+1,25,AMOUNT)
CALL THERMK(1,NPT)

RLNZT = LOG((ZT-D+ZH)/ZH) !value to calc boundary layer
resistance
RLNZU = LOG((ZU-D+ZM)/ZM)
TATIME = 0.0
TDEWT = TDWT(1) !initialize met values for first hour of day
TAIR = TAT(1)
WND = WDT(1)
CLD = CLDT(1)

IF (ISOL.EQ. 1) THEN !if solar radiation data included in input
file
    SRM = SRT(1)
ELSE !solar radiation data set to zero
    SRM = 0.0
END IF

CALL AIRDENS(TAIR,SVD_AT,TDEWT,VD_AT) !calculate atmospheric
vapour density

TTAIR = TAIR !double letter beginning indicates previous time
step

```

```

    TSMEAN = TS !surface temp
    HR = 0.0
    TT(1) = T(1)

    CALL BLR(TAIR,CLD,SLALT,VD_AT,HR,KHH,USTAR,RIB) !calculates
boundary layer resistance (ra)
    CALL INTERK(1,NPPT,KEST,UP,DOWN) !calc internodal conductivities
!
!   Storing initial values (e.g. THETA) as previous values, where
!   a double first letter implies "previous value" (e.g. TTHETA)
!

    CALL
RESET(1,NPT,DDIFFY,HH,TTHETA,KKLMID,QQI,TT,CCH,KKHMID,KKLNPT,
&
    &      KKHNPPT,DIFFY,H,THETA,KLMID,QL,T,CH,KHMID,KL(NPT),KH(NPT))

    DO I = 1,NPT
    PHPRE(I) = PH(I) !pH linear decrease following application
constrained by initial soil pH
    NPHPREFLAG = 0
    END DO

    IF (ITRACE .GT. 0) THEN !reset values used in trace gas
simulation
        DO I = 1,NPT
        AFPS(I) = THET(1) - THETA(I) !air-filled pore space
        OO2G(I) = 2.0*(10.0**(-6.0)) !mol O2/cm3 air, initializes
O2 profile
        OO2L(I) = OO2G(I)/KHO2 !mol/cm3 water
        END DO
        CALL RESET2
        CALL EQMMOD(1,NNO3L,NNO2L)
        IF (IAPPN .GT. 0) THEN
        CALL MNGMTMOD
        END IF
        TFLAG = 0 !setting tillage flag to zero until tillage day
occurs
        END IF

!-----
!
!   Multiple year loop would start here (UNSATH code)
!   NOTE: AGRIN only utilizes day loops, no multiple year option
!   Values are retained from end of previous year
!-----
!
    DO IYEAR=1,1
    HOUR = 0.0
    STORE = TMOIST
    TPREV = TMOIST
    THPREV = HSTORE
    DHPREV = HSTORE
    IDAY = NDAY
    IDBEG = NDAY+1
    CALL ZEROA(1,25,RTIME)

```

```

      CALL ZEROA(1,25,AMOUNT)

      IF (NP .GT. 0) IRDAY = METDAY

!
!   Write initial conditions to binary output file
!
      RFILE(NCHR:NCHR+3) = '.res'
      IRL = IRLMOD*MAX(110, (9+IPLANT+5)*NPT+45)

      OPEN (UNIT=LUB, FILE=RFILE, STATUS='UNKNOWN')
      CLOSE(UNIT=LUB, STATUS='DELETE')
      OPEN (UNIT=LUB, FILE=RFILE, STATUS='NEW', FORM='UNFORMATTED',
&
&   ACCESS='DIRECT', RECL=IRL)
      nh3flux = 1.0
      WRITE(LUB, REC=1) NPT, IPLANT, ITRACE, IAPPN, (Z(I), I=1, NPT), STOPHR,
&
&   NDAYS, IFILE,
      SDATE, STIME, TITLE, IDEND, NPRINT, IEVOPT, NTOTAL, IDBEG,      &
&   IVAPOR,
      ICLLOUD, IETOPT, UPPER, UPPERH, LOWER, LOWERH, IYEAR, IDAY, HOUR,      &
&
      (THETA(J), T(J), NO3(J), NH4(J), NH3(J), TANTOT(J), J=1, NPT), RN, SENFLX,
&
&   LE, SHFLUX, NH3FLUX, SLURRTANFLUX, N2OFLUX, NOFLUX, TMOIST
      HOUR = 24.0
      IREC = 1 !represents record # keeping for tracking output written
to .res file
      APLIED = 0.0
      OLD RAT = 0.0

!-----
!
!   Day Loop
!
!   IDAY = Day number
!   IDBEG = Beginning day
!   IDEND = Ending day
!-----
!
      DO IDAY=IDBEG, NDAYS
      TPREV = TMOIST
      DHPREV = HSTORE
      TOTALR = 0.
      IRRI = 0
      IPREC = 0
      CALL ZEROA(1,24,RATE)

!
!   Check for rain on current day and set times
      IF (NP .EQ. 0) GO TO 330
      IPREC = 1

!
!   Determines the water input rate (cm/h)
      IF (NP .EQ. 0) GO TO 330
      DO I=1, NP-1
      TOTALR = TOTALR+AMOUNT(I)

```



```

        ENDDO
        APLIED = APLIED+TOTALR
        J = 1
        DO I=1,24
            IF ((I-1) .GE. RTIME(1) .AND. (I-1) .LT. RTIME(NP)) THEN
                IF ((I-1) .EQ. RTIME(J)) THEN
                    RATE(I-1) = AMOUNT(J)/(RTIME(J+1)-RTIME(J))
                    J = J+1
                ELSE
                    RATE(I) = RATE(I-1)
                ENDIF
            ENDIF
        ENDDO
330  HR = 0.0
        IF (IRAD .EQ. 1) THEN
            RN = RNT(1)
        ELSE
            CLD = CLDT(1)
            SRM = SRT(1)
            CALL NETRAD(1,1,Tat(1),VD_AT,CLD,SRM,HR) !calc net rad based on
solar rad and cloud data
            END IF
        !
        ! Initialize daily cumulative totals
        !
        HOUR   = 0.0
        PTSUB  = 0.0
        PESUB  = 0.0
        TSTEPB = 0.0
        !-----
        !
        ! NTOTAL Loop
        !
        ! Program will remain in this loop until 1 day has been simulated.
        !-----
        !
        DO N=1,NTOTAL
            SPREV = TMOIST
            SHPREV = HSTORE
            NHR    = INT(1.0+(N-1)*24.0/NTOTAL)
            IF (IPREC .EQ. 1) PRAIN = RATE(NHR) !cm/h
            IF (IRRI .EQ. 1) PIRRI = RATE(NHR)
            !
            ! Set ISATUK as indicator for precipitation
            IF (RATE(NHR) .EQ. 0.) THEN
                ISATUK = 0 !There is no precipitation
            ELSE
                ISATUK = 1 !There is precipitation
                IF (OLDRAT .GT. 0.) ISATUK = 2 !There was precipitation the
last time step
            END IF
            !-----
            !
            ! Start of the DELSUB loop. The program remains here until DELSUB
            ! time has elapsed. (i.e. TSUB = DELSUB)
            ! TSTEPB = time of day (h) at beginning of time step
            ! TSTEPM = time of day (h) at midpoint of time step

```

```

!      TSTEPE = time of day (h) at end of time step
!-----
-
      TSUB = 0.0
32649 IF (DELSUB-TSUB .LE. TIMRES) GO TO 32648
      IF (DELSUB-TSUB .LT. DELMIN) DELT = DELMIN !DELSUB-TSUB
      DELSAV = DELT !hr
      TSTEPB = (NHR-1) + TSUB !HOUR+TSUB
      TSUB   = TSUB+DELMIN !hr

!
!      If application occurred on day, calculate cumulative area covered
      IF (IAPPN .GT. 0 .AND. IDAY .GE. APDAY(1) .AND. (NHR) .GE.
&
&APPNSRT(1) .AND. (NHR) .LT. APPNEND(1)) THEN
      AREACOVERED = AREACOVERED + AREATIME(1)*delmin
      END IF

!
!      Determine soil heat and moisture profiles
      CALL SOILMOD(SFLUX,KHH)

      DO i = 1,npt
      AFPS(I) = THET(1) - THETA(I)
      END DO

      IF (ITRACE .GT. 0) THEN
      IF (ITILL .GT. 0) CALL TILL (TFLAG)
      CALL DECOMPMOD(NNO3L)
      CALL NITMOD (KHH,USTAR)
      CALL DENITMOD(NNO3L,NNO2L)
      CALL TRANSMOD(TAIR,VD_AT,KHH,USTAR,NNO3L)
      CALL CBALANCE
      IF (SQL1 .GT. 0.0 ) THEN
      THICKEND = SLURRMASS1 !cm
      H2OLEFT = SLURRMASS1 !g
      END IF
      END IF

!
!      Store final values as previous values
      CALL
RESET(1,NPT,DDIFFY,HH,TTHETA,KKLMID,QQ,TT,CCH,KKHMID,KKLNPT,      &
&      KKHNP,DIFFY,H,THETA,KLMID,QL,T,CH,KHMID,KL(NPT),KH(NPT))

      IF (ITRACE .GT. 0) THEN
      CALL RESET2
      DO I = 1,NPT
      BBIONIT(I) = BIONIT(I)
      BBIODENIT(I) = BIODENIT(I)
      OO2G(I) = O2G(I)
      OO2L(I) = O2L(I)
      END DO
      NH4SOIL1 = NH4SOIL2
      NH3SOIL1 = NH3SOIL2
      TANSOIL1 = TANSOIL2
      NO3SOIL1 = NO3SOIL2
      END IF

```

```

TMOIST = SMOIST

GO TO 32649

!-----
!      End of the DELSUB Loop.  (TSUB = DELSUB)
!      Daily totals are updated
!-----
32648 HOUR   = HOUR+DELSUB
      OLDRAT = RATE(NHR)

      TDEWT = TDWT(NHR)
      TAIR  = TAT(NHR)
      WND   = WDT(NHR)
      IF (ISOL.EQ. 1) THEN
          SRM = SRT(NHR)
          CLD = CLDT(NHR)
      ELSE
          SRM = 0.0
          RN  = RNT(NHR)
      END IF

      CALL AIRDENS(TAIR,SVD_AT,TDEWT,VD_AT)

!
!      Write DELSUB summary to binary output file
!
      IF (NPRINT.EQ. 1) THEN
          IREC = IREC+1
          WRITE(LUB,REC=IREC) IDAY,NHR, (THETA(J),QL(J),QHC(J),
&
&          T(J),J=1,NPT),RN,SENFLX,LE,SHFLUX,SPREV,TMOIST,SHPREV,
&
&          hSTORE,(NO3(J),NH4(J),NH3(J),NH4S(J),NH4L(J),NH3G(J),NH3L(J)    &
&          ,TANTOT(J),J=1,NPT),NH3FLUX,SLURRTANFLUX,N2OFLUX,NOFLUX
          IF (IDAY.EQ. IDEND.AND. N.EQ. NSTOP) THEN
              FINISH = .TRUE.
              GO TO 32673
          ENDIF
      ENDIF

!
!      Estimate new DELT to start the next DELSUB period
!
      DELT = DELMIN

      WRITE(LUS,18) IDAY,NHR,Nh3FLUX,n2oflux,N2OG(1)
18      FORMAT(2I,5E10.3)
      ENDDO

!-----
!      End of the NTOTAL Loop for this day
!
!      Add daily total to simulation total
!-----

32673 IF (FINISH) GO TO 32706
      IDAYACTUAL = IDEND - NDAYS + IDAY

```

```

        IF (IDAYACTUAL .EQ. IDEND) GO TO 32706
        CALL ZEROA(1,25,RTIME)
        CALL ZEROA(1,25,AMOUNT)
        READ(LUI)
METDAY,IRTYPE,EFICEN,NP,NPP,(RTIME(J),AMOUNT(J),J=1,NP),
&      (TDWT(J),J=1,24),(TAT(J),J=1,24),(WDT(J),J=1,24)
        IF (ISOL .EQ. 1) READ(LUI) (SRT(J),J=1,24)
        IF (ICLOUD .EQ. 1) READ(LUI) (CLDT(J),J=1,24)
        IF (IRAD .EQ. 1) READ(LUI) (RNT(J),J=1,24)
        IF (NP .GT. 0) IRDAY = METDAY
        IF (IAPPN .GT. 0) THEN
            IF(APDAY(1) .EQ. IDAY) THEN !resets application info for
appropriate day
                DO I = 1,NAPPN
                    APDAY(I) = APDAY(I+1)
                    APPNEND(I)=APPNEND(I+1)
                    APPNDEN(I)=APPNDEN(I+1)
                    CNAPPN(I)=CNAPPN(I+1)
                    IF(APPNA(I+1) .EQ. 0.0) APPNA(I+1) = APPNA(I)
                    IF(PHAPPN(I+1) .EQ. 0.0) PHAPPN(I+1) = PHAPPN(I)
                    PHAPPN(I) = PHAPPN(I+1)
                    APPNA(I)=APPNA(I+1)
                    APPNRATE(I)=APPNRATE(I+1)
                    NTOTAPPN(I) = NTOTAPPN(I+1)
                    PHAPPN(I) = PHAPPN(I+1)
                    OMAPPN(I) = OMAPPN(I+1)
                    DMAPPN(I)=DMAPPN(I+1)
                    NO3APINIT(I) = NO3APINIT(I+1)
                    NH4APINIT(I) = NH4APINIT(I+1)
                    CRESAPINIT(I) = CRESAPINIT(I+1)
                END DO
            END IF
        END IF
32706 ENDDO
!-----
-
!      End of the Day Loop for this simulation
!
!      Write final simulation summary to binary output file
!-----
-

        WRITE(LUB,REC=IREC) IDAY,G,IPLANT,APLIED,TMOIST,HSTORE
        ENDDO
        WRITE(*,*) ' Simulation completed.'
        CLOSE(UNIT=LUB)
        CLOSE(UNIT=LUI,STATUS='DELETE')
999  STOP
!-----
-
!      End of program AGRIN MAIN
!-----
-

        END

        SUBROUTINE SOILMOD(SFLUX,KHH)
        INCLUDE 'agringlob.inc'

```

```

        DIMENSION SUBQL(M1),A1(M1),A2(M1),A3(M1)
        FUNVD(TD) = EXP(46.440973-(6790.4985/TD)-6.02808*LOG(TD)) !calc
vapour density as function of temp
        INCLUDE 'agrininit.inc'

        CALL INTERK(1,NPPT,KEST,UP,DOWN)
        UPPER = 0
        SSVD_S = FUNVD(T(1)) !g/cm3, soil surface saturated vapour
density
        CALL RELHUM(RHUMID,HEAD) !cal relative humidity at soil surface
        VVD_S = SSVD_S*RHUMID !g/cm3, soil surface vapour density

!       During precipitation, surface evaporation set to zero
!
        IF (ISATUK .GT. 0) THEN
            IF (ISATUK .EQ. 1) THEN
!
!       For the first time step of a rainfall event,
!
                TSUB = TSUB-DELMIN
                DELT = DELMIN
                IF (DELT .LT. DELMIN) DELT = DELMIN
                TSUB = TSUB+DELT
            ENDIF
            SFLUX = RATE(NHR) !cm/h, surface flux equals precip rate
        ENDIF
        ISAVUP = UPPER

!-----
!       Decrease DELT loop when solution unacceptable
!-----
150    DELSAV = DELMIN !h
        IN = 0
        TSTEPM = TSTEPB+0.5*DELMIN
        TSTEPE = TSTEPB+DELMIN
!
!       Set met values to hourly value
        TDEWT = TDWT(NHR)
        TAIR = TAT(NHR)
        WND = WDT(NHR)
        CLD = CLDT(NHR)
        IF (ISOL .EQ. 1) THEN
            SRM = SRT(NHR)
        ELSE
            SRM = 0.0
        END IF
        CALL AIRDENS(TAIR,SVD_AT,TDEWT,VD_AT)
        ITSUCC = 0

!-----
!
!       Predictor-Corrector Loop (while IN .LT. INMAX )
!
!       This implicit scheme solves the partial differential equation
!       for the change in head

```

```

!-----
-
!
!       This loop continues until 10 iterations or successful iteration
!
32626 IF (IN .GE. 10 .OR. ITSUCC .EQ. 1) GO TO 32625
      IN = IN+1
      DEL = 1.0/DELSAV !1/h
      HOUR = NHR
      IF (IRAD .EQ. 1) THEN
        RN = RNT(NHR)
      ELSE
        CALL NETRAD(2,IN,TAT(NHR),VD_AT,CLD,SRT(NHR),HOUR)
      END IF
      IF (IN .GT. 1) THEN
        CALL THERMK(1,NPT)
        CALL INTERK(1,NPPT,KEST,UP,DOWN)
      ENDIF
      NPPT = NPT-1
!
!       Calculate coefficients for simulation of change in moisture
content
!
556   DO II=2,NPT-1
      I      = II-1
      III     = II+1
      Z31     = (Z(III)-Z(I))/2.0 !cm
      FZZ1    = 1./(Z31*ZZ(I)) !1/cm
      FZZ2    = 1./(Z31*ZZ(II)) !1/cm
      AVD1    = 0.5*(DIFFY(I)+DIFFY(II)) !cm2/h
      AVD2    = 0.5*(DIFFY(II)+DIFFY(III))
      ZK1     = -AVD1*FZZ1 !1/h
      ZK2     = -AVD2*FZZ2 !1/h
      A1(II)  = ZK1 !1/h
      A3(II)  = ZK2
      A2(II)  = DEL-ZK1-ZK2 !1/(cm h)
      ZY(II)  = DEL*TTHETA(II) - (KLMID(II)-KLMID(I))/Z31
    ENDDO
!-----
-
!       Surface node calculations
!-----
-
      VDSLHS = 0.0
      VDSRHS = 0.0
      CALL BLR(TAIR,CLD,SLALT,VD_AT,HOUR,KHH,USTAR,RIB)
      IF (ISATUK .EQ. 0 .AND. UPPERH .EQ. 0) THEN
        SVD_S = FUNVD(TS)
        CALL RELHUM(RHUMID,HEAD)
        VD_S = SVD_S*RHUMID
!
!       Because water and vapor density are in g/cm3 and RH is in s/m,
!       the calculated evaporation rate is multiplied by 3.6E5 cm s/m hr
!       to yield a SFLUX value with units of cm/hr.
!
!       The VDSLHS term is used to modify the A2 term in the coefficient
!       matrix to account for the x-terms in the expansion of

```

```

!      exp(x) to 1+x+x^2/2&... in the calculation of VD_S.
!
      TSMEAN = 0.5*(TT(1)+TS)
      HOUR = NHR
      CALL BLR(TAIR,CLD,SLALT,VD_AT,HOUR,KHH,USTAR,RIB)
      TERMH1 = RHUMID
      TERM = TERMH1
      VDSRHS = 1.0-OSMPOT*MGR/TS
      NX = 4+3E-6*HEAD
      DO I = 2,NX
        TERM = TERM*TERMH1/I
        VDSRHS = VDSRHS+TERM
      END DO
      VDSRHS = SVD_S*VDSRHS
      RSOIL = 30.+(3.5*((THET(1)/THETA(1))**2.3))
      RSOIL1 = 6.2*(USTAR**-0.67)
      RHLE = RH+RSOIL+RSOIL1
      SFLUX = 1.0*3.6D5*(VD_AT-VVD_S)/(WATDEN*RHLE) !cm/h
      VDSLHS = 1.0*(MGR/TS)*3.6D5*SVD_S/(2*WATDEN*RH) !cm/h
      SFLUX1 = SFLUX
      SFLUX2 = SFLUX
    ENDIF
    IF (ISATUK .GT. 0) SFLUX1=RATE(NHR)

!
!      After application and until slurry water has
evaporated/infiltrated, calculate
!      evaporation from surface based on slurry and infiltrate slurry
into first soil node

      IF((IAPPN .GT. 0 .AND. IDAY .EQ. APDAY(1) .AND. (NHR) .GE.
&
&APPNSRT(1)) .OR. THICKNEW .GT. 0.0) THEN

      IF (IDAY .EQ. APDAY(1) .and. (NHR) .EQ. APPNSRT(1) .AND. THICKNEW
&
& .EQ. 0.0) THEN !for first time step, set infiltration capacity
as fraction of initial value
      THICKNEW = 1.0
      H2OMASS(1) = APPNRATE(1)*((100.-DMAPPN(1))/100.)*APPNDEN(1) !g
water/ha
      THICKADDED=H2OMASS(1)*DELSAV/(APPNEND(1)-APPNSRT(1))/(10.**8.)
!cm added over entire field for first time step
      QLN = 2.+3.*0.56
      QLHF = QLN*(-19.61)/(QLN-1)
      QLCHI = (THICKADDED-QLHF)*(THET(1)-theta(1))/(0.5*SK(1))
      TOW = DELSAV/(DELSAV+QLCHI)
      SQL1 = 0.5*SK(1)*((TOW**(-0.5))*((2.**0.5)/2.)) + (2./3.)
&
& - ((TOW**0.5))*((2.**0.5)/6.)) + (TOW*(1-(2**0.5))/3.)) !cm/h
infiltrates from slurry layer
      RED = 0.05
      SFLUX3 = RED*SQL1 !soil infiltration capacity
      SORP = 0.5
      SFLUX3 = RED*(0.5*SORP*(DELSAV**(-0.5)) + 0.363*SK(1))
    END IF

```

```

      IF (THICKNEW .GT. 0.0) THEN !if water still present at slurry
surface
      IF((NHR) .GE. APPNEND(1)) THICKADDED = 0.0
      VD_S = SVD_S
      RSOIL = 30.+(3.5*((1.)**2.3)) !for saturated conditions, assumed
until slurry layer gone
      RSOIL1 = 6.2*(USTAR**-0.67)
      RHLE = RH+RSOIL+RSOIL1
      SFLUX21 = 1.0*3.6D5*(VD_AT-VD_S)/(WATDEN*RHLE) !cm/h from
application area
      SFLUX = (SFLUX2*(APPNA(1)-AREACOVERED)*(10.**8.)+
&
      & SFLUX21*AREACOVERED*(10.**8.))/(APPNA(1)*(10.**8.))
!cm/h over entire field
      THICKNEW =THICKADDED+H2OLEFT !cm over entire field
      SFLUX1 = SFLUX3

      IF (SFLUX3 .GT. (THICKNEW/DELSAV+SFLUX)) THEN !ensure
infiltration rate doesn't surpass water available at surface
      SFLUX1 = (THICKNEW/DELSAV + SFLUX)
      END IF

      THICKLOST = (SFLUX-SFLUX1)*DELSAV !g/cm2 or cm lost to
infiltration and evaporation over entire field
      SLURRMAS1 = THICKNEW + THICKLOST !CM water left over entire
field

      END IF

      END IF

!
! Surface node equation for flux b.c.
!
      Z1 = ZZ(1)/2.0
      AVD1 = 0.5*(DIFFY(1)+DIFFY(2))
      Z11 = -AVD1/(Z1*Z1*2.0) !1/h
      A1(1) = 0.0
      A3(1) = Z11 !1/h
      A2(1) = DEL-Z11 !1/(cm h)
      ZY(1) = DEL*TTHETA(1) - (KLMID(1)-SFLUX1)/Z1
      ISTART = 1

      NPPT = NPT -1
      ZN = (ZZ(NPPT))/2.0
      AVD1 = 0.5*(DIFFY(NPPT)+DIFFY(NPT))
      ZK1 = -AVD1/(ZN*ZN*2.0) !1/(cm h)
      A3(NPT) = 0.0
      IF (LOWER .EQ. 1) QLAST = 0.5*(KL(NPT)+KKLNPT) !cm/h
      A1(NPT) = ZK1
      A2(NPT) = DEL-ZK1 !1/(cm h)
      ZY(NPT) = DEL*TTHETA(NPT) - (-KLMID(NPPT)+QLAST)/ZN
      NPPT = NPT
!

```



```

!      Solution of tridiagonal matrix
!
      CALL TRIDAG(ISTART,NPPT,A1,A2,A3,ZY,HSOL)
!-----
!
!      Solution estimate complete for this iteration
!-----
-
      NPPT = NPT-1

      IGO150 = 0

      DO I=1,NPT
        THETA(I) = HSOL(I)
        IF (THETA(I) .GT. THET(1)) THETA(I) = THET(1)
      ENDDO

      IF (IN .LT. INMAX) THEN
        CALL DIFFUSIVITY(1,NPT,THETA,DIFFY)
        CALL POLYKH(1,NPT,THETA,KL,KH)
        DO I = 1,NPT
          KLMID(I) = 0.5*(KL(I)+KL(I+1))
        END DO
      ELSE
        CALL DIFFUSIVITY(1,NPT,THETA,DIFFY)
      ENDIF
      EXCESS = 0.0
      IGO150 = 0
      CALL FLUX(VD_AT,FV)
      CALL HEATFLOW(1,SFLUX,TAIR,FV)
      CALL THERMK(1,NPT)
      IF (IGO150 .EQ. 1) GO TO 795
      CALL THERMK(1,NPT)
      IN = IN+1
      DEL = 1.0/DELSAV !1/h
      HOUR = NHR
      IF (IRAD .EQ. 1) THEN
        RN = RNT(NHR)
      ELSE
        CLD = CLDT(NHR)
        SRM = SRT(NHR)
        CALL NETRAD(2,IN,TAT(NHR),VD_AT,CLD,SRM,HOUR)
      END IF
      GO TO 32626
!-----
-
!      End of the Predictor-Corrector Loop
!-----
-
32625 SUBAST = SUBAST+1
      IGO150 = 0
!
!      Fluxes are calculated at all column segments
!
      CALL FLUX(VD_AT,FV)
      CALL HEATFLOW(2,SFLUX,TAIR,FV)
!

```

```

! Estimate total water storage in the profile (SMOIST) and the
! mass balance error (DIFMAX)
!
SMOIST = 0.0
DO I=1,NPT
    SMOIST = SMOIST+THETA(I)*THICK(I) ! !cm
ENDDO
SSFLUX = SFLUX1*DELSAV !cm
DIFMAX = TMOIST+SSFLUX-QT(NPT)-SMOIST
!
! Reduce the time step if the mass balance error is not within
! limits (when ISWDIF .EQ. 1)
!
IF (THETA(1) .LT. THET(1)) CALL DELCHK
795 IF (IGO150 .EQ. 1) THEN
    CALL RESET(1,NPT,C,H,THETA,KLMID,QL,T,CH,KHMID,KL(NPT),KH(NPT),
&
&    CC,HH,TTHETA,KKLMID,QQ,TT,CCH,KKHMID,KKLNPT,KKHNP)
    DO I = 1,NPT
        DDIFFY(I) = DIFFY(I)
    END DO
    DO I =1,NPT
        IF (ITRACE .GT. 0) AAFPS(I) = AFPS(I)
    END DO
    UPPER = ISAVUP
    GO TO 150
ENDIF
!-----
! End of convergence loop for water flow
! Time step successful, all conditions satisfied.
! Old water flow parameters are reset to new values.
! DELSUB water and heat totals are updated.
!-----
!
IF (ISATUK .EQ. 1) ISATUK = 2
SUBSTP = SUBSTP+1
SUBTIM = SUBTIM+DELSAV
DO I=1,NPT
    SUBQL(I) = SUBQL(I)+QL(I)
ENDDO
IF (SSFLUX .GT. 0.0) SUBINF = SUBINF+SSFLUX
IF (SSFLUX .LT. 0.0) SUBE = -SSFLUX
SUBPE = SUBPE+PESUB*DELSAV
IF (RATE(NHR) .GT. 0.0 .OR. HPOND .GT. 0.0) THEN
    SUBRAN = SUBRAN+DELSAV*PRAIN
    SUBIRR = SUBIRR+DELSAV*PIRRI
    RUNOFF = 0.0
    IF (PIRRI*DELSAV .GT. SSFLUX) RUNOFF = PIRRI*DELSAV-SSFLUX
    IF (PRAIN*DELSAV .GT. SSFLUX) RUNOFF = PRAIN*DELSAV-SSFLUX
    IF (RUNOFF .GT. 0.0) SUBRUN = SUBRUN+RUNOFF
ENDIF
KKLNPT = KL(NPT)
CALL DIFFUSIVITY(1,NPT,THETA,DIFFY)
CALL POLYKH(1,NPT,THETA,KL,KH)
!-----

```

```

!      HEATFLOW subroutine is called to update
!      the DELSUB total values for heat-related terms
!-----
-
      CALL HEATFLOW(3,SFLUX,TAIR,RV)
      HSTORE = SHSTORE
      KKHNPNT = KH(NPT)
      CALL THERMK(1,NPT)
      RETURN
999  WRITE(LUS,'(A)') ' Program terminated prematurely in SOILMOD'
      IF (LUSLOW) WRITE(LOUT,'(A)')
&
      &' Program terminated prematurely in SOILMOD'
      STOP
!-----
-
!      End of subroutine SOILMOD
!-----
-
      END

      SUBROUTINE BLR(RTAIR,RCLD,RSLALT,RVD_AT,RHOUR,KHH,RUSTAR,RIB)
!-----
-
!      Called by AGRIN MAIN
!
!      Calculates boundary layer resistance (RH [s/m]) to heat and vapor
!      as a function of wind speed and measurement height, air
!      temperature and measurement height, zero plane displacement,
!      roughness lengths for heat and momentum, and surface temperature
!-----
-
      INCLUDE 'agringlob.inc'
      REAL*8 KM2,KM,KMKH
      IF (WND .le. 0.01) THEN
!      --when wind is zero, RH calculated as pure diffusion
!      --the factor of 10000 converts cm^2 to m^2
      RH = 10000.0*ZT/VAPDIF
      GO TO 20
      ENDIF
      IRHLIM = 5
      PSIM = 0.
      PSIH = 0.
      TSMEAN = 0.5*(TT(1)+T(1))
      DO I = 1,IRHLIM
      USTAR = VK*WND/(RLNZU+PSIM)
      RH = (RLNZT+PSIH)/(VK*USTAR)
      IF (I .EQ. 1) THEN
      RHO = RH
      RHMIN = 0.1*RH
      RHMAX = 10.0*RH
      ELSE
      IF (RH .GT. RHMAX) THEN
      RH = RHMAX
      GO TO 20
      ELSE IF (RH .LT. RHMIN) THEN
      RH = RHMIN

```

```

        GO TO 20
    ENDIF
ENDIF
IF (I .LT. IRHLIM) THEN
    ZETA = -(VK*ZT*GRAV/(CHA*RTAIR*USTAR*USTAR*USTAR))*
&
    &      (CHA*(TSMEAN-RTAIR)/RH)
    IF (TSMEAN .LT. RTAIR) THEN
        PSIH = 4.7*ZETA
        PSIM = PSIH
    ELSE
        PSIH = -2*LOG((1.0+SQRT(1.0-16.0*ZETA))/2.0)
        PSIM = 0.60*PSIH
    ENDIF
ENDIF
ENDDO

20    RH1 = 10000.0*ZT/VAPDIF !pure diffusion
    IF (RH .GT. RH1) RH = RH1 !pure diffusion set as limit to
resistance
    RETURN

```

```

!-----
-
!      End of subroutine BLR
!-----
-

```

END

SUBROUTINE DELCHK

```

!-----
-
!      Called by AGRIN MAIN
!
!      Adjusts the time step according to the mass and heat balance
error
!      Specifically, it will increase or decrease the time step
!      according to the ratio DMAXBA/DIFMAX
!
!      - if R = 0, the time step size is not changed
!      - if the time step size equals DELMIN and the solution
!        was unsuccessful (i.e., DIFMAX > DMAXBA), the program is
!        stopped rather than accepting the solution and moving on
!        (as was done in Version 2.0)
!      - if 0.9 < R < 1.0, R = 0.9; this change prevents the slow
!        decrease of time step reduction when DIFMAX is close to DMAXBA
!-----
-

```

```

INCLUDE 'agringlob.inc'
IF (IDAY .EQ. TILLDAY) GO TO 1000
DMAXBA = 0.000000000001
DMAXHE = 1000000.0
IF (DIFMAX .EQ. 0) THEN
    RWATER = 20.0
ELSE

```

```

      RWATER = DMAXBA/ABS(DIFMAX)
    ENDIF
    R = RWATER
    IF (DMAXHE .GT. 0 ) THEN
      IF (HEATBAL .EQ. 0) THEN
        RHEAT = 20.0
      ELSE
        IF (SFLUX1 .GT. 0.0) THEN
          XHE = DMAXHE*1000.0
          RHEAT = XHE/ABS(HEATBAL)
        ELSE
          RHEAT = DMAXHE/ABS(HEATBAL)
        END IF
      ENDIF
      R = MIN(RWATER,RHEAT)
    ENDIF
    IF (R .LT. 1.0) THEN
!-----
!
!   Decrease the time step
!-----
!
      IF (DELT .LE. DELMIN) THEN
        WRITE(*,*) ' Convergence criterion not met using DELMIN'
        WRITE(*,*) ' Simulation stopped in DELCHK'
        WRITE(*,6000)
      IDAY,ISATUK,DMAXBA,DIFMAX,RWATER,DMAXHE,HEATBAL,&
        &      RHEAT,HOURL+TSUB-DELT,DELT,SFLUX1
        STOP
      ENDIF
105    RPRIM = R*R
      IF (RPRIM .GT. 0.9) RPRIM = 0.9
      IF (RPRIM .LT. 0.5) RPRIM = 0.5
      TSUB = TSUB - DELT
      DELT = DELT * RPRIM
      IF (DELT .LT. DELMIN) DELT = DELMIN
      IGO150 = 1
      TSUB = TSUB + DELT
      GO TO 1000
    ELSE
!-----
!
!   Increase the time step
!-----
!
      RPRIM = 0.5*(1+R)
      IF (RPRIM .GT. RFACT) RPRIM = RFACT
      DELT = DELT*RPRIM
      IF (DELT .GT. DELMAX) DELT = DELMAX
      TLEFT = DELSUB-TSUB
      IF (TLEFT .GT. 0. .AND. TLEFT .LE. 2.0*DELT+TIMRES) THEN
        IF (TLEFT .LE. DELT+TIMRES) THEN
          DELT = TLEFT
        ELSE
          DELT = TLEFT/2.0
        ENDIF
      ENDIF
    ENDIF

```

```

        ENDIF
1000 RETURN
!-----
!
!   Format statements
!-----
!
6000 FORMAT(
&
&   ' IDAY   = ',I3,T24,   ' ISWDIF = ',I1,1P,/,
&
&   ' DMAXBA = ',E12.5,T24,' DIFMAX = ',E12.5,T47,' RWATER = ',E12.5/,
&
&   ' DMAXHE = ',E12.5,T24,' HEATBAL = ',E12.5,T47,' RHEAT  = ',E12.5/,
&
&   ' TDONE  = ',E12.5,T24,' DELT   = ',E12.5,T47,' SFLUX  = ',E10.3)
!-----
!
!   End of subroutine DELCHK
!-----
!
        END

        SUBROUTINE NETRAD(IDAILY, INH, RTAIR, RVD_AT, RCLD, RSRM, RHOURL)
!-----
!
!   Called by AGRIN MAIN
!
!   Calculates net radiation (RN [W/m2])
!   as a function of latitude, time of year, time of day,
!   air and surface temperature, atmospheric vapor density, albedo,
!   cloud cover, surface and air emissivities, and extraterrestrial
!   solar flux) in W/m2.
!-----
!
        INCLUDE 'agringlob.inc'
        IF (ISOL .EQ. 1) ST = RSRM !W/m2 !SEXT*SR_FRAC
        IF (ST .LT. 0) ST = 0.0
!
!   ALBEDO and EMISS_S calculations are taken from van Bavel
!   and Hillel (1976)
!
        AVETHE = (THETA(1)+TTHETA(1))/2.0
        IF (AVETHE .LT. 0.1) THEN
            ALBEDO = 0.25
        ELSE IF (AVETHE .GT. 0.25) THEN
            ALBEDO = 0.1
        ELSE
            ALBEDO = 0.1+0.25-AVETHE
        ENDIF
        EMISS_A = 4.174*RVD_AT**(1.0/7.0) !unitless
        IF (RCLD .GT. 0) EMISS_A = (1.0-0.84*RCLD)*EMISS_A+0.84*RCLD
        EMISS_S = 0.9+0.18*AVETHE
        IF (EMISS_A .GT. 1.0) EMISS_A = 1.0
        IF (INH .EQ. 1) TAQ = RTAIR*RTAIR*RTAIR*RTAIR !K4
        TSMEAN = 0.5*(TT(1)+T(1))
        TSQ = TSMEAN*TSMEAN*TSMEAN*TSMEAN !K4

```

```

      RN = (1.0-0.1)*ST+SB*(EMISS_A*TAQ-EMISS_S*TSQ)
      RETURN
!-----
!      End of subroutine NETRAD
!-----
      END

      SUBROUTINE POLYKH (IBEGIN, IEND, RTHETA, RKL, RKH)
!-----
!      Called by AGRIN IN, AGRIN MAIN
!
!      Calculates the conductivity (RKL) of each node as a function of
!      the head value (HEAD) for that node
!-----
      INCLUDE 'agringlob.inc'
      DIMENSION RKL(M1), RKH(*), RTHETA(*), BB(IEND)
      DO I=IBEGIN, IEND

      RSATMA = SATMA(1) !m
      RTHETM = THET(1)
      SKM = SK(1) !cm/hr
      BM = B(1)
!
!      Calculate hydraulic conductivity

      RKL(I) = SKM*((RTHETA(I)/RTHETM)**((2.0*BM) + 3.0)) !cm/h

!
!      Calculate thermal conductivity
      D12 = 0.03+0.1*(BLKDEN**2.)
      BB(I) = 1.06*BLKDEN*RTHETA(I)
      A12 = 0.65 - 0.78*BLKDEN + 0.6*(BLKDEN**2.)
      C12 = 1. +2.6*(CLY**(-0.5))

      RKH(I) = (A12 + 1.06*BLKDEN*THETA(I)*THETA(I) - (A12-D12)*EXP(-
&
&      (C12*THETA(I))**4.))*36. !J/S/M/K TO J/h/cm/K

      IF (RKL(I) .LT. 0.0) THEN
          WRITE(*, 6000) IN, I, IDAY, TSTEPB, TTHETA(I), THETA(I), RKL(I)
          STOP
      ENDIF

      ENDDO
      RETURN
6000  FORMAT(/,
&      &' Subroutine POLYKH detected an invalid conductivity value',/,
&
&      &I13, ' = Iteration number (IN)',/,
&
&      &I13, ' = Node number (N)',/,
&

```

```

&I13,' = Simulation day (IDAY)',/,
&
&1PE13.5,' = Completed time of day (TSTEPB)',/,
&
&E13.5,' = Previous theta THTH(I)',/,
&
&E13.5,' = Current theta TH(I)',/,
&
&E13.5,' = Calculated conductivity RKL(I)',/)
!-----
-
!      End of subroutine POLYKH
!-----
-
      END
      SUBROUTINE THERMK(IBEGIN,IEND)
!-----
-
!      Called by AGRIN IN and AGRIN MAIN
!
!      Calculates soil and vol. heat capacity
!-----
-
      INCLUDE 'agringlob.inc'
      DO I=IBEGIN,IEND
          MATI = MAT(I)
          THETAI = THETA(I)
          CH(I) = CHW*THETAI+CHSOIL(I) !*blkden/1000.0 !J/cm3/K
      ENDDO
      RETURN
!-----
-
!      End of subroutine THERMK
!-----
-
      END

      SUBROUTINE TRIDAG(IF,L,A,BBB,RC,RD,V)
!-----
-
!      Called by HEATFLOW, SOILMOD, PROFMOD and AGRIN MAIN
!
!      Solves the tridiagonal solution matrix
!-----
-
      INCLUDE 'agringlob.inc'
      DIMENSION A(*),BBB(*),RC(*),RD(*),V(*),BETA(M1),GAMM(M1)
      DATA BETA/M1*0/,GAMM/M1*0/
      BETA(IF) = BBB(IF)
      GAMM(IF) = RD(IF)/BETA(IF)
      IFP1 = IF+1
      DO I=IFP1,L
          II = I - 1
          BETA(I) = BBB(I) - A(I)*RC(II)/BETA(II)
          GAMM(I) = (RD(I)-A(I)*GAMM(II))/BETA(I)
      ENDDO
      V(L) = GAMM(L)

```



```

      LAST = L - IF
      DO K = 1, LAST
        I = L - K
        V(I) = GAMM(I) - RC(I)*V(I+1)/BETA(I)
      ENDDO
      RETURN
!-----
!
!      End of subroutine TRIDAG
!-----
!
      END

      SUBROUTINE TIMEX
!-----
!
!      Called by AGRIN IN and AGRIN MAIN
!
!      Queries the operating system and returns the time and date
!      SDATE = Date in format 01 Jan 1993 (dd mmm yyyy)
!      STIME = Time in format 01:02:03.42 (hh:mm:ss.ss)
!-----
!
      INCLUDE 'agringlob.inc'
      CHARACTER*3 MON(12)*3, REAL_CLOCK(3)*12
      INTEGER DATE_TIME(8)
      DATA MON /'Jan', 'Feb', 'Mar', 'Apr', 'May', 'Jun', 'Jul',
&
& 'Aug', 'Sep', 'Oct', 'Nov', 'Dec'/
      CALL DATE_AND_TIME(REAL_CLOCK(1), REAL_CLOCK(2),
&
& REAL_CLOCK(3), DATE_TIME)
      SDATE(1:2) = REAL_CLOCK(1)(7:8)
      SDATE(3:3) = CHAR(32)
      SDATE(4:6) = MON(DATE_TIME(2))
      SDATE(7:7) = CHAR(32)
      SDATE(8:11) = REAL_CLOCK(1)(1:4)
      STIME(1:2) = REAL_CLOCK(2)(1:2)
      STIME(3:3) = CHAR(58)
      STIME(4:5) = REAL_CLOCK(2)(3:4)
      STIME(6:6) = CHAR(58)
      STIME(7:11) = REAL_CLOCK(2)(5:9)
      RETURN
!-----
!
!      End of subroutine TIMEX
!-----
!
      END

      SUBROUTINE HEATFLOW(INH, SFLUX, RTAIR, RFV)
!-----
!
!      Called by AGRIN MAIN
!
!      INH = 1 solves heat balance equations

```

```

!      INH = 2  calculates fluxes and heat balance error for current
!              time step solution
!      INH = 3  time step solution accepted; DELSUB values updated
!-----
-
      INCLUDE 'agringlob.inc'
      DIMENSION A1H(M1),A2H(M1),A3H(M1),ZYH(M1)
      GO TO (100,200,300) INH
100  NPPT = NPT-1
      DEL = 1./DELSAV
!
!      Calculate coefficients for simulation of change in temperature
!
      DO II=2,NPPT
          I      = II-1
          III     = II+1
          Z31     = (Z(III)-Z(I))/2.0
          KH1     = -KHMID(I)/(Z31*ZZ(I))
          KH2     = -KHMID(II)/(Z31*ZZ(II))
          AVCH    = CH(II) !0.5*(CCH(II)+CH(II))
          A2H(II) = AVCH*DEL-KH1-KH2
          A1H(II) = KH1
          A3H(II) = KH2
          TG1     = (TT(II)-TT(I))/ZZ(I)
          TG2     = (TT(III)-TT(II))/ZZ(II)
          ZYH(II) = AVCH*TT(II)*DEL !-((-KHMID(II)*TG2+KHMID(I)*TG1)/Z31
          DELZ31  = 1/(DELSAV*Z31*2)
      ENDDO
!
!      Surface node equation for heat flux b.c.
!      Surface fluxes such as net radiation, sensible heat, and latent
!      heat are calculated using the average time-step temperature,
!      Tavg = 0.5*(Tj + Tj-1). The surface flux units are W/m2
!
      SENFLX = CHA*((T(1)-TAIR(1)))/RH !W/m2
      SSFLUX = SFLUX*DELSAV
      LE      = -(LHV0+CHV*(0.5*(TS+TT(1))-T0))*SSFLUX/(DELSAV*0.36)
!W/m2
!
!      When evaporation occurs, SSFLUX (cm) is converted into LE (W/m2)
!
      IF (SSFLUX .LT. 0) THEN
          LE = -(LHV0+CHV*(0.5*(TS+TT(1))-T0))*SSFLUX/(DELSAV*0.36)
!W/m2
          !LE = RFV !
          SHFLUX = RN-SENFLX-LE
      ELSE
          IF (ISATUK .GT. 0) LE = 0.0
          SHFLUX = RN-SENFLX
      ENDIF

      Z1      = ZZ(1)
      KH2     = -KHMID(1)/(thick(1)*Z1)!-KHMID(1)/(Z1*Z1)
      AVCH    = CH(1) !0.5*(CH(1)+CCH(1))
      A1H(1)  = 0.0
      A2H(1)  = AVCH*DEL-KH2

```

```

      A3H(1) = KH2
      TG2 = (TT(2)-TT(1))/Z1
      ZYH(1) = AVCH*TT(1)*DEL-(-1.*SHFLUX*.36)/Z1      !(-
KKHMID(1)*TG2-2.*SHFLUX*.36)/Z1

      ISTART = 1
!
!      Lower node: constant temperature

      ZYH(NPPT) = ZYH(NPPT)-A3H(NPPT)*T(NPT)
      A3H(NPPT) = 0.0

!
!      Solution of tridiagonal matrix
!
      CALL TRIDAG(ISTART,NPPT,A1H,A2H,A3H,ZYH,T)

!-----
!
!      Solution estimate complete for this iteration
!-----
!
!      T limits are -40 C (-40 F) lower and 90 C (194 F) upper.
!      If T goes outside these limits, the time step is reduced.
!      Future option: add convergence criteria for temperature?
!

      DO I=1,NPT
      IF (T(I) .LT. 233 .OR. T(I) .GT. 363) THEN
      IF (DELT .GT. DELMIN) THEN
      TSUB = TSUB-DELT
      DELT = MAX(0.5*DELT,DELMIN)
      TSUB = TSUB+DELT
      IGO150 = 1
      ELSE
      WRITE(*,*) ' T limits exceeded and DELT < DELMIN'
      WRITE(LUS,15)T(1)
15      FORMAT ('T(1) = ', E10.3)
      WRITE(*,*) ' Simulation stopped '
      STOP
      ENDIF
      ENDIF
      ENDDO

!-----
!
!      End of the iteration loop
!-----
!
      GO TO 900

!-----
!
!      INH = 2
!      Calculate fluxes and heat balance error for this time step
!      heat flux across the surface (SHFLUX [W/m2])
!      heat fluxes within the soil (QHcvw [J/cm2/h])
!-----

```

```

200 DO II=2,NPT
      I = II-1
      ZI = ZZ(I)
      TG = (T(II)-T(I))/ZI !K/cm
      TTG = (TT(II)-TT(I))/ZI !K/cm
      QHC(I) = 0.5*(-KHMID(I)*TG-KKHMID(I)*TTG) !J/cm2/h
    ENDDO

!
! Calculate bottom conductive heat flux, QHC(NPT), [J/cm2/h]
!

      QHC(NPT) = QHC(NPT-1) !W/cm2
      THCKTM = THICK(NPT)/DELSAV

!
! Estimate heat storage in the profile (SHSTORE) and the heat
! balance error (HEATBAL) in J/m2.
!

      SHSTORE = 0.0
      HGEN = 0.0
      DO I=1,NPT
        SHSTORE = SHSTORE+CH(I)*(T(I)-T0)*THICK(I) !J/cm2
        HGEN = HGEN
      ENDDO
      HGEN = HGEN*36.0
      SHSTORE = SHSTORE*10000.0 !J/m2
      X = SHFLUX*3600.0*DELSAV
      Y = QHC(NPT)*10000.0*DELSAV
      X1 = HSTORE
      X2 = SHSTORE
      HEATBAL = (SHFLUX*3600.0+10000.0*(HGEN+QHW0-QHW(NPT)
&
&      -QHC(NPT)))*DELSAV+HSTORE-SHSTORE !J/m2
      DHSTORE = 0.0
      DO I=1,NPT
        DHSTORE = DHSTORE+0.5*(CH(I)+CCH(I))*(T(I)-TT(I))*THICK(I)
      ENDDO
      HEATBL = (SHFLUX*0.36+HGEN+QHW0
&
&      -QHW(NPT)-QHC(NPT))*DELSAV-DHSTORE
!-----
!
! End of convergence loop for HEATFLOW.
!-----
!
      GO TO 900
!-----
!
! INH = 3
! Time step solution is accepted, DELSUB totals are updated
! The surface heat fluxes are converted from [W/m2] to [J/m2],
! other fluxes are [J/cm2]
! Old heat flow parameters are reset to new values
!-----
300 SUBHBE = SUBHBE+HEATBAL

```

```

        SUBLE = SUBLE+LE*3600*DELSAV
        SUBRN = SUBRN+RN*3600*DELSAV
        SUBSHF = SUBSHF+SHFLUX*3600*DELSAV
        SUBSEN = SUBSEN+SENFLX*3600*DELSAV
        SUBQHW0 = SUBQHW0+QHW0*DELSAV
        DO I=1,NPT
            SUBQHC(I) = SUBQHC(I)+QHC(I)*DELSAV
            SUBQHW(I) = SUBQHW(I)+QHW(I)*DELSAV
        ENDDO
900    RETURN
!-----
!
!      End of subroutine HEATFLOW
!-----
!
      END

      SUBROUTINE AIRDENS(RTAIR,RSVD_AT,RTDEWT,RVD_AT)
!-----
!
!      Called by AGRIN MAIN
!
!      Calculates the atmospheric and saturated atmospheric density
!-----
!
      INCLUDE 'agringlob.inc'
      FUNVD(TD) = EXP(46.440973-(6790.4985/TD)-6.02808*LOG(TD))
      RSVD_AT = FUNVD(RTAIR) !g/cm3
      RVD_AT = FUNVD(RTDEWT) !g/cm3
      RETURN
!-----
!
!      End of subroutine AIRTMP
!-----
!
      END
      SUBROUTINE ZEROA(IBEGIN,IEND,ARRAY)
!-----
!
!      Called by AGRIN MAIN
!
!      Sets ARRAY to zero
!-----
!
      INCLUDE 'agringlob.inc'
      DIMENSION ARRAY(M1)
      DO I=IBEGIN,IEND
          ARRAY(I) = 0.0
      ENDDO
      RETURN
!-----
!
!      End of subroutine ZEROA
!-----
!
      END
      SUBROUTINE ZEROI(K1,K2,K3,K4)

```

```

!-----
!
!   Called by AGRIN MAIN
!
!   Sets INTEGER parameters to zero
!-----
-
      INCLUDE 'agringlob.inc'
      K1 = 0.0
      K2 = 0.0
      K3 = 0.0
      K4 = 0.0
      RETURN
!-----
!
!   End of subroutine ZEROI
!-----
-
      END
      SUBROUTINE ZEROR(R1,R2,R3,R4,R5,R6,R7,R8,R9,R10,R11,R12,R13)
!-----
!
!   Called by AGRIN MAIN
!
!   Sets REAL parameters to zero
!-----
-
      INCLUDE 'agringlob.inc'
      R1 = 0.0
      R2 = 0.0
      R3 = 0.0
      R4 = 0.0
      R5 = 0.0
      R6 = 0.0
      R7 = 0.0
      R8 = 0.0
      R9 = 0.0
      R10 = 0.0
      R11 = 0.0
      R12 = 0.0
      R13 = 0.0
      RETURN
!-----
!
!   End of subroutine ZEROR
!-----
-
      END
      SUBROUTINE INTERK(IBEGIN,IEND,KEST,UP,DOWN)
!-----
!
!   Called by AGRIN MAIN
!
!   1) Computes internodal conductivity, KLMID, based on KEST options
!   2) Computes internodal thermal conductivity, KHMID, using
!       arithmetic averaging

```

```

!-----
-
      INCLUDE 'agringlob.inc'
      LOGICAL LMDIFF
      MM = 0
      DO I=IBEGIN,IEND
!
!       Compute KLMID
!
      RKL1 = KL(I)
      RKL2 = KL(I+1)
      KEST = 1
!
!       Arithmetic mean of KL, KEST=1
!
      IF (KEST .EQ. 1) THEN
          KLMID(I) = (RKL1+RKL2)*0.5
!
!       Harmonic mean of KL, KEST=2
!
      ELSE IF (KEST .EQ. 2) THEN
          KLMID(I) = 2*(RKL1*RKL2/(RKL1+RKL2))
!
!       Geometric mean of KL, KEST=3
!
      ELSE IF (KEST .EQ. 3) THEN
          KLMID(I) = (RKL1*RKL2)**0.5
          IF (KLMID(I) .EQ. 0) KLMID(I) = EXP((LOG(RKL1)+LOG(RKL2))/2)
      ENDIF
!
!       Compute internodal thermal conductivities [J/cm/hr/K]
!
      KHMID(I) = (KH(I)+KH(I+1))*0.5
      ENDDO
      RETURN
!-----
-
      End of subroutine INTERK
!-----
-
      END

      SUBROUTINE
      RESET(IBEGIN,IEND,AA1,AA2,AA3,A4,A5,A6,A7,A8,A9,A10,R1, &
          & R2,R3,R4,R5,R6,R7,R8,R9,R10)
!-----
-
      Called by AGRIN MAIN
!
!       Copy R values into A. Used to
!       a) initialize parameters at start of iteration loop
!       b) reset parameters after a time step reduction
!
!       Parameter Number (array A or R)
!       1 C
!       2 H
!       3 THETA

```

```

!      4  KLMID
!      5  QL
!      6  T
!      6  CH
!      8  KHMID
!      9  KL(NPT)
!     10  KH(NPT)
!-----
-
      INCLUDE 'agringlob.inc'
      DIMENSION AA1(M1),AA2(M1),AA3(M1),A4(M1),A5(M1),A6(M1),A7(M1),
&
&
A8(M1),R1(M1),R2(M1),R3(M1),R4(M1),R5(M1),R6(M1),R7(M1),R8(M1)
      DO I=IBEGIN,IEND
          AA1(I) = R1(I)
          AA2(I) = R2(I)
          AA3(I) = R3(I)
          A4(I) = R4(I)
          A5(I) = R5(I)
          A6(I) = R6(I)
          A7(I) = R7(I)
          A8(I) = R8(I)
      ENDDO
      A10 = R10
      A9 = R9
      RETURN
!-----
-
!      End of subroutine RESET
!-----
-
      END

      SUBROUTINE RESET2
!
!      Resets values used when chemical species
!
      INCLUDE 'agringlob.inc'
      DO I=1,NPT
          NNH4(I) = NH4(I)
          NNH4L(I) = NH4L(I)
          NNH4S(I) = NH4S(I)
          NNH3(I) = NH3(I)
          NNH3G(I) = NH3G(I)
          NNH3L(I) = NH3L(I)
          NNOG(I) = NOG(I)
          NNOL(I) = NOL(I)
          NNO(I) = NO(I)
          NNO2L(I) = NO2L(I)
          NNO2(I) = NO2(I)
          NN2OL(I) = N2OL(I)
          NN2OG(I) = N2OG(I)
          NN2O(I) = N2O(I)
          NN2L(I) = N2L(I)
          NN2G(I) = N2G(I)
          NN2(I) = N2(I)

```



```

NN2OFLUX = N2OFLUX
TtANTOT(I) = TANTOT(I)
TTANL(I) = TANL(I)
NNO3(I) = NO3(I)
NNO2(I) = NO2(I)
PPH(I) = PH(I)
CCRES(I) = CRES(I)
CCBIO(I) = CBIO(I)
CCHUM(I) = CHUM(I)
CCPASS(I) = CPASS(I)
BBIONIT(I) = INITBIO(I)
BBIODENIT(I) = IDENITBIO(I)
CCO2G(I) = CO2G(I)
CCO2(I) = CO2(I)
NNO3L(I) = NO3L(I)
NNO2L(I) = NO2L(I)
HHION(I) = HION(I)
AAFPS(I) = AFPS(I)
ENDDO
RETURN

```

```

!-----
-
!      End of subroutine RESET2
!-----
-
END

```

```

SUBROUTINE TILL (TFLAG)

```

```

!
!      Creates uniform profiles up to tillage depth of 10cm
!

```

```

INCLUDE 'agringlob.inc'
IF(IDAY.EQ. TILLDAY .AND. NHR.EQ. 12 .AND. TFLAG.EQ. 0) THEN
  THETATOTAL = 0.0
  TEMPTOTAL = 0.0
  O2GTOTAL = 0.0
  O2LTOTAL = 0.0
  BIONITTOTAL = 0.0
  BIODENITTOTAL = 0.0
  TNH4TOTAL = 0.0
  TNH4LTOTAL = 0.0
  TNH4STOTAL = 0.0
  TNH3TOTAL = 0.0
  TNH3GTOTAL = 0.0
  TNH3LTOTAL = 0.0
  TTANTOTAL = 0.0
  TTANLTOTAL = 0.0
  TNO3TOTAL = 0.0
  TNO3LTOTAL = 0.0
  TPHTOTAL = 0.0
  TCRESTOTAL = 0.0
  TCHUMTOTAL = 0.0
  TCPASSTOTAL = 0.0
  TCBIOTOTAL = 0.0
  TCO2G = 0.0
  TCO2 = 0.0
  THIONL = 0.0

```

```

TAFPS = 0.0
NODENUM = 0
DO I = 1,NPT
IF (Z(I) .LE. 10.0) THEN
    TNH4TOTAL = TNH4TOTAL + NH4(I)
    THETATOTAL = THETATOTAL + THETA(I)
    TEMPTOTAL = TEMPTOTAL + T(I)
    O2GTOTAL = O2GTOTAL + O2G(I)
    O2LTOTAL = O2LTOTAL + O2L(I)
    BIONITTOTAL = BIONITTOTAL + BIONIT(I)
    BIODENITTOTAL = BIODENITTOTAL + BIODENIT(I)
    TNH4LTOTAL = TNH4LTOTAL + NH4L(I)
    TNH4STOTAL = TNH4STOTAL + NH4S(I)
    TNH3TOTAL = TNH3TOTAL + NH3(I)
    TNH3GTOTAL = TNH3GTOTAL + NH3G(I)
    TNH3LTOTAL = TNH3LTOTAL + NH3L(I)
    TTANTOTAL = TTANTOTAL + TANTOT(I)
    TTANLTOTAL = TTANLTOTAL + TANL(I)
    TNO3TOTAL = TNO3TOTAL + NO3(I)
    TNO3LTOTAL = TNO3LTOTAL + NO3L(I)
    TPHTOTAL = TPHTOTAL + PH(I)
    TCRESTOTAL = TCRESTOTAL + CRES(I)
    TCHUMTOTAL = TCHUMTOTAL + CHUM(I)
    TCPASSTOTAL = TCPASSTOTAL + CPASS(I)
    TCBiotOTAL = TCBiotOTAL + CBIO(I)
    TCO2G = TCO2G + CO2G(I)
    TCO2 = TCO2 + CO2(I)
    THIONL = THIONL + HIONL(I)
    TAFPS = TAFPS + AFPS(I)
    NODENUM = NODENUM + 1
END IF
END DO
DO I = 1,NPT
IF (Z(I) .LE. 10.0) THEN
    NH4(I) = TNH4TOTAL/NODENUM
    THETA(I) = THETATOTAL/NODENUM
    T(I) = TEMPTOTAL/NODENUM
    O2G(I) = O2GTOTAL/NODENUM
    O2L(I) = O2LTOTAL/NODENUM
    BIONIT(I) = BIONITTOTAL/NODENUM
    BIODENIT(I) = BIODENITTOTAL/NODENUM
    NH4L(I) = TNH4LTOTAL/NODENUM
    NH4S(I) = TNH4STOTAL/NODENUM
    NH3(I) = TNH3TOTAL/NODENUM
    NH3G(I) = TNH3GTOTAL/NODENUM
    NH3L(I) = TNH3LTOTAL/NODENUM
    TANTOT(I) = TTANTOTAL/NODENUM
    TANL(I) = TTANLTOTAL/NODENUM
    NO3(I) = TNO3TOTAL/NODENUM
    NO3L(I) = TNO3LTOTAL/NODENUM
    PH(I) = TPHTOTAL/NODENUM
    CRES(I) = TCRESTOTAL/NODENUM
    CHUM(I) = TCHUMTOTAL/NODENUM
    CBIO(I) = TCBiotOTAL/NODENUM
    CPASS(I) = TCPASSTOTAL/NODENUM
    CO2G(I) = TCO2G/NODENUM
    CO2(I) = TCO2/NODENUM

```

```

        HIONL(I) = THIONL/NODENUM
        AFPS(I) = TAFPS/NODENUM
    END IF
END DO
TFLAG = 1
END IF

RETURN

!-----
!
!   End of subroutine TILL
!-----
-

END

SUBROUTINE DIFFUSIVITY(IBEGIN,IEND,RTHETA,RDIFFY)
!-----
!
!   Called by AGRIN IN, AGRIN MAIN
!
!   Calculates the water content (THETA) and moisture capacity (C)
!   of each node as a function of the head value (H) for that node
!-----
-

    INCLUDE 'agringlob.inc'
    DIMENSION RTHETA(*),RDIFFY(*)
    INCLUDE 'agrininit.inc'

    DO I=IBEGIN,IEND

        SATM = SATMA(1) !m
        BM   = B(1)
        SKM   = SK(1) !cm/h
        THETM = THET(1)
        RDIFFY(I)=(BM*SKM*(SATM*100.0)/THETM)*(RTHETA(I)/THETM)**(BM+3.0)
!cm2/h
    END DO

    RETURN

!-----
!
!   Format Statements
!-----
-

6000  FORMAT(
&
& ' ERROR: Liquid water diffusivity must be positive, MAT
No.',I3,/,&
& '          Node = ',I4,', RC = ',1PE15.7,', WATCONT = ',E15.7)
6010  FORMAT(/,
&
& ' Program execution stopped in subroutine RETENT ',/,
&
& ' because of negative moisture capacity(s) for',I4,', nodes')
!-----
-

```

```

!      End of Subroutine RETENT
!-----
-
      END

      SUBROUTINE FLUX(RVDA_T,RFV)
!-----
-
!      Called by AGRIN MAIN
!
!      Calculates liquid water fluxes between nodes
!-----
-
      INCLUDE 'agringlob.inc'
      CALL ZEROA(1,NPT,QL)
      CALL ZEROA(1,NPT,QT)
      DO II=2,NPT
        I      = II-1
        III    = II+1
        ZI      = ZZ(I)
        PG      = (THETA(II) - THETA(I))/ZI
        PPG     = (TTHETA(II) - TTHETA(I))/ZI
        QL(I)
=DELSAV*0.5*(KLMID(I)+DIFFY(I)*PG+KKLMID(I)+DDIFFY(I)*PPG) !CM
        QT(I) = QL(I)
      ENDDO

!      Deep drainage flux
!
      IF (LOWER .EQ. 2 .OR. LOWER .EQ. 5) THEN
        QL(NPT) = QT(NPT-1)
      ELSE
        QL(NPT) = QLAST*DELSAV !cm
      ENDIF
      QT(NPT) = QL(NPT)
!-----
-
!      End of subroutine FLUX
!-----
-
      END

      SUBROUTINE WELCOME(name)
!-----
-
!      Called by AGRIN IN, AGRIN MAIN, and AGRIN OUT
!
!      Writes program header with version number and contact person
!-----
-
      INCLUDE 'agringlob.inc'
      CHARACTER name*7
      WRITE(LUS,10) name
10    FORMAT(/,
&

```

```

&      '      ',A12,,
&
&      '      Contact:',/,
&
&      '      Jessica Beuning',/,
&
&      '      University of Guelph',/,
&
&      '      Guelph, ON',/,
&
&      '      email jbeuning@uoguelph.ca',/)
RETURN
!-----
!      End of subroutine WELCOME
!-----
-
END

SUBROUTINE RELHUM(RHOUT,RHEAD)
!-----
!      Called by AGRIN MAIN
!
!      Calculates the relative humidity using suction head,
!      temperature, and osmotic potential (in suction head units)
!-----
-
INCLUDE 'agringlob.inc'
IF (THETA(1) .GE. THET(1)) THEN
    RHOUT = 1.0D0
ELSE
    RHEAD = SATMA(1)*100.*((THETA(1)/THET(1))**-B(1))
    RHOUT = EXP(-(RHEAD+OSMPOT)*MGR/T(1))
ENDIF
RETURN
!-----
!      End of subroutine RELHUM
!-----
-
END

SUBROUTINE EQMMOD(IFLAG,RNO3L,RNO2L)
!-----
!      Called by AGRIN MAIN
!
!      Simulates 3 equilibrium processes:
!      1) Calculates ammonium dissociation based on TAN and pH
!      2) Calculates ammonia gas production based on TAN and Henry's
Law
!      3) Calculates ammonium adsorption based on total ammonium and
Freundlich isotherm
!-----
-
INCLUDE 'agringlob.inc'

```

```

        DIMENSION YY(M1),YY1(M1),RNO3L(*),RNO2L(*),NH4FROMIN(M1),NH41(M1)
&
& ,TANN(M1),NNH3L1(M1),RNH4PROD(M1),NH4L1(M1),NH4PROD(M1),NH31(M1)
        REAL*8 NH4FROMIN,NNH41,NNH3L1,NH4L1,NH4PROD,NH31,NH41
        INCLUDE 'agrininit.inc'

        IF (IFLAG.EQ. 1) THEN !initial condition
        NH4SOIL1 = 0.0
        NH3SOIL1 = 0.0
        TANSOIL1 = 0.0
        NO3SOIL1 = 0.0
        DO I = 1,NPT
        B1 = KADS/10000.0

!
!      Adsorption algorithm first to determine free ammonium
        NH4L(I) = NH4(I)/(THETA(I)+(BLKDEN*(KADS/10000.0))) !g/cm3
        NH4S(I) = (KADS/10000.0)*(NH4L(I)) !g/g

!
!      Dissociation algorithm to determine NH3 in soil soln
        B1 = 9018
        B2 = B1/100000.0
        Y1 = 272992000
        Y2 = Y1/100000.0
        KDNH4(I) = 10.0**(-(B2 + Y2/T(I)))
        HION(I) = 10.0**(-PH(I)) !mol/L
        NH3L(I) = KDNH4(I)*(NH4L(I)*1000.0/14.0)/HION(I) !mol/L

!
!      Henry's Law for the partial pressure of NH3
        B1 = 1605590
        B2 = 8621060
        B3 = 2567670
        B4 = 35388
        B5 = B1/10000.0
        B6 = B2/1000.0
        B7 = B3/100000.0
        B8 = B4/1000000.0
        KHNH3(I) = EXP(B5 - (B6/T(I)) - B7*(LOG(T(I))) +

&
&      B8*T(I)) ! atm L/mol
        NH3G(I) = KHNH3(I)*NH3L(I) !atm
        B1 = 82057
        B2 = B1/1000000.0
        NH3G(I) = NH3G(I)/(B2*T(I)) !mol/Lair
        B1 = 14/1.0
        B2 = 1000/1.0
        B3 = B1/B2
        NH3G(I) = NH3G(I)*(B3) !g/cm3 air

!
!      Convert ammonia in soil soln to g/cm3
        NH3L(I) = NH3L(I)*(B3) !g/cm3 water
        tTANL(I) = NH3L(I) + NH4L(I) !g-N/cm3 water

!
!      Set values to values for previous time step
        NNH3L(I) = NH3L(I)
        NNH3G(I) = NH3G(I)
        NNH4S(I) = NH4S(I)

```

```

NNH4L(I) = NH4L(I)
NNH3(I) = NH3G(I)*AFPS(I) + NH3L(I)*THETA(I)
!
! Calculate initial tan soil storage
NH4SOIL1 = NH4SOIL1 + NH4(I)*THICK(I)
NH3SOIL1 = NH3SOIL1 + NNH3(I)*THICK(I)
TANSOIL1 = NH4SOIL1 + NH3SOIL1
!
! Apply adsorption isotherm to NO3, NO2, assume no adsorption
RNO3L(I) = NO3(I)/THETA(I)
RNO2L(I) = NO2(I)/THETA(I)
NO3SOIL1 = NO3SOIL1 + NO3(I)*THICK(I)

END DO
ELSE
DO I = 1,npt
TANN(I) = (NH4L(I) + NH3L(I))*1000.0/14.0 !mol/L

!
! Henry's Law for the partial pressure of NH3
KHNH3(I) = 1./(10.**(-1.69+1477.7/T(1))) !cm3 WATER/cm3air
!
! Dissociation algorithm to determine NH3 in soil soln
B1 = 9018
B2 = B1/100000.0
Y1 = 272992000
Y2 = Y1/100000.0
KDNH4(I) = 10.0**(-(B2 + Y2/T(I)))
NH3L(I) = KDNH4(I)*TANN(I)/(HION(I) + KDNH4(I)) !mol/L
NH4L(I) = (TANN(I) - NH3L(I))*14.0/1000.0 !g/cm3 water
NH3L(I) = NH3L(I)*14.0/1000.0 !g/cm3 water
NH31(I) = NH3G(I)*AFPS(I) + THETA(I)*NH3L(I)
NH3G(I) = (KHNH3(I)*NH31(I)/THETA(I))/(1.0+(KHNH3(I)*AFPS(I)
&
& /THETA(I))) !g/cm3 air
NH3L(I) = NH3G(I)/KHNH3(I) !g/cm3 water
NH41(I) = NH4S(I)*BLKDEN + NH4L(I)*THETA(I)
NH4L(I) = NH41(I)/(((KADS/10000.0)*BLKDEN)+THETA(I)) !g/cm3 water
NH4S(I) = NH4L(I) * KADS/10000.0 !G/G
NH3(I) = AFPS(I)*NH3G(I) + NH3L(I)*THETA(I)
NH4(I) = BLKDEN*NH4S(I) + THETA(I)*NH4L(I)

END DO

END IF
!-----
!
! End of subroutine EQMMOD
!-----
-
END

SUBROUTINE NITMOD (KHH,RUSTAR)

```

```

!-----
!
!      Called by AGRIN MAIN
!
!      Calculates nitrification of ammonium to nitrate based on nitrifier
dynamics
!      and soil environment (redox status, T, theta, pH). Also
calculates nitrous
!      oxide and nitric oxide production resulting from nitrification.
!-----
!
      INCLUDE 'agringlob.inc'
      DIMENSION UTEMPNIT(M1),TDEGC(M1),UWATNIT(M1),DOCTONIT(M1),
&
&
&      GRWTHNIT(M1),DTHNIT(M1),NH4TONIT(M1),KPH(M1),KN2(M1),KNIT(M1)
      REAL*8 NH4TONIT,KPH,KN2,KNIT
      INCLUDE 'agrininit.inc'
      CALL O2STATUS
      DELT = DELSAV
      DO I = 1,NPT
!      Calculate temperature and moisture functions
      TDEGC(I) = T(I)-273.16
      UTEMPNIT(I)= 3.503*((60.0-TDEGC(I))/25.78)*EXP(3.503*(TDEGC(I)-
&
&      34.22)/25.78)
      IF (THETA(I)/thet(1) .GT. 0.05) THEN
        UWATNIT(I) = 0.8 + 0.21*(1.0-THETA(I)/THET(1))
      ELSE
        UWATNIT(I) = 0
      END IF
!
!      Calculate nitrifier biomass relative growth and death rates
      DOCTONIT(I) = THETA(I)*DDOC(I)*AVF(I) !assuming no DOC adsorbed
      GRWTHNIT(I)=GMAXNIT*(
(DOCTONIT(I)/(1.0+DOCTONIT(I)))+(UWATNIT(I)/
&
&      (1+UWATNIT(I))) ) !hr-1
      DTHNIT(I)
=DMAXNIT*BBIONIT(I)/((5.0+(DOCTONIT(I))/(1+UWATNIT(I)))) !hr-1
!
!      Calculate nitrifier biomass at end of time step and net increase
in biomass
      BIONIT(I) = BBIONIT(I)*(EXP(UTEMPNIT(I)*UWATNIT(I)*DELT*
&
&      (GRWTHNIT(I)- DTHNIT(i)))) !g C/cm3 soil
!
!      Calculate nitrification rate, transformation of NH4-N to NO3-N
      NH4TONIT(I) = NNH4L(I)*AVF(I) !g/cm3 soil
      NH4L(I) = NNH4L(I)*EXP(-RMAXNIT*DELT*BIONIT(I)*PH(I)) !g/cm3
water
      RNIT(I) = THETA(I)*(NH4L(I)-NNH4L(I))/DELT !g N/cm3 soil/hr
!
!      Calculate N2O and NO produced from nitrification
      NONIT(I) = -0.0025*RNIT(I) !g N/cm3 soil/hr
      N2ONIT(I) = -0.0006*RNIT(I) !g N/cm3 soil/hr

```



```

END DO
!-----
!
!   End of subroutine NITMOD
!-----
-

END

SUBROUTINE O2STATUS
!-----
!
!   Called by NITMOD
!
!   Calculates soil O2 profile and anaerobic soil fraction.
!-----
-

INCLUDE 'agringlob.inc'
DIMENSION O2G1(M1),RO21(M1)
REAL*8 KH1O2
INCLUDE 'agrininit.inc'
DEL = 1.0/DELSAV !1/h
AAA = NINT(1.5*100.0)
AAA = AAA/100.0
BBB = INT((10.0**(-10.0))*10.0**10.0)
AAA = AAA*BBB/(10.0**10.0)

ALPHA = NINT(1.26*1000.0)
ALPHA = ALPHA/1000.0
BETA = NINT(0.6*100.0)
BETA = BETA/100.0
GAMMA = NINT(0.6*100.0)
GAMMA = GAMMA/100.0
GAMMA1 = NINT(0.85*100.0)
GAMMA1 = GAMMA1/100.0
AIRRAD = NINT(10.0**(-4.0)*100000.0) !m
AIRRAD = AIRRAD/100000.0
CHI = 10.0**4.0
DEL = 1.0/DELSAV !1/h
!
!   Calculate diffusivity and net source terms
DO I = 1,NPT
  B1 = NINT(VO2*10.0**10.0)
  SRCEO2(I) = -VO2*3600./(100.**3.) !in mol O2/cm3 soil/h
  AFPS(I) = THET(1)-THETA(I)
  DO2(I) = ( AFPS(I)**3.33)/(THET(1)**2.0 ) *DO2A !cm2/h
END DO
!

O2G(1) = O2AIR
O2L(1) = O2G(1)/KHO2
OO2G(1) = O2G(1)
OO2L(1) = O2L(1)
CALL PROFO2

```

```

!      Calculate fractions of anaerobic and aerobic microsites
DO I=1,NPT
  IF (O2G(I) .LT. 0.0) O2G(I) = 0.0
!
!      Convert consumption rate to mol/m3/s and O2 to mol/m3
O2G1(I) = O2G(I)*(100.0**3.0) !mol/m3 air
ANVF(I) = EXP(-AAA*(O2G1(I)**GAMMA)*(AIRRAD**(-ALPHA))*(VO2**
&
&  (-BETA))*((THETA(I)+(AFPS(I)*CHI)**GAMMA1))
AVF(I) = 1.0 - ANVF(I)
END DO

!-----
!      End of subroutine O2STATUS
!-----
END

SUBROUTINE DECOMPMOD(NNO3L)
!-----
!      Called by AGRIN MAIN
!
!      Calculates change in SOC concentrations due to decomposition
based on soil
!      environment. Also calculates free inorganic N and DOC for use in
nitrification
!      and denitrification modules.
!-----
INCLUDE 'agringlob.inc'
DIMENSION UCLAY(M1),UWAT(M1),UTEMP(M1),TDEGC(M1),HINM(M1),
&
& NRESPOT(M1),KRES(M1),KBIO(M1),KHUM(M1),HRES(M1),DCRESDTACT1(M1),
&
& HBIO(M1),HHUM(M1),NAVAIL(M1),DCRESDTPOT(M1),ctobio(m1),
&
& DCRESDTACT(M1),TOBIO(M1),NTOPASS(M1),DCRESDTPOT1(M1),
&
&
& NTOBIO(M1),NRATIO(M1),NHUM(M1),NACT(M1),NTOBIO1(M1),NRESPOT1(M1),
&
& NMINRATIO(M1),CACT(M1),CDIFF(M1),NDIFF(M1),NINRES(M1),
&
& COUTBIO(M1),NOUTBIO(M1),CTOHUM(M1),NTOHUM(M1),CTOPASS(M1),
&
& NBIO(M1),NNHUM(M1),CINHUM(M1),NINHUM(M1),CTOBIO1(M1),
&
&
& COUTHUM(M1),NOUTHUM(M1),NRESINPUT(M1),CINRES(M1)
REAL*8 KRES,KBIO,KHUM,NRESPOT,NAVAIL,NTOBIO,NINRES,NRESPOT1,
&
& NRATIO,NACT,NMINRATIO,NOUTBIO,NTOHUM,NBIO,NDIFF,NRESINPUT,
&
& NNHUM,NINHUM,NOUTHUM,NTOPASS,NHUM,NTOBIO1
INCLUDE 'agrininit.inc'

```

```

DO I = 1,NPT
!
! Calculate the correction functions based on soil clay content,
water content, and
! temperature. Correct the decomposition rates for actual
conditions and convert to
! appropriate units.
!
      IF (CLY.LE. 0.25) THEN
        B1 = 2
        UCLAY(I) = 1.0 - (B1/100.0)*CLY
      ELSE
        UCLAY(I) = 0.995
      END IF

      IF (THETA(I)/THET(1) .LE. 0.1) THEN
        UWAT(I) = 0.0
      ELSE IF (THETA(I)/THET(1) .GT. 0.1 .AND. THETA(I)/THET(1) .LT.
&
&      0.6) THEN
        UWAT(I) = 2.0*THETA(I)/THET(1) - 0.2
      ELSE IF (THETA(I)/THET(1) .EQ. 0.6) THEN
        UWAT(I) = 1.0 !Optimum water conditions
      ELSE IF (THETA(I)/THET(1) .GT. 0.6 .AND. THETA(I)/THET(1) .LE.
&
&      0.8) THEN
        UWAT(I) = -2.5*THETA(I)/THET(1) + 2.5
      ELSE
        UWAT(I) = -0.5*THETA(I)/THET(1) + 0.9
      END IF

      B1 = 27316
      TDEGC(I) = T(I) - (B1/100.0)
      IF (TDEGC(I) .LE. 0.0) THEN
        UTEMP(I) = 0.0
      ELSE IF (TDEGC(I) .GT. 0.0 .AND. TDEGC(I) .LE. 30.0) THEN
        UTEMP(I) = 0.0333*TDEGC(I)
      ELSE IF (TDEGC(I) .GT. 30.0 .AND. TDEGC(I) .LE. 40.0) THEN
        UTEMP(I) = 1.0
      ELSE
        UTEMP(I) = -0.04*TDEGC(I) + 2.6
      END IF

      B2 = (int(KRES0*1000.0))/1000.0
      KRES(I) = (B2/24.0)*UWAT(I)*UTEMP(I) !h-1
      B2 = (NINT(KBIO0*1000.0))/1000.0
      KBIO(I) = (B2/24.0)*UWAT(I)*UTEMP(I)
      B2 = (int(KHUM0*1000000.0))/1000000.0
      KHUM(I) = (B2/24.0)*UCLAY(I)*UWAT(I)*UTEMP(I)
      B2 = (int(HRES0*1000.0))/1000.0
      HRES(I) = (B2/24.0)*UWAT(I)*UTEMP(I)
      B2 = (NINT(HBIO0*1000000.0))/1000000.0
      HBIO(I) = (B2/24.0)*UCLAY(I)*UWAT(I)*UTEMP(I)
      B2 = (int(HHUM0*10000000.0))/10000000.0
      HHUM(I) = (B2/24.0)*UCLAY(I)*UWAT(I)*UTEMP(I)
!

```

```

! Calculate any incoming slurry residue and its effect on CNRES
IF (IAPPN .GT. 0 .AND. APDAY(1) .EQ. IDAY) THEN
  IF((NHR-1) .GE. APPNSRT(1) .AND. (NHR-1) .LT. APPNEND(1)) THEN
    CRESINPUT(1) = (CRESAPINIT(1)*DELSAV/(100.*100.))/THICK(1) !g/cm3
    NRESINPUT(1)=(CRESAPINIT(1)*DELSAV/(100.*100.))/CNAPPN(1)/THICK(1
  )
    ELSE
    CRESINPUT(1) = 0.0
    NRESINPUT(1) = 0.0
    END IF
  ELSE
  CRESINPUT(1) = 0.0
  NRESINPUT(1) = 0.0
  END IF
!
! Calculate organic C concentration in residue pool based on
potential decomposition
!
  SRES1 = (INT(SRES*1000.0))/1000.0
  HRES1 = (INT((1-SRES-SRESVL)*1000.0))/1000.0
  CRESPOT(I) = CCRES(I)*SRES1*EXP(-
KRES(I)*DELMIN)+CCRES(I)*(HRES1)*
& EXP(-HRES(I)*DELMIN)
  CRESPOT1(I) = CCRES1(I)*SRESVL*EXP(-KRES(I)*DELMIN) !g C cm-3
soil
  IF (CNRES1(I) .EQ. 0.0) CNRES1(I) = CNRESVL
  NRESPOT(I) = CRESPOT(I)/CNRES
  NRESPOT1(I) = CRESPOT1(I)/CNRES1(I) !g N /cm3 soil
!
! Calculate free nitrogen available for decomposition process (not
adsorbed)
  NAVAIL(I) = (NNH4L(I) + NNO3L(I) + NNO2L(I))*THETA(I)+
&
& NNRES(I) + NNRES1(I) - NRESPOT(I) - NRESPOT1(I) !g N/cm3 soil
!
! Calculate reduction on potential decomposition based on available
N and use to calculate
! actual decomposition and C flows out of residue pool
!
  B1 = (INT(0.2*100.0))
  B2 = (INT(7.2*100.0))
  UCN(I) = (B1/100.0) +(B2/100.0)/((CCRES(I)+CCRES1(I)-CRESPOT(I)-
&
& CRESPOT1(I))/NAVAIL(I))
  IF (UCN(I) .GT. 1.0) UCN(I) = 1.0
  DCRESDTPOT(I)=-KRES(I)*SRES1*CRESPOT(I)-
(HRES1)*HRES(I)*CRESPOT(I)
  DCRESDTPOT1(I) = -KRES(I)*SRESVL*CRESPOT1(I) !g C/Cm3/h, very
labile pool
  DCRESDTACT(I) = UCN(I)*DCRESDTPOT(I)
  DCRESDTACT1(I) = UCN(I)*DCRESDTPOT1(I)
  COUTRES(I) = -DCRESDTACT(I)*DELMIN !actual C produced from decomp
in g C/CM3
  COUTRES1(I) = -DCRESDTACT1(I)*DELMIN !very labile pool

```

```

CTOBIO(I) = COUTRES(I)*fnbio !C flow to biomass pool, g C /cm3
CTOBIO1(I) = COUTRES1(I)*FNBIO !out of very labile pool
C2PRES(I) = COUTRES(I) - CTOBIO(I) !CO2 produced, g C /cm3
C2PRES1(I) = COUTRES1(I) - CTOBIO1(I)

!
! Calculate N flows out of residue pool based on C flows
NMINRES(I) = C2PRES(I)/CNRES !g N cm-3, N mineralized to NH4,
associated with CO2 prodn
NMINRES1(I) = C2PRES1(I)/CNRES1(I)
! Adjust NH4 concentrations for mineralization
NH4L(I) = NNH4L(I) + NMINRES(I)/THETA(I)+NMINRES1(I)/THETA(I)
IF (NH4L(I) .LT. 0.0) NH4L(I) = 0.0
NTOBIO(I) = CTOBIO(I)/CNRES !g N cm-3, N to biomass pool
NTOBIO1(I) = CTOBIO1(I)/CNRES1(I)

!
! Adjust N in biomass pool based on incoming N from last time step
CINBIO(I) = CCBIO(I) !total C in biomass pool, g C/cm3
NINBIO1(I) = NNBIO(I) !total N before adjustment g N/cm3, this
should include inflows
IF (NINBIO1(I) .EQ. 0.0) NINBIO1(I) = CINBIO(I)/CNBIO
NRATIO(I) = CINBIO(I)/CNBIO !g N/cm3
IF (NRATIO(I) .GT. 0.0) THEN
  NACT(I) = NINBIO1(I)/NRATIO(I) !ratio
ELSE
  NACT(I) = 0.0
END IF
NMINRATIO(I) = NACT(I) - 1
! Net mineralization due adjustments based on incoming flows,
negative value indicates immobilization (likely to occur here)
NMINBIO1(I) = NMINRATIO(I)*NRATIO(I) !g N/cm3

!
! If not enough N available to immobilize, adjust C flow from
residue to biomass pool
!
IF (NMINBIO1(I) .LT. 0) THEN !Immobilization occurs, likely
  IF ((NH4L(I) + NNO3L(I) + NNO2L(I))*THETA(I) .LT. -NMINBIO1(I))
    &
    & THEN !not enough inorganic N for immobilization
      NMINBIO1(I) = -(NH4L(I) + NNO3L(I) + NNO2L(I))*THETA(I) !g/cm3
soil

      NINBIO(I) = NINBIO1(I) + NTOBIO(I) + NTOBIO1(I) + NTOBIOR1(I) + NTOBIOR2(I)
-&
      & NMINBIO1(I)
      CACT(I) = NINBIO(I)*CNBIO !Actual carbon needed
      CDIFF(I) = CINBIO(I) - CACT(I) !Excess carbon in pool that needs
to be reduced
      CTOBIO(I) = CTOBIO(I) + CTOBIO1(I) - CDIFF(I) !Adjusted C flow
from res pool
      CRES(I) = CRES(I) + CDIFF(I)
      END IF
    ELSE
      NINBIO(I) = NINBIO1(I) - NMINBIO1(I)
      END IF

!
! Calculate decomposition in biomass pool based on incoming C
flows. Calculate C,N flows out.

```

```

SBIO1 = NINT(SBIO*1000000.0)
SBIO2 = SBIO1/1000000.0
HBIO1 = INT((1-SBIO)*1000000.0)
HBIO2 = HBIO1/1000000.0
CBIO(I) = CCBIO(I)*SBIO2*EXP(-KBIO(I)*DELT)+CCBIO(I)*(HBIO2)*
&
& EXP(-HBIO(I)*DELT) !g C/cm3, incoming minus outgoing
COUTBIO(I) = CCBIO(I) - CBIO(I) !gC/cm3, C flow out, initial
minus undecomposed portion

NOUTBIO(I) = COUTBIO(I)/CNBIO !gN/cm3
B1 = INT(FNBIO1*100.0)
CTOBIOR1(I) = COUTBIO(I)*(B1/100.0) !gC/cm3, recycled back into
biomass pool, part of DOC pool
B1 = INT(FNHUM*100.0)
CTOHUM(I) = COUTBIO(I)*(B1/100.0) !gC/cm3, flow out to humads
pool
C2PBIO(I) = COUTBIO(I) -CTOBIOR1(I)-CTOHUM(I) !gC/cm3, CO2
production
NTOBIOR1(I) = CTOBIOR1(I)/CNBIO !gN/cm3
NTOHUM(I) = CTOHUM(I)/CNBIO !gN/cm3
NMINBIO2(I) = C2PBIO(I)/CNBIO !Net mineralization due to CO2
production

! Adjust NH4l for immobilization that likely occurred or immobilize
NO3 if not enough NH4
IF (NMINBIO1(I) .LT. 0.0 .AND. ABS(NMINBIO1(I)) .GT.(NH4L(I)
&
& *THETA(I))) THEN
NDIFF(I) = (-NMINBIO1(I)) - NH4L(I)*THETA(I)
NH4L(I) = NH4L(I) + (-(-NMINBIO1(I)-NDIFF(I))+ NMINBIO2 (I))
&
& /THETA(I)
NO3L(I) = NNO3L(I) - NDIFF(I)/THETA(I)
ELSE
NH4L(I) = NH4L(I) + NMINBIO1(I)/THETA(I) + NMINBIO2(I)/THETA(I)
!Adjusted NH4 for net mineralization in biomass pool, g/cm3 H2O
NO3L(I) = NNO3L(I)
NBIO(I) = CBIO(I)/CNBIO !gN/cm3
END IF

IF (NH4L(I) .LT. 0.0) NH4L(I) = 0.0

!
! Adjust N in humads based on incoming C,N flows. Similar
algorithm to that used for biomass pool.
!
NNHUM(I) = CCHUM(I)/CNHUM
CINHUM(I) = CCHUM(I)
NINHUM(I) = NNHUM(I)
NRATIO(I) = CINHUM(I)/CNHUM
IF (NRATIO(I) .GT. 0.0) THEN
NACT(I) = NINHUM(I)/NRATIO(I)
ELSE
NACT(I) = 0.0
END IF
NMINRATIO(I) = NACT(I) -1

```

```

!      Net mineralization due to any adjustments required from incoming
flows, negative value indicates immobilization
!      Should be zero if biomass and humads pool have same C/N ratio
      NMINHUM1(I) = NMINRATIO(I)*NRATIO (I)
!
!      If not enough N available to immobilize, adjust C flow from
residue to biomass pool
!
      IF (NMINHUM1(I) .LT. 0) THEN !i.e. immobilization occurs
        IF ((NH4L(I) + NNO3L(I) +NNO2L(I))*THETA(I) .LT. -NMINHUM1(I))
&
&      THEN
        NMINHUM1(I) = -(NH4L(I) + NNO3L(I) +NNO2L(I))*THETA(I)
        NINHUM(I) = NNHUM(I) + NTOHUM(I) - NMINHUM1(I)
        CACT(I) = NINHUM(I)*CNHUM !Actual carbon needed
        CDIFF(I) = CINHUM(I) - CACT(I) !excess carbon in pool that needs
to be eliminated
        CTOHUM(I) = CTOHUM(I) - CDIFF(I) !Adjusted C flow from res pool
        CBIO(I) = CBIO(I) + CDIFF(I)
        END IF
      ELSE
        NINHUM(I) = NNHUM(I) + NTOHUM(I) - NMINHUM1(I)
      END IF
!
!      Calculate decomposition in humads pools and C flows out
!
      SHUM1 = NINT(SHUM*100.0)/100.0
      HHUM1 = NINT((1-SHUM)*100.0)/100.0
      CHUM(I) = CCHUM(I)*SHUM1*EXP(-KHUM(I)*DELT)+CCHUM(I)*
&
&      (HHUM1)* EXP(-HHUM(I)*DELT) !C (g/CM3) in pool at end of
time step
      COUTHUM(I) = CCHUM(I) - CHUM(I) !C (g/cm3)leaving pool due to
decomposition
      NOUTHUM(I) = COUTHUM(I)/CNHUM
      B1 = NINT(FNBIOR2*100.0)
      CTOBIOR2(I) = COUTHUM(I)*(B1/100.0) !recycled into biomass pool
      NTOBIOR2(I) = CTOBIOR2(I)/CNHUM
      B1 = NINT(FNPASS*100.0)
      CTOPASS(I) = COUTHUM(I)*(B1/100.0)
      NTOPASS(I) = CTOPASS(I)/CNHUM
      C2PHUM(I) = COUTHUM(I) - CTOBIOR2(I) - CTOPASS(I)
      NMINHUM2(I) = C2PHUM(I)/CNHUM !Net min due to CO2 production
      NHUM(I) = CHUM(I)/CNHUM
      CPASS(I) = CCPASS(I)
!
!      Adjust NH4l for immobilization or immobilize NO3 if not enough
NH4
      IF (NMINHUM1(I) .LT. 0.0 .AND. ABS(NMINHUM1(I)) .GT. (NH4L(I)
&
&      *THETA(I))) THEN
        NDIFF(I) = (-NMINBIO1(I)) - NH4L(I)*THETA(I)
        NH4L(I) = NH4L(I) + (NMINHUM1(I)+ NMINHUM2 (I))/THETA(I)
        NO3L(I)= NNO3L(I) - NDIFF(I)/THETA(I)
      ELSE
        NH4L(I) = NH4L(I) + NMINHUM1(I)/THETA(I) + NMINHUM2(I)/THETA(I)
        NO3L(I) = NNO3L(I)

```

```

END IF

IF (NH4L(I) .LT. 0.0) NH4L(I) = 0.0
END DO

!
! Calculate DOC profile and CO2 profile
DO I =1,NPT
  DDOC(I) = CTOBIOR1(I) + CTOBIOR2(I) !g/cm3 soil (not water!)
  RCO2P(I) = (C2PRES(I)+C2PRES1(I)+C2PBIO(I)+C2PHUM(I))/DELT
!g/cm3 soil

! Determine rate of net mineralization
RNH4MIN(I) = THETA(I)*(NH4L(I) - NNH4L(I))/DELMIN !g N/cm3
soil/h, neg value means losing nh4 to immobilization
!
! Determine organic C in pools at end of time step

NNRES1(I) = CCRES1(I)/CNRES1(I)
NNRES(I) = CCRES(I)/CNRES
CCRES(I) = CCRES(I) - COUTRES(I)
CCRES1(I) = CCRES1(I) - COUTRES1(I) + CRESINPUT(I)
NNRES(I) = NNRES(I) - COUTRES(I)/CNRES
NNRES1(I) = NNRES1(I) - COUTRES1(I)/CNRES1(I) + NRESINPUT(I)
NNBIO(I) = CCBIO(I)/CNBIO-COUTBIO(I)/CNBIO+CTOBIOR1(I)/CNBIO +
&
& CTOBIOR2(I)/CNHUM + CTOBIO(I)/CNRES + CTOBIO1(I)/CNRES1(I)
CCBIO(I) = CCBIO(I) - COUTBIO(I) + CTOBIO(I) + CTOBIO1(I) +
&
& CTOBIOR1(I) + CTOBIOR2(I)

CNRES1(I) = CCRES1(I)/NNRES1(I)
IF (CNRES1(I) .eq. 0.0 .OR. NNRES1(I) .EQ. 0.0) CNRES1(I)=CNRESVL
CCHUM(I) = CCHUM(I) - COUTHUM(I) + CTOHUM(I)
NNHUM(I) = (CCHUM(I) - COUTHUM(I))/CNHUM + CTOHUM(I)/CNBIO
CCPASS(I) = CCPASS(I) + CTOPASS(I)

END DO

!-----
-
! End of subroutine DECOMPMOD
!-----
-

END

SUBROUTINE TRANSMOD(RTAIR,RVD_AT,KHH,RUSTAR,NNO3L)
!-----
-
! Called by AGRIN MAIN
!
! Simulates species movement in soil profile, including surface
fluxes
!-----
-

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INCLUDE 'agringlob.inc'
DIMENSION DNH3A(M1),DDNH3A(M1),NH4LAPPN(M1),NH3LAPPN(M1)
REAL*8 KH1NH3,DHNH3GAIR,SCNH3,BLKNH3DIFF,DCO2GAIR,SCCO2,KH1CO2,
&
& BLKCO2,BLKCO2DIFF,CO2FLUX,DNOAIR,SCNO,KH1NO,BLKNO,BLKNODIFF,
&
& DN2OAIR,SCN2O,BLKN2O,BLKN2ODIFF,KH1N2O,DN2AIR,SCN2,KH1N2,BLKN2,
&
& BLKN2DIFF,NO3LOST,NH4LAPPN,NH3LAPPN,NO3LEFT,NO3LSLURR,NOTOTAL,
&
& N2OTOTAL,N2TOTAL
INCLUDE 'agrininit.inc'
DEL = 1.0/DELSAV !1/h
PR = CPAIR*UAIR/KAIR
DNH3GAIR = (1.7*10**(-5.0)*(1.03**(RTAIR-293.0)))*100.0*100.0
!cm2/s
DCO2GAIR = DCO2A/3600. !cm2/s
DNOAIR = DNOA/3600.0
DN2OAIR = DN2OA/3600.0
DN2AIR = DN2A/3600.0
!
! Bulk transfer coefficient for chemical species volatilization
RBNH3 = 6.2*(RUSTAR**-0.67)
RCNH3 = 0.0
BLKCNH3 = 1.0/(RBNH3+RH+RCNH3) !m/s
BLKCO2 = BLKCNH3
BLKNO = BLKCNH3
BLKN2O = 1./rh !BLKCNH3
BLKN2 = BLKCNH3
!
! Determine if less than pure diffusion coefficient
BLKNH3DIFF = DNH3GAIR/(10000.0*ZT)
BLKCO2DIFF = DCO2GAIR/(10000.0*ZT)
BLKNODIFF = DNOAIR/(10000.0*ZT)
BLKN2ODIFF = DN2OAIR/(10000.0*ZT)
BLKN2DIFF = DN2AIR/(10000.0*ZT)
IF (BLKCNH3 .LT. BLKNH3DIFF) BLKCNH3 = BLKNH3DIFF
IF (BLKCO2 .LT. BLKCO2DIFF) BLKCO2 = BLKCO2DIFF
IF (BLKNO .LT. BLKNODIFF) BLKNO = BLKNODIFF
IF (BLKN2O .LT. BLKN2ODIFF) BLKN2O = BLKN2ODIFF
IF (BLKN2 .LT. BLKN2DIFF) BLKN2 = BLKN2DIFF
!
! Calculate diffusivities and net source terms for each species
DO I = 1,NPT
KHNH3(I) = 10.**(-1.69+1477.7/T(1)) !cm3air/cm3H2O
KHNH3(I) = 1./KHNH3(I) !cm3 H2O/cm3 air
!
! Calculate net source terms
SRCECO2(I) = RCO2P(I) !in g C/cm3/h
SRCETAN(I) = 0.0 + RNH4MIN(I) + RNIT(I) !
SRCENO3(I) = 0.0 -RNIT(I) + RNO3DENIT(I)*THETA(I) !
SRCEH(I) = 0.0 -RNIT(I)/7.0-RCO2P(I)/12.0 +RVOL(I)/14.0
!mol/cm3 soil/h or g/cm3/h because MW = 1 g/mol
SRCENO(I) = RNODENIT(I)*THETA(I) + NONIT(I) !g/cm3soil/h
SRCENO2(I) = RNO2DENIT(I)*THETA(I)
SRCEN2O(I) = RN2ODENIT(I)*THETA(I) + N2ONIT(I)
SRCEN2(I) = RN2DENIT(I)*THETA(I)
!

```

```

!      Check that initial profile exists
      IF (CCO2G(I) .EQ. 0.0) CCO2G(I) = (C2PRES(I)+C2PBIO(I)+C2PHUM(I))
&
      &      /AFPS(I) !g/cm3 air
      HHIONL(I) = (10**(-PPH(I)))/1000.0 !mol/cm3 water
!
!      Calculate diffusivities
      DCO2(I) = ( (AFPS(I)**(10.0/3.0))/(THET(1)**2) )*DCO2A !cm2/h
      DNH3A(I) = (1.7*10.0**(-5.0)*(1.03**(T(I)-293.0)))*100.0*100.0
!cm2/s
      DNH3(I) = ( (AFPS(I)**(10.0/3.0))/(THET(1)**2) )*DNH3A(I)*3600.0
!cm2/h
!      DDOCL1(I) = ((THETA(I)**(10.0/3.0))/(THET(1)**2))*DDDOCL
      DNH4L(I) = 9.8*(10.0**(-10.0))*100.*100.*3600.*(1.03**(T(I)-273.))
!cm2/h, in pure water
      DNH4(I) = ((THETA(I)**(10.0/3.0))/(THET(1)**2))*DNH4L(I)
      DNO3(I) = ((THETA(I)**(10.0/3.0))/(THET(1)**2))*DNO3L
      DNO2(I) = ((THETA(I)**(10.0/3.0))/(THET(1)**2))*DNO2L
      DH(I) = ((THETA(I)**(10.0/3.0))/(THET(1)**2))*DHL
      DDH(I) = ((THETA(I)**(10.0/3.0))/(THET(1)**2))*DHL
      DNO(I) = ( (AFPS(I)**(10.0/3.0))/(THET(1)**2) )*DNOA !cm2/h
      DN2O(I) = ( (AFPS(I)**(10.0/3.0))/(THET(1)**2) )*DN2OA !cm2/h
      DN2(I) = ( (AFPS(I)**(10.0/3.0))/(THET(1)**2) )*DN2A !cm2/h

      END DO

!
!      After application and until slurry water has
      evaporated/infiltrated, calculate
!      volatilization and surface infiltration based on slurry thickness
      IF(IAPPN .GT. 0 .AND. IDAY .GE. APDAY(1) .AND. (NHR) .GE.
&
&APPNSRT(1) .AND. THICKNEW .GT. 0.0) THEN
      IF (NHR .GE. APPNEND(1)) then
      NH4APINIT(1) = 0.0
      NO3APINIT(1) = 0.0
      END IF
      KHNH3(1) = (10.0**(-1.69+1477.7/T(1))) !cm3 air/cm3water
      VOLH2O = THICKNEW*APPNA(1)*(10.0**8.) !cm3 water in slurry layer
      TANCONC(1) = (NH4APINIT(1)*DELSAV + TANLEFT)/VOLH2O !g/cm3 water
      KDNH4(1) = 10.0**(-0.09018-2729.2/T(1))
      NH3LAPPN(1) = (TANCONC(1)*1000./14.)/(1.+ ((10.0**(-PHAPPN(1)))/
&
& KDNH4(1))) !mol/L
      NH4LAPPN(1) = (TANCONC(1)*1000./14. - NH3LAPPN(1)) !mol/L
      NH3LAPPN(1) = NH3LAPPN(1)*14.0/1000.0 !g/cm3 water
      NH4LAPPN(1) = NH4LAPPN(1)*14./1000.
      NH3GSURF = NH3LAPPN(1)/KHNH3(1) !g/cm3 air in equilibrium
      NH3FLUX1 = BLKCNH3*3600.0*100.0*(NH3AIR-NH3GSURF) !g/cm2/h from
      application area
      SLURRTANFLUX = TANCONC(1)*SFLUX1 !g/cm2soil/h OVER ENTIRE field
      SLURRTANFLUX1 = SLURRTANFLUX*APPNA(1)/AREACOVERED !over
      application area
      NH3FLUXMAX = -(TANCONC(1)*VOLH2O/APPNA(1)/DELSAV-SLURRTANFLUX)
!over field, max nh3flux is constrained by how much TAN applied and how
much TAN infiltrates
      NH3FLUX = NH3FLUX1*AREACOVERED/(APPNA(1)) !averaged over field

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```

      IF (NH3FLUX .lt. NH3FLUXMAX) THEN
        NH3FLUX=NH3FLUXMAX
      END IF

      IF (NH3FLUX .GT.0.0) THEN !infiltrating faster than can
volatilize, volatilization from soil surface concentration
        NH3FLUX=BLKCNH3*3600.0*100.0*(NH3AIR-NNH3G(1))
        SLURRTANFLUX = NH3FLUX+SLURRTANFLUX !boundary condition balance
between two rates at soil surface
        NH3FLUX1 = 0 !from slurry surface
      END IF

      TANINIT = TANCONC(1)*VOLH2O !mass of TAN at beginning of time
step
      TANLEFT = TANINIT-(SLURRTANFLUX-NH3FLUX)*DELSAV*appna(1)*
&
      &      (10.**8.) !g TAN left after infiltration and volatilization
      IF (TANLEFT .LT. 0.0) TANLEFT = 0.0
!
!      Calc nitrate flux into soil from slurry
      NO3LSLURR = (NO3APINIT(1)*DELSAV + NO3LEFT)/VOLH2O !gN/cm3 water
      NO3FLUX = SFLUX1*NO3LSLURR !g/cm2/h, over entire field
      NO3FLUX1 = NO3FLUX*appna(1)/areacovered !g/cm2/h, over
application area only
      NO3LEFT = NO3LSLURR*VOLH2O - NO3FLUX*DELSAV*APPNA(1)*(10.**8.)
!g left

      END IF

      CALL PROFTAN(TTANL,TANL,NH3AIR,TANFLUXBOT,KADS)
      CALL PROFAQ (NNO3L,NO3L,NO3RAIN,NO3FLUX,NO3FLUXBOT,DNO3,KDNO3,
&
      &      SRCENO3)
      CALL PROFAQ (NNO2L,NO2L,NO2RAIN,NO2FLUX,NO2FLUXBOT,DNO2,KDNO2,
&
      &      SRCENO2)
      CALL PROFGAS (NNOL,NOL,DNOA,NOAIR,BLKNO,NOFLUX,DNO,KHNO, SRCENO)
      CALL PROFGAS (NN2OL,N2OL,DN2OA,N2OAIR,BLKN2O,N2OFLUX,DN2O,KHN2O,
&
      &      SRCEN2O)
      CALL PROFGAS (NN2L,N2L,DN2A,N2AIR,BLKN2,N2FLUX,DN2,KHN2, SRCEN2)
      CALL PROFAQHION (HHIONL,HIONL,HIONRAIN,HFLUX,HFLUXBOT,DH,KDHION,
&
      &      SRCEH)

      DO I = 1,NPT
!
!      Determine phase partitioning for chemical species
      PH(I) = -LOG10(HIONL(I)*1000.)
      PHSOIL(I) = PH(I)
      IF(IAPPN .GT. 0 .AND. IDAY .GE. APDAY1 .AND. NPHPREFLAG.EQ.0)
THEN !gradient based on Chantigny et al. (2004)
        IF (IDAY .EQ. APDAY1 .AND. NHR .LT. APPNSRT(1)) THEN
          GO TO 111
        END IF

```

```

      IF (IDAY .EQ. APDAY1) THEN !during application
        IF (Z(I) .LE. 0.0) PH(I) = PHAPPN(1)

      ELSE IF (IDAY .GE. (APDAY1+1)) THEN
        IF (Z(I) .LE. 0.0) then
          IF (PH(I) .LT. PHPRE(I)) THEN
            PH(I) = PHPRE(I)
            NPHPREFLAG = 1 !stops program from doing these calcs once pH
is restored to initial soil pH
            GO TO 111
          END IF
          PH(I) = PPH(1) - 0.02*delt !0.0208*DELT

        END IF

      END IF

    END IF

    IF (Z(I).GT.0.0.AND.Z(I).LE. 2.5) THEN
      PH(I)=PH(I-1)-0.4*(Z(I)-Z(I-1))
      IF (PH(I) .LT. PHSOIL(I)) PH(I) = PHSOIL(I)
    END IF
    IF(Z(I).GT.2.5) THEN
      PH(I)=PH(I-1)-0.2*(Z(I)-Z(I-1))
      IF (PH(I) .LT. PHSOIL(I)) PH(I) = PHSOIL(I)
    END IF
  END IF
111  NH3G(I) = TANL(I)*KHNH3(I)/(1.+HION(I)/KDNH4(I)) !g/cm3 air
      NH3L(I) = NH3G(I)/KHNH3(I)
      NH4L(I) = TANL(I) - NH3L(I)
      NH4S(I) = (KADS/10000.)*NH4L(I)
      NH3(I) = AFPS(I)*NH3G(I) + THETA(I)*NH3L(I)
      NH4(I) = THETA(I)*NH4L(I) + NH4S(I)*BLKDEN
      NO2(I) = NO2L(I)*THETA(I)
      NOG(I) = NOL(I)*KHNO
      NO(I) = NOL(I)*THETA(I) + NOG(I)*AFPS(I)
      N2OG(I) = N2OL(I)*KHN2O
      N2O(I) = N2OL(I)*THETA(I) + N2OG(I)*AFPS(I)
      N2G(I) = N2L(I)*KHN2
      N2(I) = N2L(I)*THETA(I) + N2G(I)*AFPS(I)
      NO3(I) = NO3L(I)*THETA(I) + 0.0
      TANTOT(I) = NH4(I) + NH3(I) !g/cm3 soil
      RVOL(I) = (NH3G(I)-NNH3G(I))*AFPS(I)/DELT
    END DO

!-----
-
!   End of subroutine TRANSMOD
!-----
-
      END

      SUBROUTINE PROFO2
!-----
-
!   Called by AGRIN MAIN

```

```

!
!   Simulates TAN movement in soil profile using finite difference
approximation
!-----
-
      INCLUDE 'agringlob.inc'
      DIMENSION Y(M1),YY(M1),A1C(M1),A2C(M1),A3C(M1),ZYC(M1)
      REAL*8 SURFFLUX,KON,AIRCON,lwrflx
      INCLUDE 'agrininit.inc'
      DEL = 1/DELT
      NPPT = NPT-1

      DO II=2,NPPT
        I = II-1
        III = II+1
        Y(II) = THETA(II) + AFPS(II)*KHO2 !cm3 H2O/cm3 soil
        Z31 = Z(III)-Z(I)
        DO21 = 0.5*(DO2(I)+DO2(II))
        DO22 = 0.5*(DO2(II)+DO2(III))
        DIFF1 = DO21*KHO2
        DIFF2 = DO22*KHO2
        A1C(II) = (-DIFF1)/(THICK(II)*ZZ(I)) !1/h
        A3C(II) = (-DIFF2)/(THICK(II)*ZZ(II)) !1/h
        A2C(II) = Y(II)*DEL + (DIFF2/ZZ(II) + DIFF1/ZZ(I))/THICK(II)
!1/h
        AVS = SRCEO2(II) !mol/cm3 soil/h
        ZYC(II) = Y(II)*(OO2L(II))*DEL + AVS !mol/cm3 soil/h
      END DO

!
!   Lower node, unit gradient
      NPPT = NPT -1
      ZN = ZZ(NPPT)
      A3C(NPT) = 0.0
      DO21 = 0.5*(DO2(NPPT)+DO2(NPT))
      DIFF1 = DO21*KHO2
      A1C(NPT) = (-DIFF1)/(THICK(NPT)*ZN) !1/h
      Y(NPT) = THETA(NPT) + AFPS(NPT)*KHO2 !cm3 H2O/cm3 soil
      AVS = SRCEO2(NPT) !g/cm3 soil/h
      A2C(NPT) = Y(NPT)*DEL+(DIFF1)/(THICK(NPT)*ZN) !1/h
      ZYC(NPT) = Y(NPT)*OO2L(NPT)*DEL+AVS !g/cm3 soil/h

!
!   Flux conditiion for constant atmospheric concentration at top node
      ZYC(2) = ZYC(2) - A1C(2)*O2L(1)
      A1C(2) = 0.0

!
!   Solution of tridiagonal matrix
      CALL TRIDAG(2,NPT,A1C,A2C,A3C,ZYC,O2L)
      DO I = 1,NPT
        IF(O2L(I) .LT. 0.0) O2L(I) = 0.0
        O2G(I) = O2L(I)*KHO2
      END DO

!-----
-
!   End of subroutine PROFO2
!-----
-

```

END

```
SUBROUTINE PROFTAN(CCONC, CONC, AIRCONC, LWRFLX, KON)
!-----
!
!   Called by AGRIN MAIN
!
!   Simulates TAN movement in soil profile using finite difference
approximation
!-----
!
      INCLUDE 'agringlob.inc'
      DIMENSION
CCONC(M1), CONC(M1), Y(M1), YY(M1), A1C(M1), A2C(M1), A3C(M1),      &
&      ZYC(M1)
      REAL*8 SURFFLUX, KON, AIRCON, lwrflx
      DEL = 1/DELT
      NPPT = NPT-1
!
!   After application and until slurry water has
evaporated/infiltrated, calculate
!   volatilization and surface infiltration based on slurry thickness
      IF(IAPPN.GT. 0 .AND. IDAY.GE. APDAY(1) .AND. (NHR).GE.
&
&APPNSRT(1) .AND. THICKNEW.GE. (10.**-5.)) THEN
      SURFFLUX1 = SLURRTANFLUX
      GO TO 123
      END IF

      NH3FLUX = BLKCNH3*3600.0*100.0*(AIRCONC-NNH3G(1))
      SURFFLUX1 = NH3FLUX
!
!   Surface node equation for flux b.c.
123  TANFLUXTOP = SURFFLUX1
      Z1      = ZZ(1)
      A1C(1)  = 0.0
      AFPS2 = 0.5*(AFPS(1)+AFPS(2))
      KHNH3(1) = 1./((10.**(-1.69+1477.7/T(1))) !cm3 WATER/cm3AIR
      KHNH3(2) = 1./((10.**(-1.69+1477.7/T(2))) !cm3 WATER/cm3AIR
      KDNH4(1) = 10.**(-0.09018-2729.2/T(1))
      KDNH4(2) = 10.**(-0.09018-2729.2/T(2))
      HION(1) = 10.**(-PH(1))
      HION(2) = 10.**(-PH(2))
      QL2 = 0.5*(QL(1)+QL(2))/DELT !cm/h, Jw, 1.5
      DNH41 = 0.5*(DNH4(1)+DNH4(2)) !DAQ, 1.5
      DNH31 = 0.5*(DNH3(1)+DNH3(2)) !DG, 1.5
      DKHNH31 = 0.5*(KHNH3(1)+KHNH3(2)) !Kh, 1.5
      DKDNH41 = 0.5*(KDNH4(1)+KDNH4(2)) !Kd, 1.5
      DHION1 = 0.5*(HION(1)+HION(2))
      DNH3CON1 = DKHNH31/(1. + DHION1/DKDNH41)
      DIFF1 = DNH41 + DNH31*DNH3CON1
      A3C(1) = (-0.5*DIFF1)/(THICK(1)*Z1) + 0.25*QL2/THICK(1) !CM3
H2O/cm3soil/h
      PG2      = (CCONC(2)+CCONC(1)) !g/cm3 H2O
```

```

      Y(1) = THETA(1) + (BLKDEN*KON/10000.) + AFPS(1)*KHNH3(1)/
&
&      (1.+(HION(1)/KDNH4(1))) !cm3 H2O/cm3 soil
      AVS = SRCETAN(1) !g/cm3 soil/h
      A2C(1) =
(Y(1)/DELT)+(0.5*DIFF1/(THICK(1)*Z1))+(0.25*QL2/THICK(1)) !1/h
      ZYC(1) = Y(1)*DEL*CCONC(1)+AVS + (1.0*SURFFLUX1/THICK(1)) !g/cm3
soil/h

      DO II=2,NPPT
      I = II-1
      III = II+1
      HION(II) = 10.**(-PH(II))
      HION(I) = 10.**(-PH(I))
      HION(III) = 10.**(-PH(III))
      KHNH3(I) = 1./(10.**(-1.69+1477.7/T(I))) !cm3 WATER/cm3AIR
      KHNH3(II) = 1./(10.**(-1.69+1477.7/T(II))) !cm3 WATER/cm3AIR
      KHNH3(III) = 1./(10.**(-1.69+1477.7/T(III))) !cm3 WATER/cm3AIR
      KDNH4(I) = 10.**(-0.09018-2729.2/T(I))
      KDNH4(II) = 10.**(-0.09018-2729.2/T(II))
      KDNH4(III) = 10.**(-0.09018-2729.2/T(III))
      DKHNH31 = 0.5*(KHNH3(I)+KHNH3(II))
      DKDNH41 = 0.5*(KDNH4(I)+KDNH4(II))
      DHION1 = 0.5*(HION(I)+HION(II))
      DKHNH32 = 0.5*(KHNH3(III)+KHNH3(II))
      DKDNH42 = 0.5*(KDNH4(III)+KDNH4(II))
      DHION2 = 0.5*(HION(III)+HION(II))
      DNH3CON1 = DKHNH31/(1.+(DHION1/DKDNH41)) !cm3 water/cm3air
      DNH3CON2 = DKHNH32/(1.+(DHION2/DKDNH42)) !cm3 water/cm3air
      Y(II) = THETA(II) + (BLKDEN*KON/10000.) + AFPS(II)*KHNH3(II)/
&
&      (1.+(HION(II)/KDNH4(II))) !cm3 H2O/cm3 soil
      Z31 = Z(III)-Z(I)
      FZZ1 = 1./(Z31*ZZ(I))
      FZZ2 = 1./(Z31*ZZ(II))
      QL2 = 0.5*(QL(II)+QL(III))/DELT !cm/h
      QL1 = 0.5*(QL(I) + QL(II))/DELT
      AFPS1 = 0.5*(AFPS(I)+AFPS(II))
      AFPS2 = 0.5*(AFPS(III)+AFPS(II))
      DNH41 = 0.5*(DNH4(II)+DNH4(I))
      DNH42 = 0.5*(DNH4(II)+DNH4(III))
      DNH31 = 0.5*(DNH3(II)+DNH3(I))
      DNH32 = 0.5*(DNH3(II)+DNH3(III))
      DIFF1 = DNH41 + DNH31*DNH3CON1
      DIFF2 = DNH42 + DNH32*DNH3CON2
      A1C(II) = (-0.5*DIFF1)/(THICK(II)*ZZ(I)) - 0.25*QL1/THICK(II)
!1/h
      A3C(II) = (-0.5*DIFF2)/(THICK(II)*ZZ(II)) + 0.25*QL2/THICK(II)
!1/h
      A2C(II) = Y(II)*DEL + ((0.5*DIFF2/ZZ(II))+ (0.5*DIFF1/ZZ(I))-
&
&      0.25*QL1+0.25*QL2)/THICK(II) !1/h
      AVS = SRCETAN(II) !G/cm3 soil/h
      ZYC(II) = Y(II)*(CCONC(II))*DEL +AVS !G/cm3 soil/h

      END DO
      !

```

```

!      Lower node, unit gradient
      NPPT = NPT -1
      ZN      = ZZ(NPPT)
      A3C(NPT) = 0.0
      LWRFLX = CCONC(NPT)*0.5*((QL(NPT)+QL(NPT))/DELT) !g/cm2/h
      QL1 = 0.5*(QL(NPPT)+QL(NPT))/DELT !cm3 H2O/cm2/h
      AFPS1 = 0.5*(AFPS(NPPT)+AFPS(NPT))
      KHNH3(NPPT) = 1./(10.**(-1.69+1477.7/T(NPPT))) !cm3 WATER/cm3AIR
      KHNH3(NPT) = 1./(10.**(-1.69+1477.7/T(NPT))) !cm3 WATER/cm3AIR
      KDNH4(NPPT) = 10.**(-0.09018-2729.2/T(NPPT))
      KDNH4(NPT) = 10.**(-0.09018-2729.2/T(NPT))
      HION(NPPT) = 10.**(-PH(NPPT))
      HION(NPT) = 10.**(-PH(NPT))
      DNH41 = 0.5*(DNH4(NPPT)+DNH4(NPT))
      DNH31 = 0.5*(DNH3(NPPT)+DNH3(NPT))
      DKHNH31 = 0.5*(KHNH3(NPT)+KHNH3(NPPT))
      DKDNH41 = 0.5*(KDNH4(NPT)+KDNH4(NPPT))
      DHION1 = 0.5*(HION(NPPT)+HION(NPT))
      DNH3CON = DKHNH31/(1.+(DHION1/DKDNH41)) !cm3 water/cm3air
      DIFF1 = DNH41+DNH31*DNH3CON
      A1C(NPT) = (-0.5*DIFF1)/(THICK(NPT)*ZN) - 0.25*QL1/THICK(NPT)
!1/h
      Y(NPT) = THETA(NPT) + (BLKDEN*KON/10000.) + AFPS(NPT)*KHNH3(NPT)/
&
&      (1.+(HION(NPT)/KDNH4(NPT))) !cm3 H2O/cm3 soil
      AVS = SRCETAN(NPT) !g/cm3 soil/h
      A2C(NPT)=Y(NPT)*DEL+(0.5*DIFF1)/(THICK(NPT)*ZN)-
.25*QL1/THICK(NPT) !1/h
      ZYC(NPT) = Y(NPT)*CCONC(NPT)*DEL+AVS+(-LWRFLX)/THICK(NPT) !g/cm3
soil/h
!
!      Solution of tridiagonal matrix
      CALL TRIDAG(1,NPT,A1C,A2C,A3C,ZYC,CONC)
      DO I = 1,NPT
      IF(CONC(I) .LT. 0.0) CONC(I) = 0.0
      END DO

!-----
!      End of subroutine PROFTAN
!-----
-
      END

      SUBROUTINE
      PROFAQ(CCONC,CONC,RAINCONC,SURFFLUX,LWRFLX,DC,KON,SRCE)
!-----
-
!      Called by AGRIN MAIN
!
!      Simulates aqueous speccies movement in soil profile using finite
difference approximation
!-----
-
      INCLUDE 'agringlob.inc'

```



```

      DIMENSION
CCONC(M1),CONC(M1),Y(M1),YY(M1),A1C(M1),A2C(M1),A3C(M1),      &
      &      ZYC(M1),DC(M1),SRCE(M1)
      REAL*8 SURFFLUX,RAINCONC,LWRFLX,KON
      DEL = 1/DELT
!
!      After application and until slurry water has
evaporated/infiltrated, calculate
!      surface infiltration based on slurry thickness
      IF(IAPPN .GT. 0 .AND. IDAY .GE. APDAY(1) .AND. (NHR) .GE.
&
&APPNSRT(1) .AND. THICKNEW .GE. (10.**-5.)) THEN
      SURFFLUX2 = SURFFLUX !boundary condition is nitrate flux from
slurry
      GO TO 123
      END IF

      IF (RATE(NHR) .GT. 0.0) THEN
      SURFFLUX2 = SFLUX1*RAINCONC !infiltration from preicpitation
      SURFFLUX = SURFFLUX2
      ELSE
      SURFFLUX2 = 0.0
      SURFFLUX = 0.0
      END IF

!
!      Surface node equation for flux b.c.
123  Z1      = ZZ(1)
      A1C(1) = 0.0
      QL2 = 0.5*(QL(1)+QL(2))/DELT !cm/h,Jw,1.5
      DC1 = 0.5*(DC(1)+DC(2)) !DAQ,1.5
      DIFF1 = DC1
      A3C(1) = (-DIFF1)/(THICK(1)*Z1) + 0.5*QL2/THICK(1) !CM3
H2O/cm3soil/h
      Y(1) = THETA(1) + BLKDEN*KON !cm3 H2O/cm3 soil
      A2C(1) = (Y(1)/DELT) + (DIFF1/(THICK(1)*Z1)) + (0.5*QL2/THICK(1))
!1/h
      AVS = SRCE(1)
      ZYC(1) = Y(1)*DEL*CCONC(1)+AVS + (1.0*SURFFLUX2/THICK(1)) !g/cm3
soil/h

!      Interior nodes
      DO II=2,NPT-1
      I = II-1
      III = II+1
      Y(II) = THETA(II) + (BLKDEN*KON) !cm3 H2O/cm3 soil
      Z31      = Z(III)-Z(I)
      QL2 = 0.5*(QL(II)+QL(III))/DELT !cm/h
      QL1 = 0.5*(QL(I) + QL(II))/DELT
      DC1 = 0.5*(DC(II)+DC(I))
      DC2 = 0.5*(DC(II)+DC(III))
      DIFF1 = DC1
      DIFF2 = DC2
      A1C(II) = (-DIFF1)/(THICK(II)*ZZ(I)) - 0.5*QL1/THICK(II) !1/h
      A3C(II) = (-DIFF2)/(THICK(II)*ZZ(II)) + 0.5*QL2/THICK(II) !1/h
      A2C(II) = Y(II)*DEL + ( DIFF2/ZZ(II)) + (DIFF1/ZZ(I))-0.5*QL1
+ &

```

```

&      0.5*QL2)/THICK(II) !1/h
      AVS = SRCE(II)
      ZYC(II) = Y(II)*(CCONC(II))*DEL +AVS !G/cm3 soil/h
END DO

!
!      Lower node, unit gradient
      NPPT = NPT -1
      ZN      = ZZ(NPPT)
      A3C(NPT) = 0.0
      LWRFLX = CCONC(NPT)*0.5*((QL(NPT)+QL(NPT))/DELT) !g/cm2/h
      QL1 = 0.5*(QL(NPPT)+QL(NPT))/DELT !cm3 H2O/cm2/h
      DC1 = 0.5*(DC(NPPT)+DC(NPT))
      DIFF1 = DC1
      A1C(NPT) = (-DIFF1)/(THICK(NPT)*ZN) - 0.5*QL1/THICK(NPT) !1/h
      Y(NPT) = THETA(NPT) + (BLKDEN*KON) !cm3 H2O/cm3 soil
      A2C(NPT) = Y(NPT)*DEL+(DIFF1)/(THICK(NPT)*ZN) - .5*QL1/THICK(NPT)
!1/h
      AVS = SRCE(NPT)
      ZYC(NPT) = Y(NPT)*CCONC(NPT)*DEL+AVS+(-LWRFLX)/THICK(NPT) !g/cm3
soil/h
!
!      Solution of tridiagonal matrix
      CALL TRIDAG(1,NPT,A1C,A2C,A3C,ZYC,CONC)
      DO I = 1,NPT
      IF(CONC(I) .LT. 0.0) CONC(I) = 0.0
      END DO

!-----
-
!      End of subroutine PROFAQ
!-----
-
      END

      SUBROUTINE PROFAQHION(CCONC,CONC,RAINCONC,SURFFLUX,LWRFLX,DC,KON,
&
&      SRCE)
!-----
-
!      Called by AGRIN MAIN
!
!      Simulates H ion aqueous species movement in soil profile using
finite difference approximation
!-----
-
      INCLUDE 'agringlob.inc'
      DIMENSION
CCONC(M1),CONC(M1),Y(M1),YY(M1),A1C(M1),A2C(M1),A3C(M1),
&
&      ZYC(M1),DC(M1),SRCE(M1)
      REAL*8 SURFFLUX,RAINCONC,LWRFLX,KON
      DEL = 1/DELT

      IF (RATE(NHR) .GT. 0.0) THEN
      SURFFLUX2 = SFLUX1*RAINCONC !infiltration from preicpitation
      SURFFLUX = SURFFLUX2
      ELSE

```

```

SURFFLUX2 = 0.0
SURFFLUX = 0.0
END IF

!
! Surface node equation for flux b.c.
123 Z1 = ZZ(1)
A1C(1) = 0.0
QL2 = 0.5*(QL(1)+QL(2))/DELT !cm/h, Jw, 1.5
DC1 = 0.5*(DC(1)+DC(2)) !DAQ, 1.5
DIFF1 = DC1
A3C(1) = (-DIFF1)/(THICK(1)*Z1) + 0.5*QL2/THICK(1) !CM3
H2O/cm3soil/h
Y(1) = THETA(1) + ((BLKDEN/1000.)*BUFFCAP/(HHIONL(1)*2.302)) !cm3
H2O/cm3 soil
A2C(1) = (Y(1)/DELT) + (DIFF1/(THICK(1)*Z1)) + (0.5*QL2/THICK(1))
!1/h
AVS = SRCE(1)
ZYC(1) = Y(1)*DEL*CCONC(1)+AVS + (1.0*SURFFLUX2/THICK(1)) !g/cm3
soil/h

! Interior nodes
DO II=2,NPT-1
I = II-1
III = II+1
Y(II) = THETA(II) + ((BLKDEN/1000.)*BUFFCAP/(HHIONL(II)*2.302))
!cm3 H2O/cm3 soil
Z31 = Z(III)-Z(I)
QL2 = 0.5*(QL(II)+QL(III))/DELT !cm/h
QL1 = 0.5*(QL(I) + QL(II))/DELT
DC1 = 0.5*(DC(II)+DC(I))
DC2 = 0.5*(DC(II)+DC(III))
DIFF1 = DC1
DIFF2 = DC2
A1C(II) = (-DIFF1)/(THICK(II)*ZZ(I)) - 0.5*QL1/THICK(II) !1/h
A3C(II) = (-DIFF2)/(THICK(II)*ZZ(II)) + 0.5*QL2/THICK(II) !1/h
A2C(II) = Y(II)*DEL + (DIFF2/ZZ(II)) + (DIFF1/ZZ(I))-0.5*QL1
+ &
& 0.5*QL2)/THICK(II) !1/h
AVS = SRCE(II)
ZYC(II) = Y(II)*(CCONC(II))*DEL +AVS !G/cm3 soil/h
END DO

!
! Lower node, unit gradient
NPPT = NPT -1
ZN = ZZ(NPPT)
A3C(NPT) = 0.0
LWRFLX = CCONC(NPT)*0.5*((QL(NPT)+QL(NPT))/DELT) !g/cm2/h
QL1 = 0.5*(QL(NPPT)+QL(NPT))/DELT !cm3 H2O/cm2/h
DC1 = 0.5*(DC(NPPT)+DC(NPT))
DIFF1 = DC1
A1C(NPT) = (-DIFF1)/(THICK(NPT)*ZN) - 0.5*QL1/THICK(NPT) !1/h
Y(NPT) = THETA(NPT) +
((BLKDEN/1000.)*BUFFCAP/(HHIONL(NPT)*2.302)) !cm3 H2O/cm3 soil
A2C(NPT) = Y(NPT)*DEL+(DIFF1)/(THICK(NPT)*ZN) - .5*QL1/THICK(NPT)
!1/h

```

```

      AVS = SRCE(NPT)
      ZYC(NPT) = Y(NPT)*CCONC(NPT)*DEL+AVS+(-LWRFLX)/THICK(NPT) !g/cm3
soil/h
!
!      Solution of tridiagonal matrix
      CALL TRIDAG(1,NPT,A1C,A2C,A3C,ZYC,CONC)
      DO I = 1,NPT
      IF(CONC(I) .LT. 0.0) CONC(I) = 0.0
      END DO

!-----
!      End of subroutine PROFAQHION
!-----

      END

      SUBROUTINE PROFGAS(CCONC,CONC,DA,AIRCONC,BLK,SURFFLX,DC,KON,SRCE)
!-----
!      Called by AGRIN MAIN
!
!      Simulates aqueous speccies movement in soil profile using finite
      difference approximation
!-----

      INCLUDE 'agringlob.inc'
      DIMENSION
      CCONC(M1),CONC(M1),Y(M1),YY(M1),A1C(M1),A2C(M1),A3C(M1),      &
      &      ZYC(M1),DC(M1),SRCE(M1)
      REAL*8 AIRCONC,LWRFLX,KON,SURFFLX,BLK,DA,NGASTOTAL
      DEL = 1/DELT

!
!      Surface node equation for flux b.c.
123  Z1      = ZZ(1)
      SURFFLX = DA*(AIRCONC-CCONC(1)*KON)/THICK(1)      !g/cm2 soil/h
      A1C(1)  = 0.0
      DC1 = 0.5*(DC(1)+DC(2)) !Dg,1.5
      DIFF1 = DC1
      A3C(1)  = (-DIFF1*KON)/(THICK(1)*Z1) !CM3 WATER/cm3soil/h
      Y(1) = THETA(1) + AFPS(1)*KON !cm3 H2O/cm3 soil
      A2C(1) = (Y(1)/DELT) + (DIFF1*KON/(THICK(1)*Z1)) !l/h
      AVS = SRCE(1)
      ZYC(1) = Y(1)*DEL*CCONC(1)+AVS + (1.0*SURFFLX/THICK(1)) !g/cm3
soil/h

!      Interior nodes
      DO II=2,NPT-1
      I = II-1
      III = II+1
      Y(II) = THETA(II) + (AFPS(I)*KON) !cm3 H2O/cm3 soil
      Z31 = Z(III)-Z(I)
      DC1 = 0.5*(DC(II)+DC(I))
      DC2 = 0.5*(DC(II)+DC(III))
      DIFF1 = DC1

```

```

        DIFF2 = DC2
        A1C(II) = (-DIFF1*KON)/(THICK(II)*ZZ(I)) !1/h
        A3C(II) = (-DIFF2*KON)/(THICK(II)*ZZ(II)) !1/h
        A2C(II)=Y(II)*DEL+(DIFF2*KON/ZZ(II)+DIFF1*KON/ZZ(I))/THICK(II)
!1/h
        AVS = SRCE(II)
        ZYC(II) = Y(II)*(CCONC(II))*DEL +AVS !G/cm3 soil/h
    END DO
!
! Lower node, unit gradient
    NPPT = NPT -1
    ZN = ZZ(NPPT)
    A3C(NPT) = 0.0
    LWRFLX = 0.0 !g/cm2/h
    DC1 = 0.5*(DC(NPPT)+DC(NPT))
    DIFF1 = DC1
    A1C(NPT) = (-DIFF1*KON)/(THICK(NPT)*ZN) !1/h
    Y(NPT) = THETA(NPT) + (AFPS(I)*KON) !cm3 H2O/cm3 soil
    A2C(NPT) = Y(NPT)*DEL+(DIFF1*KON)/(THICK(NPT)*ZN) !1/h
    AVS = SRCE(NPT)
    ZYC(NPT) = Y(NPT)*CCONC(NPT)*DEL+AVS+(-LWRFLX)/THICK(NPT) !g/cm3
soil/h
!
! Solution of tridiagonal matrix
    CALL TRIDAG(1,NPT,A1C,A2C,A3C,ZYC,CONC)
    DO I = 1,NPT
        IF(CONC(I) .LT. 0.0) CONC(I) = 0.0
    END DO

!-----
! End of subroutine PROFGAS
!-----
END

SUBROUTINE MNGMTMOD
!-----
! Called by AGRIN MAIN
!
! Initializes water, residue and N application rates
!-----

    INCLUDE 'agringlob.inc'
    DIMENSION APPNTIME(NAPPN)
    INCLUDE 'agrininit.inc'

    DO I = 1,NAPPN
!
! Calculate application H+,NH4,NH3,NO3, N total, organic C (to
residue C pool)
        INITMOIST(I) = 1.0-DMAPPN(I)/100.0 !g H2O/g slurry
        APPNTIME(I) = APPNRATE(I)/(APPNEND(I) - APPNSRT(I)) !L/ha/h
        AREATIME(I) = APPNA(I)/(APPNEND(I) - APPNSRT(I)) !ha/h
        SLURRMASS(I) =INITMOIST(I)*1.*APPNTIME(I)*APPNDEN(I)/10000.
!g/m2/h

```

```

      NH4APINIT(I) = NH4APPNRATE(I)*AREATIME(I)*1000. !g N/h
      CRESAPINIT(I) = (OMAPPN(I)/100.0)*APPNDEN(I)*APPNTIME(I)/10000.
!gC/m2/h soil
      NO3APINIT(I) = NO3APPN(I)*APPNRATE(I)*AREATIME(I) !gN/h
      APDAY1 = APDAY(1)

      END DO

!-----
-
!      End of subroutine MNGMTMOD
!-----
-

      END

      SUBROUTINE CBALANCE
      INCLUDE 'agringlob.inc'
!
!      species balance
      TANSOIL2 = 0.0
      NO3SOIL2 = 0.0
      SRCETANTOT = 0.0
      SRCENO3TOT = 0.0

      DO I =1,NPT
      TANSOIL2 = TANSOIL2 + TANTOT(I)*THICK(I)
      NO3SOIL2 = NO3SOIL2 + NO3(I)*THICK(I)
!      SRCENH4TOT = SRCENH4TOT + SRCENH4(I)*DELT*THICK(I)
!      SRCENO3TOT = SRCENO3TOT + SRCENO3(I)*DELT*THICK(I)
      END DO
      TANBAL = TANSOIL1 - TANSOIL2 + SRCETANTOT + (TANFLUXTOP*DELT) -
&
&      (TANFLUXBOT*DELT)
      NO3BAL = NO3SOIL1 - NO3SOIL2 + SRCENO3TOT + (NO3FLUX*DELT) -
&
&      (NO3FLUXBOT*DELT) !g/cm2

!
!-----
-
!      End of subroutine CBALANCE
!-----
-

      END

      SUBROUTINE DENITMOD (NNO3L,NNO2L)
!-----
-
!      Called by AGRIN MAIN
!
!      Calculates denitrification in anaerobic soil fraction. Simulates
NOx
!      consumption/production and N2 production from denitrification
process.
!-----
-

```

```

        INCLUDE 'agringlob.inc'
        DIMENSION DOCD(M1),NO3D(M1),NO2D(M1),NOD(M1),N2OD(M1),UNO3(M1),
&
&
UNO2(M1),UNO(M1),UTOTAL(M1),UN2O(M1),FTEMP(M1),FPH1(M1),FPH2(M1),&
& FPH3(M1),TDEGC(M1),DBIODENITDT(M1),OXIDETOT(M1),DNO3DT(M1),
&
&
DNO2DT(M1),DNODT(M1),DN2ODT(M1),NTOTALHALF(M1),NO31(M1),NO21(M1),
&
& DCO2DTD(M1),NASSD(M1),NNTOTAL(M1),K1NO3(M1),K2NO3(M1),K3NO3(M1),
&
& K4NO3(M1),K1NO2(M1),K2NO2(M1),K3NO2(M1),K4NO2(M1),K1NO(M1),
&
& K2NO(M1),K3NO(M1),K4NO(M1),K1N2O(M1),K2N2O(M1),K3N2O(M1),
&
& K4N2O(M1),UUNO3(M1),UUNO2(M1),UUNO(M1),UUN2O(M1),UUTOTAL(M1),
&
&UNO3HALF(M1),UNO2HALF(M1),UNOHALF(M1),UN2OHALF(M1),UTOTALHALF(M1),&
& BIODENITHALF(M1),NO3HALF(M1),NO2HALF(M1),NOHALF(M1),N2OHALF(M1),
&
& NO1(M1),N2O1(M1),BBIODENIT1(M1),BIODENIT1(M1)
        REAL*8 NO3D,NO2D,NOD,N2OD,K1NO3,K2NO3,K3NO3,K4NO3,K1NO2,K2NO2,
&
& K3NO2,K4NO2,K1NO,K2NO,K3NO,K4NO,K1N2O,K2N2O,K3N2O,K4N2O,NO31,
&
& NO21,NO1,N2O1,NNTOTAL,NTOTALHALF,NO2HALF,NO3HALF,NOHALF,
&
& N2OHALF
        INCLUDE 'agrininit.inc'
        DEL = 1.0/DELSAV !1/h
        DO I = 1,NPT
!
!       Calculate substrates allocated to denitrification
!       Substrate units must be in g cm-3 water, while biomass per dry
soil concentration
        DOCD(I) = DDOC(I)*ANVF(I)/THETA(I) !g cm-3 water
        BBIODENIT1(I) = BBIODENIT(I) !*ANVF(I)
!       Apply Henry's Law to get aqueous concentrations here
        NO3D(I) = NNO3L(I)*ANVF(I) !G/CM3 WATER
        NO2D(I) = NNO2L(I)*ANVF(I)
        NOD(I) = NNOL(I)*ANVF(I) !g/cm3 water
        N2OD(I) = NN2OL(I)*ANVF(I)
!
!       Calculate relative growth rates for each species
        UNO3(I) = UNO3MAX*(DOCD(I)/(KCD+DOCD(I)))*(NO3D(I)/(KND+NO3D(I)))
!1/h
        UNO2(I) = UNO2MAX*(DOCD(I)/(KCD+DOCD(I)))*(NO2D(I)/(KND+NO2D(I)))
        UNO(I) = UNOMAX*(DOCD(I)/(KCD+DOCD(I)))*(NOD(I)/(KND+NOD(I)))
        UN2O(I) = UN2OMAX*(DOCD(I)/(KCD+DOCD(I)))*(N2OD(I)/(KND+N2OD(I)))
!
!       Calculate temperature and pH factors
        TDEGC(I) = T(I) - 273.16
        FTEMP(I) = 2**((TDEGC(I)-22.5)/10.0)
        FPH1(I) = 0.4*(PH(I)-2.5)
        FPH2(I) = 0.4*(PH(I)-3.0)

```

```

      FPH3(I) = 0.4*(PH(I) - 3.5)
!
!   Calculate total relative growth rate
      UTOTAL(I) = FTEMP(I)*(FPH1(I)*UNO3(I) + FPH2(I)*UNO2(I) +
&
& FPH2(I)*UNO(I) + FPH3(I)*UN2O(I)) !1/h
!
!   Calculate biomass at end of time step
      BIODENIT1(I) = BBIODENIT1(I)*EXP((UTOTAL(I)-(MCD*YCD))*DELT) !g
cm-3 soil
      DBIODENITDT(I) = BIODENIT1(I)*(UTOTAL(I)-MCD*YCD) !g cm-3 soil h-
1
!
!   Calculate consumption of DOC, CO2 production, and N assimilation
rates
      RDOCDENIT(I) = BBIODENIT1(I)*zz(i)*((UTOTAL(I)/YCD)+MCD) !g cm-3
soil h-1
      RCO2DENIT(I) = (RDOCDENIT(I) - UTOTAL(I)*BBIODENIT1(I)) !g CO2-C
cm-3 soil h-1
      RNASSDENIT(I) = UTOTAL(I)*BBIODENIT1(I)/CNDEN !g N cm-3 soil h-1
!
!   Calculate N oxide consumption rates
      OXIDETOT(I) = NO3D(I)+NO2D(I)+NOD(I)+N2OD(I)
      DNO3DT(I)=(UNO3(I)/YNO3)+MNO3*NO3D(I)/OXIDETOT(I))*BBIODENIT1(I)
!gN/cm3WATER/h
      DNO2DT(I)
= ((UNO2(I)/YNO2)+MNO2*NO2D(I)/OXIDETOT(I))*BBIODENIT1(I)
      DNODT(I) = ((UNO(I)/YNO)+MNO*NOD(I)/OXIDETOT(I))*BBIODENIT1(I)
      DN2ODT(I)
= ((UN2O(I)/YN2O)+MN2O*N2OD(I)/OXIDETOT(I))*BBIODENIT1(I)
!   Net rate change of aqueous concentrations
      RNO3DENIT(I) = -DNO3DT(I)-RNASSDENIT(I)
      RNO2DENIT(I) = DNO3DT(I)-DNO2DT(I)
      RNODENIT(I) = DNO2DT(I) - DNODT(I)
      RN2ODENIT(I) = DNODT(I) - DN2ODT(I)
      RN2DENIT(I) = DN2ODT(I)
      BIODENIT(I) = BBIODENIT(I) + DBIODENITDT(I)*DELT

      END DO
!-----
!
!   End of subroutine DENITMOD
!-----
-
      END

```

A.5 AGRIN OUT source code

```

      PROGRAM AGRIN OUT
!-----
!
!   Calls ...

```



```

!
! Processes the binary output file (*.RES) generated by AGRIN MAIN.
!-----
-
      INCLUDE 'agringlob.inc'
      DATA DOV/1.0/
      CALL WELCOME('AGRIN OUT',DOV)
20  WRITE(LUS,6010)
      READ(LUR,5000) TMFILE
      IF (INDEX(TMFILE(1:1),'0') .GT. 0) STOP
      NCHR = INDEX(TMFILE,' ')
      TMFILE(NCHR:NCHR+3) = '.res'
      OPEN(UNIT=LUI,FILE=TMFILE,STATUS='OLD',FORM='UNFORMATTED',
&
&      ACCESS='DIRECT',RECL=100,ERR=900)
      READ(LUI,REC=1) NPT,IPLANT,ITRACE,IAPPN
      CLOSE(LUI)
      IRL = IRLMOD*MAX(110,(9+IPLANT+5)*NPT+45)
      OPEN(UNIT=LUI,FILE=TMFILE,STATUS='OLD',FORM='UNFORMATTED',
&
&      ACCESS='DIRECT',RECL=IRL,ERR=900)
      INQUIRE(UNIT=LUI,NAME=RFILE)
      READ(LUI,REC=1) NPT,IPLANT,ITRACE,IAPPN,(Z(I),I=1,NPT),STOPHR,
&
&      NDAYS,IFILE,
      SDATE,STIME,TITLE,IDEND,NPRINT,IEVOPT,NTOTAL,IDBEG,      &
&      IVAPOR,
      ICLOUD,IETOPT,UPPER,UPPERH,LOWER,LOWERH,IYEAR,IDAY,HOUR,      &
&
      (THETA(J),T(J),NO3(J),NH4(J),NH3(J),TANTOT(J),J=1,NPT),RN,SENFLX
&
&      ,LE,SHFLUX,NH3FLUX,SLURRTANFLUX,N2OFLUX,NOFLUX,TMOIST

      MAXREC = 3+(IDEND-IDBEG+1)*(1+NTOTAL*NPRINT)-
&
&      NINT(NPRINT*NTOTAL*(1-STOPHR/24.))
      DO I=1,MAXREC
          READ (LUI,REC=I,ERR=48)
          ENDDO
48  IF (I-1 .NE. MAXREC) WRITE(LUS,6111) I-1,MAXREC-I+1
      IREC = 2
      WRITE(LUS,*)
50  WRITE(LUS,6020)
      READ(LUR,*) IOPT
      IF (IOPT .LT. 1 .OR. IOPT .GT. 6) IOPT = 0

!
! Call the chosen option
!
      GO TO (999,100,200), IOPT+1
100  CALL LISTDATA
      GO TO 50
200  CLOSE (LUI)
      GO TO 20
900  WRITE(LUS,6040) TMFILE
      GO TO 20
999  STOP ' '

```

```

!-----
-
!      FORMAT Statements
!-----
-
5000  FORMAT(A80)
6000  FORMAT(/,
&
&      &' Program AGRIN provides several options for',/,
&
&      &' processing the output file (i.e., a *.res file)'/)
6010  FORMAT('/' Enter output filename without ".res" extension',/,
&
&      &' (or "0" to terminate the program) ==> ', $)
6020  FORMAT(' COMMAND LEVEL: The processing options are...',/,
&
&      &'      0) Exit the program',/,
&
&      &'      1) Create data vs time files',/,
&
&      &'      2) Change the current *.res file',/,
&
&      &' Enter the number of your choice ==> ', $)
6040  FORMAT('/' No record of file ',A50,/,
&
&      &' Try again...'/)
6111  FORMAT('/' CAUTION: Be advised that this results file contains ',
&
&      &'only',I5,/,T12,'records, which is',I5,' less than it ',
&
&      &'should have if simulating',/,T12,' at least one year.'/)
!-----
-
!      End of program agrin in
!-----
-
      END

      SUBROUTINE READREC
!-----
-
!      Called by DDSUM, INITSUM, LISTDATA, PROFILER, and REINIT
!
!      Reads the *.RES file , either DELSUB or daily
!      summary records
!-----
-
      INCLUDE 'agringlob.inc'
      IERROR = 0

      READ(LUI,REC=IREC,ERR=200) IDAY,NHR, (THETA(J),QL(J),QHC(J),
&
&      T(J),J=1,NPT),RN,SENFLX,LE,SHFLUX,SPREV,TMOIST,SHPREV,
&
&      hSTORE,(NO3(J),NH4(J),NH3(J),NH4S(J),NH4L(J),NH3G(J),NH3L(J) &
&      ,TANTOT(J),J=1,NPT),NH3FLUX,SLURRTANFLUX,N2OFLUX,NOFLUX

```

```

100  RETURN
200  WRITE(LUS,6000) IREC
      IERROR = 1
      GO TO 100
!-----
!
!      FORMAT Statements
!-----
6000  FORMAT(/' Record No. ',I5,' could not be read'/)
!-----
!
!      End of subroutine READREC
!-----
-
      END

      SUBROUTINE LISTDATA
!-----
!
!      Called by AGRIN OUT
!
!      Calls READREC
!
!      Creates data lists, such as head values at the end each time
period,
!      for output to a separate file to be used for plotting purposes.
!-----
-
      INCLUDE 'agringlob.inc'
      DIMENSION FZ(M1)
      DO I=1,NPT-1
          FZ(I) = (Z(I+1)+Z(I))/2
      ENDDO
      FZ(NPT) = Z(NPT)
      WRITE(LUS,6000)
      WRITE(LUS,6010)
!
!      Choose variable for output
!
100  NOUT = 1
      LOUT = LUS
      WRITE (LUS,6020)
      WRITE(LUS,6024)
      IF(ITRACE .GT. 0)WRITE(LUS,60241)
      WRITE(LUS,6025)
      READ(LUR,*) CHOICE
          LOUT = LUW
          WRITE(LUS,6050)
          READ(LUR,'(A)') OFILE
          OPEN (UNIT=LOUT,FILE=OFILE,STATUS='UNKNOWN')
          CLOSE(UNIT=LOUT,STATUS='DELETE')
          OPEN(UNIT=LOUT,FILE=OFILE,STATUS='NEW')
          INQUIRE(UNIT=LOUT,NAME=OFILE)
          IF (LOUT .EQ. LUW) WRITE(LOUT,6060) DOV,IFILE,RFILE,SDATE,STIME

```

```

IF (CHOICE .EQ. 1) THEN
  WRITE(LOUT,6062)
  WRITE(LOUT,6069)
ELSE IF (CHOICE .EQ. 2) THEN
  WRITE(LOUT,6072)
  WRITE(LOUT,6074)
ELSE IF (CHOICE .EQ. 3) THEN
  WRITE(LOUT,6140)
ELSE IF (CHOICE .EQ. 4) THEN
  WRITE(LOUT,6141)
ELSE IF (CHOICE .EQ. 5) THEN
  WRITE(LOUT,60721)
  WRITE(LOUT,6074)
ELSE
  WRITE(LOUT,*) ' There is no choice ',CHOICE
  WRITE(LOUT,*) ' The available choices are 1 to 5. Try again'
  GO TO 100
ENDIF
IDAY = 0
HOUR = 0.0

!
! Read variables and write to screen or file
!
DO IREC=2,MAXREC-1
  IF (IREC .EQ. 2) THEN
    READ(LUI,REC=2) IDAY,NHR,(THETA(J),QL(J),QHC(J),
&
&      T(J),J=1,NPT),RN,SENFLX,LE,SHFLUX,SPREV,TMOIST,SHPREV,
&
&      hSTORE,(NO3(J),NH4(J),NH3(J),NH4S(J),NH4L(J),NH3G(J),NH3L(J)      &
&      ,TANTOT(J),J=1,NPT),NH3FLUX,SLURRTANFLUX,N2OFLUX,NOFLUX
    JDAY = IDEND - NDAYS + 1
    IF (JDAY .GT. IDEND) GO TO 135
    IF (CHOICE .EQ. 1) THEN
      DO I = 1,NPT
        WRITE(LOUT,6100) JDAY,nhr,I,Z(I),THETA(I)
      END DO
    ELSE IF (CHOICE .EQ. 2) THEN
      DO I = 1,NPT
        WRITE(LOUT,6100) JDAY,NHR,I,Z(I),T(I)
      END DO
    ELSE IF (CHOICE .EQ. 3) THEN
      WRITE(LOUT,6093) JDAY,NHR,RN,SENFLX,LE,SHFLUX
    ELSE IF (CHOICE .EQ. 4) THEN
      WRITE(LOUT,6094) JDAY,NHR,NH3FLUX,SLURRTANFLUX,N2OFLUX,NOFLUX
    ELSE IF (CHOICE .EQ. 5) THEN
      DO I = 1,NPT
        TANTOT(I) = NH4(I) + NH3(I)
        WRITE(LOUT,6101) JDAY,NHR,I,Z(I),TANTOT(I),NO3(I)
      END DO
    ENDIF
  ELSE
    IF (IREC .GT. 2 .AND. NPRINT .EQ. 1) THEN
      IF (IREC .EQ. (2+(IDAY-IDBEG+1)*(NTOTAL+1))) GO TO 130
      IF (IDAY .EQ. IDEND .AND. IREC .EQ. MAXREC-1) GO TO 130
    ENDIF
  ENDIF

```



```

&          ' the selected choice',/,/,
&
&          ' Choose output reduction option ==> ',$,)
6040 FORMAT(/' Options for output device:',/,
&
&          ' 0) screen',/,
&
&          ' 1) file',/,
&
&          ' Choose output device option ==> ',$,)
6050 FORMAT(/' Enter output file name ==> ',$,)
6060 FORMAT(' AGRIN Version ',F4.2,/,
&
&          ' Input File: ',A65,/,
&
&          ' Results File: ',A65,/,
&
&          ' Date of Run: ',A11,/,
&
&          ' Time of Run: ',A11,/)
6062 FORMAT(' Time (day)      Hour      Node      Depth(cm)
&
&Theta(cm3 cm-3) ')
6064 FORMAT(' Time (day) ',T15,'T (K)')
6069 FORMAT(1X,11('-'),T15,6(11('-')))
6070 FORMAT(T7,'NODE =',T15,6(I7,4X))
6071 FORMAT(T2,'NODE OVER Z =',T15,6(I7,4X))
6072 FORMAT(' Day      Hour      Node      Depth(cm)
&
&Temp(K) ')
60721 FORMAT(' Day      Hour      Node      Depth(cm)
&
&[TAN](g/cm3 soil) [NO3-](g/cm3soil)')
6074 FORMAT(1X,11('-'),T15,(10('-')),T26,6(11('-')))
6076 FORMAT(T7,'NODE =',T26,6(I7,4X))
6077 FORMAT(T2,'DEPTH (cm) =',T26,1P,6(E11.4))
6078 FORMAT(T2,'DEPTH (cm) =',T15,1P,6(E11.4))
6140 FORMAT(' Surface Energy Balace Per Output Cycle (units = W/m2)',
&
&/, ' Day',T19,'Hour      RN      SENFLX      LE
&
&SHFLUX',/,1X,11('-'),T15,5(1X,10('-')),/)
6141 FORMAT(' Day      Hour      NH3flux(g/cm2/h)      SLURRY TAN
&
&FLUX      N2OFLUX      NOFLUX',/,1X,11('-'),T15,5(1X,10('-')),/)
6090 FORMAT(1P,2I,2X,1P,I,E11.3,E12.4)
6091 FORMAT(2I,2X,1P,E11.3)
6092 FORMAT(2I,2X,5E11.4)
6093 FORMAT(2I,2X,4F11.3)
6094 FORMAT(2I,2X,4E11.3)
6100 FORMAT(1P,2I,2X,1P,I,2E12.3)
6101 FORMAT(1P,2I,2X,1P,I,3E12.3)
6112 FORMAT(1P,E12.5,2X,1PE11.4,0P,4I11)
6120 FORMAT(/' The data have been written to file: ',/,1X,A60)
6260 FORMAT(80('_'),/, ' Press <RTN> to get LISTDATA options ==> ',$,)
!-----
-

```

```

!      End of subroutine LISTDATA
!-----
-
      END

      SUBROUTINE WELCOME(name,ver)
!-----
-
!      Called by AGRIN IN, AGRIN MAIN, AGRIN OUT
!
!      Writes program header with version number and contact person
!-----
-
      INCLUDE 'agringlob.inc'
      CHARACTER name*7
      WRITE(LUS,10) name,ver
10    FORMAT(/,
&
&      &'          Program ',A7,/,
&
&      &'          Version ',F4.2,/,
&
&      &'          Contact:',/,
&
&      &'          J Beuning',/,
&
&      &'          University of Guelph',/,
&
&      &'          phone: 519-824-4120 ext. 58263',/,
&
&      &'          email: jbeuning@uoguelph.ca',/)
      RETURN
!-----
-
!      End of subroutine WELCOME
!-----
-
      END

```

APPENDIX B: INPUT FILES

B.1: 1992.inp

```
1992.inp: Test of soil heat and moisture flow for bare
loam soil with net radiation data
0,0,0,0,0,                                IPLANT, ITRACE, IAPPN, IRES, ITILL
272,268,                                IFDEND, IDTBEG
5,1.0e-04,1.0,0.004,                    INMAX, DMAXBA, DELMAX, DELMIN
0,1,0,0.0,                                ICLoud, IRAD, ISOL, DMAXHE
32,                                    NPT
0.0,0.1,0.2,0.3,
0.5,0.7,0.9,1.0,
2.5,4.0,5.0,7.5,
9.5,12.0,14.5,17.0,
20.0,23.5,26.5,30.5,
34.5,39.0,43.5,47.5,
52.5,62.5,72.5,87.5,
103.0,123.0,143.0,173.0,200.0,
Loam soil properties
2.52,0.451,0.478,2.39,5.39,            SK, THET, SATMA, CHS, B
0.19,1.5,                                CLY, BLKDEN
0,                                    NDAY
0.27,0.27,0.27,0.27,
0.27,0.27,0.27,0.27,
0.27,0.27,0.27,0.27,
0.27,0.27,0.27,0.27,
0.27,0.27,0.27,0.27,
0.27,0.27,0.27,0.27,
0.27,0.27,0.27,0.27,
0.27,0.27,0.27,0.27,
280.0,282.0,285.0,285.0,
284.0,283.0,284.0,284.0,
286.0,288.0,286.0,288.0,
290.0,290.0,290.0,290.0,
293.0,293.0,293.0,293.0,
293.0,293.0,293.0,293.0,
293.0,293.0,293.0,293.0,
293.0,293.0,293.0,293.0,
0.001,0.001,7.0,7.0,0.0,45.19,        ZH, ZM, ZT, ZU, D, LAT
268.0,271.65,271.45,271.85,272.15,272.15,272.85,272.05,273.35,275.75,27
6.75,274.85,273.75,273.55,273.75,274.85,273.75,273.25,272.65,271.65,272
.75,273.15,273.55,274.15,273.95,
269.0,273.75,273.65,273.55,273.95,273.45,274.05,274.05,275.95,278.05,27
8.75,278.55,277.55,276.75,275.85,276.15,277.35,276.65,278.75,278.35,277
.45,277.05,276.55,276.95,276.95,
270.0,276.15,275.85,276.25,275.75,277.15,277.55,277.75,278.45,279.85,28
0.85,280.85,281.05,281.75,281.55,281.65,281.95,283.05,283.35,283.95,284
.55,285.55,285.85,285.85,285.85,
271.0,285.75,286.15,286.45,286.55,286.75,287.05,287.45,287.65,288.05,28
8.95,289.15,288.95,289.25,289.65,290.85,287.65,283.85,283.25,283.25,283
.55,282.55,282.65,282.55,282.35,
272.0,282.25,282.25,282.35,282.25,281.85,281.55,281.85,282.65,283.15,28
2.75,282.45,282.65,281.65,280.25,280.85,281.55,283.05,282.95,282.45,282
.75,283.75,284.15,278.85,278.35,
```


268.0,271.02,270.79,269.83,269.66,269.75,270.01,272.8,277.19,278.77,282
 .52,284.5,285.76,288.53,289.06,290.09,292.79,289.89,287.05,281.13,278.2
 6,276.44,275.45,275.13,275.11
 269.0,273.67,274.15,273.99,273.02,273.29,276.12,281,282.65,286.48,289.2
 8,291.38,293.72,293.43,294.34,294.98,292.87,290.27,284.91,283.24,279.97
 ,278.42,278.42,276.1,276.4
 270.0,274.71,274.92,274.29,275.54,275.08,276.11,280.17,282.77,285.72,28
 7.09,287.67,288.85,290.15,288.95,288.71,285.24,284.53,284.83,285.13,285
 .57,286.3,286.48,286.36,286.32
 271.0,288.35,286.58,286.77,286.82,286.84,287.27,287.79,288.41,289.57,28
 9.91,289.62,289.86,290.3,292.13,293.17,291.96,290.36,289.91,289.81,289.
 88,289.18,288.88,288.5,288.08
 272.0,287.45,286.62,286.75,284.81,282.36,282.8,285.27,287.71,290.23,290
 .71,291.4,292.55,293.27,293.32,292.25,291.4,289.11,287.23,287.21,287.13
 ,287.19,285.3,282.39,282.39
 268.0,0.09,0.14,0,0,0.1,0,0,0.89,2.55,1.7,2.1,2.53,2.27,1.53,1.63,1.44,
 1.22,1.28,1.82,0.81,0.31,1.1,0.83,0.7
 269.0,0.28,1.26,0.67,0.37,0.68,0,1.65,2.36,1.83,2.01,1.74,1.88,1.75,2.2
 1,2.55,2.38,1.12,2.87,2.28,0.38,0.73,1.03,0.05,0.86
 270.0,0.1,0.39,0.44,1.08,0.13,0.04,1.31,2.99,2.79,2.86,3.18,3.61,3.8,4.
 19,3.65,3.03,2.76,2.23,2.31,1.81,2.61,2.2,1.93,2.22
 271.0,1.44,1.01,1.37,1.2,1.55,2.26,3.47,4.15,4.45,4.72,4.4,5.58,6.06,8.
 04,9.73,10.33,9.72,7.77,8.99,11.27,11.31,9.33,7.86,7.3
 272.0,6.43,4.77,5.77,3.94,2.03,1.45,2.83,2.98,2.94,3.44,5.24,5.47,5.71,
 5.91,5.18,5.06,5.27,4.96,5.08,5.43,5.17,6.72,4.56,4.56
 268.0,-36.68,-30.67,-25.75,-25.23,-23.82,-22.56,-
 20.44,26.87,116.6,214.6,323.4,407.3,451,443.3,400.0,324,214.3,75.5,-
 42.94,-70.7,-66.5,-61.42,-53.21,-45.63
 269.0,-40.17,-34.59,-31.04,-31.35,-29.37,-
 26.83,4.18,100.1,198.5,305.4,382.5,422.1,420,383.9,310.7,206.4,67.73,-
 47.53,-75.5,-72.7,-67.65,-62.59,-60.14,-57.75
 270.0,-54.54,-45.8,-34.28,-27.86,-20.03,-
 14.38,15.32,65.08,130,239.8,158.8,148.2,184.9,210.2,139.3,69.83,23.92,7
 .69,-1.31,-3.49,-0.61,0.01,-0.3,-0.27
 271.0,0.04,0.1,0.56,0.29,-0.56,-
 0.4,10.7,22.98,76.5,116.8,52.01,42.89,45.3,52.22,210.4,182.2,69,-11.3,-
 8.95,-17.36,-6.31,-6.25,-6.08,-5.64
 272.0,-5.94,-23.59,-12.36,-24.85,-60.5,-
 62.06,1.54,71.2,185.2,297.2,376.6,432.8,440.4,394.5,316.5,204.6,46.38,-
 37.21,-41.79,-16.4,-9.07,-12.47,-56.49,-56.49
 2, NWATER
 270,5,
 17.00,0.05,
 18.00,0.05,
 19.00,0.00,
 23.00,0.02,
 24.00,0.00
 271,9,
 1.00,0.05,
 2.00,0.00,
 8.00,0.06,
 9.00,0.08,
 10.00,0.00,
 12.00,0.06,
 13.00,0.10,
 14.00,0.10,
 15.00,0.00,

B.2: richmond.inp

```
richmond.inp: Fall 2004 liquid dairy manure application to bare soil
0,1,1,0,0, IPLANT, ITRACE, IAPPN, IRES, ITILL
277,257, IFDEND, IDTBEG
1,1.0e-010,1.0,0.004, INMAX, DMAXBA, DELMAX, DELMIN
1,0,1,1000.0, ICLOUD, IRAD, ISOL, DMAXHE
32, NPT
0.0,0.1,0.2,0.3,
0.5,0.7,0.9,1.0,
2.5,4.0,5.0,7.5,
9.5,12.0,14.5,17.0,
20.0,23.5,26.5,30.5,
34.5,39.0,43.5,47.5,
52.5,62.5,72.5,87.5,
103.0,123.0,143.0,200.0,
Loam soil properties
2.52,0.451,0.478,2.39,5.39, SK, THET, SATMA, CHS, B
0.19,1.4, CLY, BLKDEN
0.35,0.35,0.35,0.35,
0.35,0.35,0.35,0.35,
0.35,0.35,0.35,0.35,
0.35,0.35,0.35,0.35,
0.35,0.35,0.35,0.35,
0.35,0.35,0.35,0.35,
0.35,0.35,0.35,0.35,
0.35,0.35,0.35,0.35,
0.35,0.35,0.35,0.35,
285.0,285.0,285.0,286.0,
286.0,286.0,287.0,287.0,
287.0,287.0,287.0,287.0,
287.0,286.0,286.0,286.0,
285.0,285.0,285.0,285.0,
285.0,284.0,283.0,283.0,
280.0,280.0,280.0,280.0,
280.0,280.0,280.0,280.0,
0.024,0.019,9.35E-07,8.1E-06,0.0,6.3,11,
RESINIT, SOCINIT, NH4INIT, NO3INIT, NO2INIT, PHINIT, NODEIN
-0.00034, -0.00027, 0.0, 0.0, 0.0, 0.0078,
RESRATE, SOCRATE, N4RATE, NO3RATE, NO2RATE, PHRATE
1,0.05, NAPPN, RED
2,22.0,11,17,78634.0,18.3,
APDAY, APPNA, APPNSRT, APPNEND, APPNRATE, NH4APPNRATE
1200.0,9.0,0.011,1.1,7.4,1.7,2.1,
APPNDEN, CNAPPN, NO3APPN, NTOTAPPN, PHAPPN, OMAPPN, DMAPPN
0.001,0.001,3.5,3.5,0.0,45.19, ZH, ZM, ZT, ZU, D, LAT
257,280.5,279.0,278.0,277.2,276.0,275.5,275.2,275.5,275.9,275.8,275.5,2
75.1,274.9,275.5,275.7,275.3,275.5,276.1,276.5,276.8,275.9,275.4,274.5,
274.8
258,276.0,275.6,275.1,275.0,274.9,274.8,274.6,276.0,277.2,277.7,279.1,2
79.8,280.9,281.6,282.0,281.0,281.2,280.9,281.3,281.8,281.2,281.0,280.5,
279.8
```

259,279.5,279.5,279.3,279.4,281.9,282.6,282.7,282.5,283.7,284.6,284.5,2
 84.8,285.0,285.0,284.8,284.7,283.9,283.8,283.7,283.7,283.3,283.0,282.8,
 282.8
 260,282.8,282.1,281.8,281.6,281.4,281.2,281.3,281.9,282.6,283.3,283.7,2
 83.8,284.3,284.2,284.0,283.9,284.2,284.1,284.4,284.9,285.7,285.7,284.8,
 282.7
 261,280.5,279.0,278.0,277.2,276.0,275.5,275.2,275.5,275.9,275.8,275.5,2
 75.1,274.9,275.5,275.7,275.3,275.5,276.1,276.5,276.8,275.9,275.4,274.5,
 274.8
 262,273.5,274.0,273.7,273.8,273.2,273.2,273.1,273.2,273.1,273.1,273.1,2
 73.1,273.1,273.1,273.1,273.1,273.1,273.1,273.1,273.1,273.1,273.1,
 273.1
 263,273.1,273.1,273.2,273.8,273.1,273.1,273.1,273.1,273.1,273.2,273.1,2
 73.2,273.1,273.1,273.1,273.1,273.1,273.1,273.2,273.2,273.2,273.1,273.1,
 273.1
 264,273.1,273.1,273.1,273.1,273.1,273.1,273.1,274.4,274.8,275.8,275.8,2
 76.0,275.4,275.6,275.0,274.9,275.6,276.0,276.3,276.2,277.3,278.1,278.1,
 277.9
 265,277.7,277.9,278.0,277.9,277.5,277.4,277.5,277.8,277.9,278.5,278.0,2
 77.6,278.4,278.1,279.2,280.2,280.4,280.0,279.8,280.1,280.3,279.9,279.0,
 279.2
 266,278.9,278.8,278.6,278.1,276.3,275.4,276.0,277.9,279.2,280.0,279.9,2
 80.3,281.2,281.7,282.0,282.4,282.7,283.2,283.0,283.8,283.6,283.4,282.4,
 281.0
 267,281.3,280.4,280.3,281.5,281.6,282.3,281.8,281.8,281.9,278.8,278.1,2
 78.3,278.6,279.1,280.1,279.6,279.8,280.3,281.1,280.1,279.7,279.0,278.9,
 278.5
 268,278.0,278.6,278.7,277.9,277.4,277.3,276.8,279.0,280.7,282.9,284.1,2
 84.8,284.8,284.5,283.7,283.2,282.1,281.4,281.4,281.9,282.8,283.1,283.1,
 283.2
 269,283.4,283.5,283.6,283.6,283.9,284.0,284.0,283.8,284.1,284.0,283.6,2
 83.2,281.8,280.7,279.5,278.7,277.2,276.8,277.3,277.6,278.0,278.3,278.0,
 277.6
 270,276.6,275.8,275.5,275.8,275.7,274.9,274.4,275.0,276.9,276.9,277.1,2
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 ,1.0,0.7,0.7,0.7,0.3,0.3,0.3
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 ,0.7,0.7,0.7,0.3,0.3,0.0
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 ,0.7,1.0,1.0,1.0,1.0,0.3,0.0
 267,0.0,0.0,0.3,0.7,1.0,0.7,0.7,0.7,0.3,0.0,0.0,0.0,0.0,0.3,0.0,0.0,0.3
 ,0.3,0.3,0.3,0.0,0.0,0.0,0.3
 268,0.3,0.3,0.3,0.3,0.3,0.3,0.7,0.7,0.7,0.3,0.3,0.7,0.7,0.7,0.7,0.7,0.7
 ,0.7,0.7,0.7,0.7,0.7,1.0,1.0
 269,1.0,1.0,1.0,1.0,1.0,1.0,1.0,1.0,0.7,0.7,1.0,1.0,0.7,0.7,0.7,0.3,0.0
 ,0.3,0.3,0.7,0.3,0.3,0.3,0.0
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 ,0.0,0.0,0.0,0.0,0.0,0.0,0.0
 271,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0
 ,0.0,0.3,0.0,0.0,0.0,0.0,0.3
 272,0.3,0.0,0.3,0.3,0.0,0.3,0.3,0.3,0.3,0.7,0.7,0.7,0.7,0.7,0.7,0.7,0.7
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 ,0.3,0.3,0.3,0.7,0.7,0.3,0.3
 274,0.0,0.0,0.0,0.3,0.3,0.7,0.7,0.7,0.7,0.7,0.7,0.7,1.0,0.7,0.7,0.7,0.7
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 ,0.7,0.3,0.0,0.3,0.7,0.3,0.3
 277,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.3,0.7,0.7,0.7,0.7,0.3
 ,0.7,0.0,7.0,0.0,0.3,0.3,0.3
 5, NWATER
 260,2,
 15.00,0.01,
 15.5,0.0,
 269,2,
 10.5,0.04,
 11.0,0.0,
 271,2,
 7.00,0.01,
 7.5,0.0,
 275,4,
 5.5,0.01,
 6.0,0.0,
 7.5,0.01,
 8.0,0.0,
 276,8,
 6.5,0.05,
 7.0,0.0,
 14.5,0.01,
 15.0,0.45,
 15.5,0.43,
 16.0,0.18,
 16.5,0.03,
 17.0,0.0,

B.3: forage.inp

forage.inp: August 2005 poultry slurry application to bare soil

0,1,1,0,	IPLANT, ITRACE, IAPPN, IRES
237,218,	IFDEND, IDTBEG
1,1.0e-010,1.0,0.004,	INMAX, DMAXBA, DELMAX, DELMIN
1,0,1,1000.0,	ICLOUD, IRAD, ISOL, DMAXHE
32,	NPT
0.0,0.1,0.2,0.3,	
0.5,0.7,0.9,1.0,	
2.5,4.0,5.0,7.5,	
9.5,12.0,14.5,17.0,	
20.0,23.5,26.5,30.5,	
34.5,39.0,43.5,47.5,	
52.5,62.5,72.5,87.5,	
103.0,123.0,143.0,200.0,	
Clay loam soil properties	
0.9,0.476,0.63,2.39,8.52,	SK, THET, SATMA, CHS, B
0.34,1.5,	CLY, BLKDEN
0.35,0.35,0.35,0.35,	
0.35,0.35,0.35,0.35,	
0.35,0.35,0.35,0.35,	

0.35,0.35,0.35,0.35,
 0.35,0.35,0.35,0.35,
 0.35,0.35,0.35,0.35,
 0.35,0.35,0.35,0.35,
 0.35,0.35,0.35,0.35,
 290.0,290.0,291.0,291.0,
 291.0,291.0,291.0,292.0,
 295.0,295.0,295.0,295.0,
 285.0,285.0,285.0,285.0,
 294.0,294.0,293.0,293.0,
 290.0,287.0,285.0,285.0,
 285.0,285.0,283.0,283.0,
 285.0,285.0,283.0,283.0,
 0.024,0.019,9.35E-07,8.1E-06,0.0,6.3,11,
 RESINIT,SOCINIT,NH4INIT,NO3INIT,NO2INIT,PHINIT,NODEIN
 -0.00034,-0.00027,0.0,0.0,0.0,0.0,0.0078,
 RESRATE,SOCRATE,N4RATE,NO3RATE,NO2RATE,PHRATE
 1,0.1, NAPPN,RED
 2,3.0,8,11,33300.0,41.0,
 APDAY,APPNA,APPNSRT,APPNEND,APPNRATE,NH4APPNRATE
 1200.0,9.0,0.017,6.6,7.7,6.5,7.0,
 APPNDEN,CNAPPN,NO3APPN,NTOTAPPN,PHAPPN,OMAPPN,DMAPPN
 0.001,0.001,3.5,3.5,0.0,45.19, ZH,ZM,ZT,ZU,D,LAT
 218,283.86,283.03,282.18,281.52,281.43,280.89,282.45,286.08,286,284.13,
 283.85,283.9,284.08,284.53,285.05,285.56,283.29,283.41,283.79,285.92,28
 6.88,287.07,286.61,286.56
 219,286.62,286.66,286.26,283.78,282.66,282.38,284.51,286.25,286.41,286.
 19,286.05,284.65,284.42,283.06,284.9,284,283.08,283.63,286.18,287.51,28
 8.24,288.14,288.67,289.28
 220,289.16,287.79,285.81,286.54,286.11,285.85,286.33,288.58,288.56,287.
 36,287.42,288.08,286.75,285.42,284.98,284.58,284.21,284.25,285.98,290.3
 3,289.2,288.94,288.75,288.13
 221,288.08,288.22,288.97,289.95,290.69,291.28,292.65,292.91,293.26,292.
 9,292.67,290.91,288.92,288.97,289.84,289.66,290.93,291.88,292.4,292.77,
 292.31,292.2,292.1,292.15
 222,292.26,292.1,292.05,291.81,291.1,291.52,292.97,294.1,293.7,294.13,2
 93.15,294.09,294.77,294.17,289.41,292.49,293.62,293.78,294.17,293.75,29
 2.84,292.04,291.7,291.55
 223,291.6,291.37,290.31,291.49,290.81,290.61,291.07,292.2,292.8,291.56,
 290.24,289.66,288.84,285.92,284.41,284.35,284.31,284.55,285.84,286.33,2
 86.33,288.47,288.2,286.61
 224,286.88,286.69,288,286.8,285.78,285.25,285.15,285.35,285.92,287.49,2
 88.76,290.32,292.13,292.57,291.03,291.39,291.76,290.36,290.99,291.84,29
 2.13,292.39,292.88,293.5
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 .13,285.5,285.36,285.69

229,285.8,286.15,287.51,287.22,287.25,286.54,285.19,282.59,280.82,280.4
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 230,279.228,278.692,277.551,278.887,279.007,279.716,281,281.94,279.842,
 278.932,278.798,279.127,279.027,279.207,279.116,278.604,279.338,280.56,
 281.55,280.96,281.49,281.21,282.09,281.6
 231,280.39,280.69,280.25,279.842,279.474,280.63,282.09,282.43,283.2,283
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 89.26,289.69,289.96,290.21
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 234,282.24,282.61,283.19,283.39,283.82,284.5,285,285.68,285.75,285.59,2
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 ,285.46,285.14,285.54,284.83
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 85.37,284.96,284.61,284.98
 218,287.81,286.98,285.82,285.83,284.39,284.29,285.73,292.22,293.67,295.
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 .28,294.62,293.6,292.9
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 ,298.58,296.86,296.11,295.79
 221,294.56,293.53,292.4,292.31,291,291.59,292.86,293.56,295.45,297.76,2
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 ,294.07,295.2,295.55,295.28,295.9,295.67,295.35,295.41,295.02,293.77,29
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 17
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 63
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 .27,4.009,4.479,4.111,2.577,3.259,3.413,2.84,2.53,0.924,0.623,0.893,0.5
 96
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 227,0.622,0.88,0.74,0.175,0.166,0.101,0.668,1.028,0.777,0.97,0.938,0.71
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 32

228,2.648,0.871,1.084,2.317,0.752,0.243,1.291,3.091,2.828,3.378,4.567,4
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 231,0.775,1.536,0.926,0.757,0.952,1.308,2.805,3.658,3.937,4.023,3.601,1
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 13
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 218,0,0,0,0,0,2.764,112.5,264.7,436.7,595.6,726,817,851,844,679.9,688.7
 ,553.2,379.5,207,21.95,0.495,0,0,0
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 ,131.1,36,59.69,19.11,0.081,0,0,0
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232,0,0,0,0,0,0,5.675,31.68,98.3,111.9,144.8,164.8,195.1,152,246.6,79,7
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 ,1,1,0.6
 236,0.6,0,0,0,0,0,0,0,0,0,0.4,0.4,0.4,0.4,0.6,0.6,0.6,0.6,0.6,0.4,0,0,0
 ,0
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 .6
 7, NWATER
 222,5
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 7.0,0.0,
 15.0,2.76,
 16.0,1.38,
 17.0,0.0,
 224,11,
 12.0,0.03,
 13.0,0.07,
 14.0,0.01,

15.0,0.09,
 16.0,0.02,
 17.0,0.0,
 18.0,0.13,
 19.0,0.09,
 20.0,0.0,
 21.0,0.01,
 22.0,0.0,
 225,2,
 4.0,0.01,
 5.0,0.0,
 226,5,
 5.0,0.04,
 6.0,0.0,
 7.0,0.03,
 8.0,0.01,
 9.0,0.0,
 231,8,
 10.0,0.02,
 11.0,0.6,
 12.0,0.11,
 13.0,0.07,
 14.0,0.17,
 15.0,0.25,
 16.0,0.08,
 17.0,0.0,
 232,6,
 1.0,0.02,
 2.0,0.18,
 3.0,0.01,
 4.0,0.13,
 5.0,0.01,
 6.0,0.0,
 233,3,
 7.0,0.23,
 8.0,0.15,
 9.0,0.0,

B.4: exappn.inp

exappn.inp: example application over growing season for dairy cattle
 slurry applied to bare loam soil

0,1,1,0,1,	IPLANT, ITRACE, IAPPN, IRES, ITILL
304,121,	IFDEND, IDTBEG
1,1.0e-010,1.0,0.004,	INMAX, DMAXBA, DELMAX, DELMIN
1,0,1,1000.0,	ICLOUD, IRAD, ISOL, DMAXHE
32,	NPT
0.0,0.1,0.2,0.3,	
0.5,0.7,0.9,1.0,	
2.5,4.0,5.0,7.5,	
9.5,12.0,14.5,17.0,	

129,277.56,276.56,276.26,275.96,276.46,276.26,277.36,277.56,277.96,279.
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 130,281.76,281.56,281.76,281.76,281.56,281.86,282.46,283.16,283.96,284.
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 131,281.26,282.06,284.46,286.66,285.86,285.56,285.86,286.06,287.16,287.
 66,287.76,288.66,287.76,287.46,287.16,283.76,280.76,279.16,277.66,276.0
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 132,270.26,269.16,267.76,265.46,264.16,264.06,263.66,263.46,263.66,263.
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 6,269.56,269.16,270.86,272.36
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 36,276.46,276.36,276.06,275.66,274.96,275.76,278.76,277.36,277.36,277.1
 6,276.86,276.66,275.86,275.76
 137,275.26,274.26,274.26,274.06,275.36,274.46,275.56,276.46,275.86,275.
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 96,279.06,279.26,280.06,280.96,280.66,280.96,280.56,280.66,280.46,280.9
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 145,278.16,278.36,277.76,277.86,277.86,278.06,277.56,276.96,276.26,275.
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 6,274.36,273.96,273.26,278.26
 146,274.46,274.46,274.86,274.86,274.86,275.26,275.46,274.06,275.56,278.
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[illegible]

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