Modelling Soil Organic Matter Dynamics – Global Challenges

K. PAUSTIAN

Natural Resource Ecology Laboratory, Colorado State University, Ft Collins, CO 80523, USA

Introduction

Soil organic matter (SOM) modelling is gaining recognition as a key part of efforts better to understand, and manage, the terrestrial carbon cycle. The influence of the terrestrial carbon cycle on greenhouse gas emissions and uptake, and the potential feedbacks on long-term climatic change, have become front page news. Major questions with far-reaching societal impacts include: what is the current role of soils as a source/sink for increased atmospheric CO_2 ?; will climate change increase CO_2 emissions from soil, resulting in a positive feedback to drive global warming?; and can soils be managed effectively to mitigate increased greenhouse gas loading? Answers to these questions require the application of models to quantify and predict SOM dynamics as a function of environmental factors and human management. Consequently, SOM modelling has played a prominent role in much of the recent research on climate change and the global carbon cycle (e.g. King *et al.*, 1997; Field and Fung, 1999; Schimel *et al.*, 2000).

The requirements for an accurate accounting of greenhouse gas emissions and sinks is central to the UN Framework Convention on Climate Change (FCCC) which requires national reporting of all major sources and sinks, including soils. Modelling will play a key role in integrating the variability and dynamics of soils, climate, topography and land use (as they affect SOM) to provide national estimates of soil C stock changes (e.g. Eve *et al.*, 2000; Tate *et al.*, 2000). SOM models have been used to estimate the potential for soils to sequester carbon and thus mitigate

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 CO_2 increases at national and regional levels (Dumanski *et al.*, 1997; Smith *et al.*, 1997a). If soil sinks are included under the Kyoto protocol, methods to quantify and verify changes in soil C at local, regional and national levels will be required. The potential for national and international trading of carbon emission offsets, making soil carbon a commodity, will necessitate that carbon changes be quantified to known levels of uncertainty. SOM modelling can play a central role in such quantification systems, but it will require a new level of integration with field measurements and other data on environmental and management factors.

Several of the SOM models currently in use today were first developed in the late 1970s and early 1980s (e.g. Jenkinson and Rayner, 1977; Parton *et al.*, 1983). Since then, many new models have been developed (see reviews by Jenkinson, 1990; Paustian, 1994; McGill, 1996) and older models have continued to evolve on a more or less continuous basis. Despite their diversity, most of these models share some basic assumptions which include the representation of SOM as multiple pools (or as a quality spectrum) with differing inherent decomposition rates, governed by first-order rate constants modified by climatic and edaphic (e.g. soil physical attributes) reduction factors. Most of these models were conceived originally to describe processes at the ecosystem or field scale. New approaches continue to be explored, and some of the major recent trends in SOM modelling and their application to environmental problems will be discussed below.

Collaborative Networks

A significant recent development in SOM modelling has been the increased level of formal and informal collaborations between different modelling groups and between modellers and experimental scientists. Whether this has occurred as a result of the greater international collaboration spurred by global change research, or simply as a result of increasing ease of communication and the maturation of the science, is perhaps not important. Whatever the case, such collaboration has facilitated the comparison and evaluation of different models and approaches, such as a recent workshop in which a number of SOM models from around the world were brought together and evaluated using a common set of long-term experimental data from a variety of climatic, soil and land use conditions (Powlson et al., 1996; Smith et al., 1997b). Such comparisons help to clearly identify the difference in structure and assumptions of existing models (Paustian, 1994; McGill, 1996) and their relative strengths and weaknesses for a particular set of circumstances. These developments mirror similar recent efforts to conduct cross-model evaluations for water quality modelling, trace gas modelling and general circulation climate modelling, to name a few examples.

Long-term field experiments have been a mainstay for the development and evaluation of soil organic matter models (Powlson, 1996). Since soil organic matter levels change relatively slowly against a large and variable background level, long-term experiments with well-documented management histories are well suited to elicit and detect changes. Many SOM models originally were developed and tested using such experiments, but often for a restricted set of ecosystem, soil or climate conditions. However, with the increased use of models for regional, national and even global applications, testing of models to determine their generality (or lack thereof) over the entire domain of their application becomes crucial. This is particularly true given that these models are used increasingly for predictive purposes to guide policy-making and management decisions. The recent compilation of many of the long-term experiment data sets for the US and Canada (Paul et al., 1997) and Europe (Powlson et al., 1998) have helped to address this need by providing data, in standardized formats, which can be used to test and validate models for broad geographic regions and multiple types of land use, management, soil and climate conditions. A formal network of global metadata, describing both long-term experimental data and SOM models, SOMNET, has been established to facilitate collaboration between modellers and data holders (Smith et al., 1997c). Further expansion of such networks and compilation of other networked field data, such as long-term ecosystem C flux estimates, will play an important role in continued improvements in our models.

Measurement and Modelling Integration

A recurrent theme in discussions about the state-of-the-art of SOM modelling is the disparity between modelled pools and analytical SOM fractions measured in the laboratory. Most models represent the heterogeneity of SOM by defining several pools, typically 3–5, each with a characteristic specific decay rate or mean residence time, usually assuming first-order kinetics (i.e. constant proportional mass loss per unit time) (see reviews by Paustian, 1994; McGill, 1996). As fresh residues and SOM fractions decompose, a portion of the residual products is more resistant to further decay, which is represented by transfers to more slowly decomposing pools, in a decomposition cascade (see Swift *et al.*, 1979). Alternatively, specific decomposition rate can be made a function of a continuous SOM quality spectrum, which varies according to characteristics of the plant residues and the duration of decay (e.g. Bosatta and Agren, 1996). In either case, the representation of the model pools (or quality spectrum) is primarily conceptual in nature.

The sum of model pools is equal to the total organic carbon, a measurable and unambiguous quantity. However, individual pools generally are only loosely associated with measurable quantities obtained through existing chemical and/or physical fractionations performed in the laboratory. Consequently, it is not possible to falsify the internal dynamics of SOM models with conceptual pool definitions via a direct comparison to measured pool changes. Thus, a closer linkage between theoretical and analytical representations of SOM heterogeneity can be advanced through revising model definitions to coincide with measurable quantities or by devising more functional laboratory fractionation procedures, or both. The phrase 'modelling the measurable or measuring the modellable' has been coined as representing the two approaches towards a closer reconciliation between theoretical and experimental work on SOM (Christensen, 1996; Elliott *et al.*, 1996).

Various attempts have been made to correlate laboratory fractions with model pool definitions and to devise more general guidelines for initializing the soil organic matter pools as defined in existing models. For example, Motavalli et al. (1994) compared laboratory measurements of C mineralization with simulations by the Century model (Parton et al., 1994) for several tropical soils. When the active and slow pools in the model were initialized using laboratory determinations of microbial + soluble C for the active pool and light fraction for the slow pool, C mineralization was consistently underestimated, although all fractions were highly significantly correlated to C mineralization in a regression analysis. In contrast, using the standard procedure for internally initializing model pools, by running the model to equilibrium with estimated climate and primary productivity driving variables, provided the best fit to measured C mineralization. Similarly, Magid et al. (1997) tested the DAISY model using field measurements of litter decomposition, soil microbial biomass and particulate organic matter (POM), and endeavoured to 'measure the modellable' ' by relating the analytical fractions and residue quality indices to model pools. They concluded 'there is no firm relationship between the standard set of measurable quality parameters of the added plant materials and an adequate parameterization of the model.' Standard measures of residue quality such as lignin/N ratios and water-soluble/insoluble fractions were not able to account for the initial N dynamics during decomposition.

An alternative approach to modelling the measurable has been proposed by Arah (2000) and others (see Gaunt *et al.*, Chapter 2.6) using analytically defined pools and measurement of ¹³C and ¹⁵N stable isotope tracers to derive parameters in the model. The approach considers all possible transformations between measured C and N pools and devises a system of equations using observed changes in total C and N and ¹³C and ¹⁵N for each fraction to solve all model unknowns. Necessary requirements of such an approach are that the analytical fractions are distinct and together account for the total carbon inventory. It must also be parsimonious (no more than 4–5 pools each for C and N) such that the model is sufficiently constrained to solve for parameter values (Arah, 2000).

Collins *et al.* (2000) used C mineralization data, total C and acid hydrolysis to estimate amounts and turnover rates for a three-pool model (representing active, slow and passive fractions) for five long-term experiments in central USA. They demonstrated that the amount of crop-derived carbon, determined from field sampling and ¹³C natural abundance methods, was well correlated with the mean residence time of the slow pool determined from laboratory fractionations. The relationship was consistent across soil depth increments (up to 1 m) within sites, but differed distinctly between forest- and prairie-derived soils.

For both approaches, measuring the modellable or modelling the measurable, the derivation and testing of SOM models has benefited substantially from the increased application of isotopic methods, particularly the use of the stable isotopes ¹³C and ¹⁵N and radioactive ¹⁴C. Isotope dynamics can be coded explicitly into models, including appropriate isotope discrimination coefficients. In particular, the use of natural abundance ¹³C has been valuable in quantifying SOM dynamics following land use change or changes in agricultural management (e.g. Balesdent et al. 1987; Six et al., 1998; Collins et al., 2000). The method relies on the difference in ¹³C natural abundance between plants with different photosynthetic pathways (usually contrasting C₃ versus C₄ plants) so that the relative mix of SOM derived from a particular vegetation can be quantified. Thus, where land use changes have occurred at a known point in time, for example C_3 forest conversion to C_4 cropland, the rate of loss of the original forest-derived SOM and the contribution of new crop-derived SOM can be inferred from changes in the ¹³C signature of the soil. The approach can be extended to make inferences about the dynamics of SOM isolates as well as whole soil. Since land use or management changes involving shifts in major vegetation types are relatively widespread and occur in nearly all types of climatic and soil conditions, the approach is well suited for testing models for general use and regional applications. However, the inferences based on stable isotope data introduce additional sources of variability and error that need to be accounted for (Veldkamp and Weitz, 1994), and accurate measures of pre-disturbance soils and the amount and type of post-disturbance plant residue inputs are required.

Radiocarbon dating of SOM and tracer methods utilizing the ¹⁴C enrichment from above-ground bomb testing have been utilized in conjunction with simulation modelling of SOM dynamics (e.g. Jenkinson *et al.*, 1987; Trumbore *et al.*, 1995), although to a lesser extent than ¹³C, due in part to the greater expense and more limited availability of ¹⁴C analysis facilities. Radiocarbon dating of SOM and SOM fractions has had a major role in the definition of recalcitrant pools in SOM models (Falloon and Smith, 2000). Initialization of the inert pool fraction in the Roth-C model is

based explicitly on ¹⁴C carbon dating, and default estimation procedures have been published by Falloon *et al.* (1998a). The inclusion of a small (~5–10% of total C), totally inert, and very old SOM fraction in the Roth-C model was based on the need to reconcile the radiocarbon age of the soil with rates of SOM turnover inferred from bomb-C measurements. In analysing ¹⁴C dynamics for a tropical and temperate soil, Trumbore (1993) concluded that the temperate soil was best represented by a relatively even distribution of organic matter in active, slow and passive pools while the tropical soil was best represented as comprised of mostly actively cycling carbon with a small, very recalcitrant pool.

Seeking a closer correspondence between theoretical and measurable fractions will continue to be a major thrust of SOM research. It should be realized that both theoretical and measurement-based depictions of SOM components are, in essence, 'models', i.e. abstractions and simplifications of reality. As new analytical procedures are developed that give functionally meaningful results, with consistent and repeatable patterns, they will doubtless influence the definition of modelled pools. Similarly, the expanded use of isotopic tracers and the availability of a richer set of field experiments will allow more robust and constrained testing of conceptually based models.

Regional Applications

Climate change issues, specifically questions about: (i) the role of soil carbon as a potential part of the 'missing' terrestrial carbon sink; (ii) climate change impact studies; (iii) the need to quantify the emissions/sinks of CO_2 from soils as part of national greenhouse gas inventories; and (iv) interest in the potential of soil C sequestration as a greenhouse gas mitigation option have helped spur the development and application of SOM modelling systems at regional and global levels (e.g. Burke et al., 1991; Donigian et al., 1994; King et al., 1997; Falloon et al., 1998b; Paustian et al., 2000; Schimel et al., 2000). The approaches used are similar in most cases and rely on the linkage of simulation models with geographically distributed databases, typically maintained in geographic information systems (GIS) which contain model-driving variables and initial conditions (i.e. inputs) and help to manage and display model output (Fig. 2.1). Typically, model-driving variables (i.e. climate, soils, vegetation and land use) define a unit area of land, or polygon, having a unique combination of driving variables to which the model is applied. Approaches vary in the spatial and temporal resolution employed, the degree to which sub-polygon distributions of soil, vegetation and land use are represented, the source of the input data and the model being used. Such approaches have enabled information and understanding of SOM, originally derived at the field level, to be scaled up



Fig. 2.1. Structure for regional modelling and integrated assessment of SOM dynamics. Ecosystem/SOM models, based on fundamental process studies, are driven by spatially distributed databases of driving variables and validated by regional networks of long-term experimental sites. For climate change impact assessment, climate models provide projected climatic driving variables for the region. Economic decisions influence the type and distribution of management systems, and the ecosystem responses to changes in management and climate provide a feedback to economic and management decision models.

to encompass geographic and political units which are relevant to decision and policy makers.

However, significant challenges remain, particularly considering the potential impact of decisions based on these types of applications. A number of authors (e.g. Elliott and Cole, 1989; Paustian et al., 1995; Powlson, 1996) have emphasized the importance of linking such applications to regionally distributed experimental databases for model validation purposes, as described earlier in this chapter. As of yet, there are few studies that have examined the influence of spatial and temporal scale on model predictions at the regional scale. Depending on the properties of the driving variables and the model functions that utilize them, aggregation errors may be more or less severe, depending on the linearity of their scaling properties (Paustian et al., 1997). Similarly, there is a need to develop and apply formalized methods for uncertainty analysis of regionalized SOM models, including differentiating between uncertainty associated with input data and uncertainty in model predictions. Decision-makers utilizing the information generated by regional modelling systems will accept uncertainty as long as they have an idea as to the degree of uncertainty and that the estimates are unbiased.

In intensively managed ecosystems, such as agriculture, management decisions by farmers have a profound influence on the structure and functioning of the ecosystem, including the amount and dynamics of soil organic matter (Antle, 1996). Management practices are to a large degree driven by economic factors. Thus, the feedbacks and interactions between biophysical and economic components that govern the larger humandominated ecosystem are fundamental to predicting potential changes in soil C amounts and dynamics. This is particularly true for assessing the potential outcome of greenhouse gas mitigation policies in which changes in soil C and other soil-derived greenhouse gases will have a direct effect on farm income. However, it is equally true for assessing the effects on soil C of climate change or other changes in policies or economics to which farmers respond. Understanding regional soil organic matter dynamics, as driven by economically based management decisions, will require a whole-ecosystem approach where the interactions between SOM, crop yields, economic returns and subsequent changes in management feedback to determine SOM and crop responses (Fig. 2.1). Integrating SOM models into such systems will provide valuable tools to guide policy and decision-making on many of the pressing environmental issues facing society.

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Soil Organic Matter 2.1 Sustainability and Agricultural Management – Predictions at the Regional Level

P.D. FALLOON¹, P. SMITH¹, J. SZABO², L. PASZTOR², J.U. SMITH¹, K. COLEMAN¹ AND S. MARSHALL³

¹Soil Science Department, IACR-Rothamsted, Harpenden, Hertfordshire AL5 2JQ, UK; ²GIS Laboratory of RISSAC, RISSAC, Herman Otto Utca 15, Budapest 1022, Hungary; and ³School of Biology, University of Nottingham, Sutton Bonnington Campus, Loughborough, Leicestershire LE12 5RD, UK

Introduction

In Europe, the potential for carbon sequestration from various changes in land management has previously been estimated using data from the Global Change and Terrestrial Ecosystems Soil Organic Matter Network (GCTE-SOMNET; Smith et al., 1996). Linear relationships between management practices and yearly changes in soil organic carbon were developed and used to estimate changes in the total carbon stock of European soils (Smith et al., 1997a,b, 1998, 2000a,b). To refine these semi-quantitative estimates, the local soil type, meteorological conditions and land use must also be taken into account. We previously have used the Rothamsted carbon model (Roth-C) linked to geographical information systems (GIS) to estimate the potential effects of afforestation on soil carbon stocks in central Hungary (Falloon et al., 1998). Further developments have involved a combined modelling approach. Our new approach is based on the CENTURY model frame and allows either the Roth-C or CENTURY soil organic matter (SOM) decomposition model to be used (Falloon et al., 1999, 2000). This allows an equal comparison of the models. The GIS-linked system integrates land use, soil and weather data with knowledge of land use history, net primary production, local agricultural practices and best estimates of the current soil organic carbon (SOC) stock.

In this chapter, we describe how these developments can be used to estimate SOM sustainability and carbon sequestration at the regional level using a dynamic simulation model linked to spatially explicit data, and show results of carbon sequestration potential estimated with a simple regression-based approach. We demonstrate the system in use for an area of central Hungary.

Methods

Our case study area (24,804 km²) in central Hungary and GIS data sets have been described in detail elsewhere (Falloon *et al.*, 1998, 2000). Here, we describe the use of the IGATE system (Fig 2.1.1; Falloon *et al.*, 2000) to compare C sequestration estimates using the Roth-C (Coleman and Jenkinson, 1996) and CENTURY (Parton *et al.*, 1988) models with estimates using simple linear regressions (Smith *et al.*, 1997a,b, 1998, 2000a,b).

The CENTURY model was validated and calibrated using 17 data sets from the GCTE-SOMNET database (Smith *et al.*, 1996) and the IBP woodlands data set (DeAngelis *et al.*, 1981). To compare the models at the regional scale, we initialized the models by running for 3000 years under native vegetation (forest: Marton *et al.*, 1989) and then 500 years of current land use. We then ran a demonstration scenario of afforestation of all arable land to (i) show the maximum possible increase in SOC stocks; and (ii) highlight the largest differences between model estimates. We used the regressions of Smith *et al.* (1997a,b, 1998, 1999a,b) to estimate changes in regional SOC stocks under the six scenarios given in Table 2.1.1, all applied to all arable land. We calculated annual CO₂ emissions offsets using 1990 national data from Marland *et al.* (1999), and scaled this to our



Fig. 2.1.1. IGATE system.

	Regression		Roth-C model		CENTURY model	
Scenario	SOC change, Tg	% annual emissions offset	SOC change, Tg	% annual emissions offset	SOC change, Tg	% annual emissions offset
Afforestation	101.8	21.66	37.00	8.00	55.00	12.00
No till	44.77	9.52	_	_	_	_
Organic manures ^a	20.00	4.26	_	_	_	_
Sewage sludge ^b	131.25	27.93	_	_	_	_
Cereal straw ^c	46.44	9.88	_	_	_	_
Ley-arable ^d	62.55	13.31	_	_	_	_

 Table 2.1.1.
 Changes in SOC stocks and CO₂ emissions offsets for the area of central Hungary.

All scenarios applied to all arable land. Annual application rates: ^a10 t ha⁻¹; ^b2.59 t ha⁻¹; ^c5.07 t ha⁻¹; ^d30% ley arable rotation.

study area. We used 1990 CO_2 emissions since 1990 is the Kyoto protocol baseline.

Finally, we investigated the sustainability of SOC stocks for a typical arable polygon of the case study area in our GIS database using the CENTURY model. We ran the model for 3000 years under native forest, then 350 years extensive arable agriculture and 100 years (1860–1960) intensive arable agriculture with the inorganic N fertilization rate set at 1960 levels (the earliest statistic from FAOSTAT, 1999). From 1960 to the present day, the model was run under intensive arable agriculture with annual N application rates set from FAOSTAT, and finally for a 100 year scenario of intensive arable agriculture with N application rates at the current level.

Results and Discussion

There was good agreement between measured and simulated SOC levels at the validation sites ($r^2 = 0.83$). The results of the model comparison and the regression estimates for the various scenarios are given in Table 2.1.1. For our demonstration scenario of afforestation of all arable land, SOC changes predicted using the regression method are significantly greater than those predicted using the Roth-C or CENTURY models, and the CENTURY model predicts a greater C sequestration estimate than Roth-C. Although some of these scenarios are unrealistic and require refinement for the study area, the magnitude of CO₂ emissions offsets indicated is encouraging.

Figure 2.1.2 shows the dynamics of SOC predicted by the CENTURY model for our investigation of SOC stock sustainability. Under native forest



Fig. 2.1.2. Historic-future SOC dynamics using fertilizer statistics (CENTURY model).

vegetation, the SOC content of the soil reached a high, steady state. Upon conversion to extensive arable agriculture, there was a steady loss of SOC. On conversion to a more intensive arable system, with a low level of N application, there was a rapid loss of SOC, which recovered following the high N application rates during the 1970s. Despite the drop in N application rates after 1990, assuming that current N application rates continue for 100 years, the model predicted a recovery and stabilization of SOC stocks. We assumed that current N application rates continue into the future since no projected figures were available. We remain uncertain regarding the sustainability of current SOC, due to the limited information on historical land use and management.

In conclusion, we have shown that different methods for estimating changes in regional SOC stocks can produce quite different results. There may be several reasons for the differences between SOC stock estimates obtained using the regressions CENTURY and Roth-C. The regression-based estimates are generalizations of data from European long-term experiments, on specific soil types and with specific cropping regimes. Reasons for differences in carbon changes resulting from the actual management scenarios investigated here have been discussed in detail by Smith *et al.* (1997a,b, 1998, 2000a,b). The long-term data sets used in the regression-based approach may not be specific to central Hungarian soil, climatic and management conditions. The dynamic modelling approaches do, however, account for local soil type, weather and management conditions, and hence we would expect different (and more site-specific) results. We would also expect different results from the two models (CENTURY and Roth-C), since they have different structures, pool sizes and turnover

times. More information is needed on historical land use and practices to allow estimates of the sustainability of current agricultural practices with regard to SOC stocks.

Acknowledgements

We would like to thank György Várallyay, Péter Csathó and Tamás Németh (RISSAC, Hungary) for assisting with input data and site information, Dr Keith Paustian and Robin Kelly (Colorado State University, USA) for advice on the CENTURY model, Dr R. Webster (IACR-Rothamsted, UK) and Professor David Jenkinson (IACR-Rothamsted, UK) for assistance with the Roth-C model and general advice. This work contributes to: the UK-BBSRC-ASD Project 'Modelling SOM Dynamics using SOMNET' (Grant: 206/A 06371) and the EU project Low Input Agriculture and Soil Sustainability in Eastern Europe (Grant: EU-COPERNICUS PL97 1006). IACR receives grant-aided support from the Biotechnology and Biological Sciences Research Council of the UK.

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Modelling of Carbon Dynamics 2.2 in a Rural Area of Central Germany

U. FRANKO AND S. SCHENK

UFZ Centre for Environmental Research, Leipzig-Halle, Germany

Introduction

Soil organic matter (SOM) is a very important component of agroecosystems. Biological, chemical and physical soil properties are strongly correlated with the carbon content of the soil, which is the usual indicator for SOM. It is very important to distinguish between the inert and the decomposable part of SOM. Turnover processes of this decomposable SOM lead to a more or less continuous flowing stream of nitrogen and other nutrients in soil. SOM changes are very slow and poorly indicated by measurements. Modelling may give faster results about the directions and amounts of soil organic matter change in the future. This chapter presents the results of a study in the Chernozem region of central Germany on the consequences of land use change for organic matter cycling and SOM dynamics.

Model and Database

The CANDY system integrates a simulation model and a database of parameters, measurement values, initial values, weather data and management data. The user interface not only provides the function for simulation control but also tools for parameter estimation, risk analysis and recommendation for fertilizer application. The simulation model works on a daily time step with modules for calculation of soil temperature, moisture content, the processes of the soil carbon–nitrogen cycle and pesticide dynamics. The model is integrated in a geographic information systems (GIS)/database environment in order to obtain inputs on weather, soil physics and agricultural management on a regional scale. A more detailed description of the construction and evaluation results of the CANDY model has been published (Franko 1996; Franko *et al.*, 1997).

A landscape unit is considered as a composition of homogeneous patches that are independent from each other with regard to the processes in the soil. The construction of the homogeneous patches is a result of an overlay of a soil map with a map of the farm fields and a map of precipitation patterns. It is very useful to use identical shapes for farm fields and precipitation patterns in order to reduce the number of patches to a reasonable level. The soil map and the farm field map as well as the map of climate structure have a database background with detailed information.

The soil mapping units are characterized by a list of soil profiles, weighted by their part in the whole area of the item. A soil profile description contains a list of horizons with their depths. The soil physical parameters of density, texture, field capacity and wilting point are assigned to each horizon.

Climatic data include air temperature, global radiation and precipitation provided by a station situated nearby. A precipitation index has been calculated for every farm field from long-term averages of regional precipitation distribution expressing the relationship of precipitation intensity between a given point in the area and the position of the climate station. During the simulation runs, this index is used in order to adapt the local precipitation data.

Farm field management is described by a date, an action, a specification and an intensity. Actions are cropping, tillage, application of fertilizer, manure or pesticides, and irrigation. Cropping data have to include the yield and/or the nitrogen uptake of the crop at harvest.

Investigation Area and Simulation Scenario

The study was performed on an area of 3850 ha of arable land on Haplic Chernozem with loess as parent material. The water-holding capacity of the upper 100 cm is ~310 mm, with 190 mm available to plants. Clay content varies between 18 and 20%. Long-term averages of air temperature and annual precipitation are 8.7° C and 520-560 mm, respectively.

Land use data for every farm field were collected for a time period from 1981 to 1996. With the re-unification of Germany, there were changes in the agriculture of Eastern Germany concerning setaside of land, reduction of animal breeding, crop rotations and yields because of improved agrochemicals and technology. An important question is how this change in land use will affect the SOM dynamics. The land use change in the investigation area is characterized by a decrease of area for root crops from 24 to 13% which is now used for oilseed rape, sunflower and as setaside land. Two percent of the former cereal area (now 60%) is now used for legume crops. The yield has increased for winter wheat from 0.64 kg m⁻² in the 1980s to 0.73 kg m⁻² in the 1990s and for sugar beet from 3.5 to 5.2 kg m^{-2} .

The simulated scenario starts in August 1980. Observed values for the required initial conditions of the model were not available. The initial content of SOM was calculated using site-specific statistical information about yields and animal concentration before 1981 assuming an even application of the organic inputs and that the organic matter content had reached a steady state. Parameters and algorithms of the necessary calculations have been published (Franko, 1997). Initial soil water content was assumed to be 60% of field capacity, and soil mineral nitrogen has been assigned according to internal standard parameters of the model that are related to the different soil units.

Evaluation of Soil Organic Matter Level

It is known from long-term experiments that land use is only responsible for changes in the decomposable part of SOM whereas the inert SOM is dependent of the site conditions. Therefore, the evaluation is restricted to the decomposable SOM pool. Recently published results of Körschens (1999) show that the effect of SOM on yield is limited to a certain level and that in different long-term experiments a SOM range of ~0.14-0.51% of decomposable carbon provides the best conditions for high-quality yields.

Could higher inputs of organic material to the soil and the subsequent increase in the carbon storage in the soil be of benefit for the global carbon cycle? A simple calculation shows that there are better solutions for the reduction of carbon dioxide emissions. Under the conditions of Chernozem in central Germany, an additional straw input of 400 g m⁻² per year will eventually lead to an increase in the SOM carbon of ~ 1.2 kg m⁻² with a maximum rate of 60 g m⁻² year⁻¹. This rate decreases with time because of the remineralization of the newly formed SOM. It takes ~100 years to reach the final level. Afterwards, no further increase will occur. At this steady state, the total input is equal to the mineralization. However, the same amount of straw can be used as an energy source in order to replace fossil fuels. The energy equivalent of 400 g of straw is ~5.6 MJ (Brenndörfer et al., 1994) – an amount equivalent to the energy gain from ~120 g of carbon in fossil fuels. This is twice as high than the maximum accumulation rate in SOM. Because of its regenerative character, the consumption of the straw as an energy source will relieve the global carbon balance per square metre of ~ 12 kg within 100 years, which is ten times better then the sequestration of carbon in soil.

The range of optimal content of decomposable carbon, published by Körschens (1999), shows a tendency for higher values in soils with a lower turnover activity. This leads to the assumption that the turnover rate of SOM could be a good indicator for SOM management. This is also reasonable because an increase in the SOM level increases the nitrogen mineralization and could also increase the nitrogen surplus. Results from the long-term experiment at Bad Lauchstädt (Körschens *et al.*, 1994) suggest that the optimal SOM level for nitrate recovery is 1.97% C_{org} (Fig. 2.2.1), which is equivalent to a decomposable carbon content of 0.42% and an annual carbon turnover of ~90 g m⁻². Using these values as a benchmark, possible ranges for the evaluation of the SOM level are presented in Table 2.2.1.

Results and Discussion

The steady increase in yields – especially after 1989 when agricultural technology improved very rapidly – leads to a continuous increase in SOM with some fluctuations due to yield decreases in years with very low precipitation



Fig. 2.2.1. Efficiency of the nitrogen usage (N_{eff}) as the relationship between N uptake and N input from mineral fertilizer and manure for 16 different treatments of the Bad Lauchstädt long-term experiment in term of dependence on the corresponding content of soil organic carbon (C_{org}). Data after Körschens *et al.* (1994).

(Fig. 2.2.2). Using the amount of decomposable SOM as an indicator, > 90% of the area is now at an optimal SOM level, and < 5% is classified as 'low' or 'high'. It is obvious that the system has not reached a steady state. Despite some decreasing trends, most of the area shows a carbon accumulation. Because of the very slow reaction time of SOM, it would be more informative to evaluate the carbon input rates in order to predict the future prospects. Taking the input rates of carbon reproducing SOM (C_{rep}) from 1993 to 1996 as an indicator, a large area has to be classified as 'very high' in terms of supply of SOM (Fig. 2.2.3).

Despite the temporary very high contents of mineral nitrogen in the soil (> 20 g m⁻²), the percolation water leaving the rooting zone meets the quality conditions for drinking water. The total nitrogen export (leaching plus gaseous losses) amounts to $4.4 \text{ g m}^{-2} \text{ year}^{-1}$ and is lower than the nitrogen import from the air which is assumed to be ~6 g m⁻² year⁻¹.

If the trend of carbon accumulation continues, a reduced nitrogen efficiency is to be expected, with subsequent increasing export of nitrogen

Table 2.2.1. Classification of the SOM content (SOM level) in terms of soil organic carbon (C_{org}), decomposable carbon (C_{dec}) and soil organic carbon reproduction rates (C_{rep}) relative to the efficiency of the nitrogen input (N efficiency) for a Haplic Chernozem in central Germany.

SOM level	N efficiency	C _{org} (%)	C _{dec} (kg m ⁻²)	C _{rep} (g m ⁻² year ⁻¹)
Very low	< 1.50	< 1.80	< 1.45	< 60
Low	1.50-1.58	1.80–1.91	1.45-1.95	60-80
Normal	> 1.58	1.91–2.03	1.95–2.45	80-100
High	1.58-1.50	2.03-2.15	2.45-2.95	100-120
Very high	< 1.50	> 2.15	> 2.95	> 120



Fig. 2.2.2. Regional average of decomposable carbon in soil.



Fig. 2.2.3. Regional classification of the SOM level according to the average carbon input.

into the environment. In order to avoid this risk and to keep the system at an optimal SOM level, it is necessary to find new solutions for organic material management that guarantee an equal distribution of the required carbon combined with an energetic usage of the surplus.

Conclusions

Model outputs show an increase in carbon storage in the soil of the investigated area due to higher inputs of organic material. Under the current conditions, the nitrogen export into the environment is lower than the nitrogen import from the atmosphere. Results of the long-term experiment at Bad Lauchstädt indicate an optimal rate of SOM turnover of ~90 g m⁻². Using this as the indicator for the evaluation of the carbon dynamics in the investigation area, a surplus of organic matter can be found that could cause an increase in nitrate exports into the environment. Surplus of organic matter could be used better for the replacement of fossil fuels in order to reduce the carbon dioxide output to the atmosphere.

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Modelling Variation in C and
N Loss and Effects on N2.3Mineralization After Grassland
Ploughing Over a Catchment1

G.M. RICHTER, G. TUCK AND J.U. SMITH

Soil Science Department, IACR-Rothamsted, Harpenden, Hertfordshire AL5 2JQ, UK

Introduction

Ploughing grassland has a great impact on organic carbon (Corg) and nitrogen (Nt) turnover, and related budgets vary considerably. Expressed as relative total N content, its decline after grassland ploughing can be approximated by a unique exponential decay function. As a generalization, 50-60% of initial nitrogen will remain under long-term arable land use (Voroney et al., 1981; Johnston et al., 1994) for loamy grassland soils. Difficulties arise for regional quantitative analysis, since long-term observations are missing, and initial values are often unknown on the landscape scale. 'Snap-shots' of the current status for soil organic matter (SOM) combine spatial and temporal variation reflecting physicochemical properties of soils and differences in management. Variable soil physical and hydrological properties may have caused enrichment and differences in the chemistry of SOM. One question is whether equilibrium C and N contents of arable soils will be reached within a period meaningful for farm management (a decade or a generation). Models, which describe the underlying dynamics as a function of soil, climate and management variables, may be able to explain the observed variability. As a first step, we attempt here to simulate SOM dynamics following ploughing up of grassland using a standard arable model (SUNDIAL) with modifications only to the soil carbon parameters as measured. These early predictions will be compared with SOM N fractions and N mineralization measurements.

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Materials and Methods

Soil samples of the A horizon were collected on several arable sites in two German catchments. They represent a series characterized by variable time elapsed since grassland ploughing (GP, 1–33 years), soil texture (sandy loam–clay loam) and SOM (h2–h4) class. Arable (A) sites were assumed to be under cultivation for at least 115 years, setting the long-term equilibrium content (Y[A]). C_{org} and N_t (Kjeldahl) were measured by dry combustion. Assuming a ploughing depth of 0.25 m and a uniform dry bulk density of the soil (1.5 g cm⁻³), the storage of C and N in the GP soils ranged from 200 to 90 t C ha⁻¹ and 18 to 7 t N ha⁻¹, actually representing two different SOM classes. The decomposable and recalcitrant fractions of potentially mineralizable N (N₀ = N_{dpm} + N_{rpm}) were determined by incubation (Richter *et al.*, 1989). A sub-sample was used to estimate carbon and nitrogen in the microbial biomass (C_{mic}, N_{mic}) by chloroform fumigation extraction (CFE; Brookes *et al.*, 1985; Vance *et al.*, 1987).

Modelling

Two approaches were used to explain the dynamics of SOM fractions after grassland ploughing in the sub-samples of sandy and clay loam. A static model (Equation 1) was used to quantify the total amount of C, N and N₀ in SOM derived from grassland (Y[G]) at any time (t_{GPA} , years) under arable cultivation before reaching an equilibrium content (Y[A]). The half-life, $t_{1/2}$, is estimated from the rate constant k (Equation 2).

$$Y = Y[A] + Y[G] \times \exp(-k \times t_{\text{GPA}})$$
(1)

$$t_{\frac{1}{2}} = \ln \frac{2}{k} \tag{2}$$

The dynamic model SUNDIAL was chosen, which is based on the Rothamsted carbon model (Roth-C; Jenkinson and Coleman, 1994) extended to include N turnover (Bradbury *et al.*, 1993). As major inputs, the model considers C and N from fertilizer (mineral and organic) and crops (stubble + straw and debris), which are partitioned between mineral (CO₂, NH₄ and NO₃) and organic pools (humus and microbial biomass) in the soil. Mineralization and immobilization of N due to decomposition of crop residues, biomass and humus are calculated from the C/N ratio of the decomposing material on a weekly basis. For the simulations of C and N turnover after grassland ploughing, humus C and fraction of microbial biomass C (C_{mic}/C_{act}) were initialized according to measurements in single samples of loam soils (Widmer, 1993; Table 2.3.1). The fraction of C_{mic} was changed in the range of low (0.028; arable) to high (0.046) to account for different mixing ratios (ploughing depth, sod depth and litter incorporation). Absolute values for C_{mic} were high compared with other locations

Management/soil type	Humus C (t ha ⁻¹)	Cmic/Cact fraction	C/N ratio	
A/sand	25	0.028	12–17	
A/loam	36	0.028	11	
A/clay	44	0.028	10	
GP/loam	90	0.032	10	
GP/humic loam	204	0.012	11.4	
Grass/loam	94	0.035	9.4	

Table 2.3.1. Parameters selected for model initialization.

(Lavahun *et al.*, 1996), but the relative difference of microbial C in grassland and arable soil was similar (20%).

Management scenarios for the simulation were based on a standard 3-year rotation, consisting of winter oilseed rape, winter wheat and winter barley (RWB), with and without residue (straw; Y/N) incorporation. Two different yield potentials were considered for the cereals (miN/maX), which were correlated with a difference in N fertilizer addition (+50 kg N ha⁻¹). Generally, a trend was accounted for in N fertilization rising between 1965 and 1985 in cereals, starting at 120 kg N ha⁻¹ and reaching a plateau of 180 and 230 kg N ha⁻¹, respectively. Simulations were also performed for 'continuous arable' (A) to check the effect of fertilization on SOM equilibria.

Results and Discussion

Measurements

Soils from areas of high water table had about twice the amount of SOM; clay soils were too variable to fit an empirical relationship (Fig. 2.3.1). For C_{org} and N_t measured in humic soils, the hypothetical equilibrium content will not be reached until 115 years of arable cultivation. Some decline can be derived from the measured N_t contents in clay soils if one identifies two different soil types (Humic Gley and Gley). For the sub-sample of loess soils (sandy loam), typically low in SOM (h2–h3), exponential decay functions could be parameterized (Table 2.3.2) as shown for total nitrogen (Fig. 2.3.1). We assumed that equilibrium was reached after 115 years. Quantifying the half-life of either fraction under arable conditions (Table 2.3.2) shows that N_t reaches its equilibrium level faster than C_{org} . The drop in carbon content is ~10% larger compared with nitrogen, in spite of returning carbon-rich residues, such as straw, with a wide C/N ratio and a comparatively slow turnover rate. Overall, mineralizable nitrogen, incarbon content C/N ratio.



Fig. 2.3.1. Spatial and temporal variation of total N in the A horizon after ploughing grassland within two catchments; \Box loam soil (h2–h3), **\blacksquare** humic loam soil (< h3) and \checkmark clay soils (h4).

Table 2.3.2. Mean parameters (± sE) and approximate half-life, $t_{1/2}$, after grassland ploughing in loam soils (h2–h3); exponential decay function: $Y = Y[A] + Y[G] \times EXP(-k \times t_{GPA})$.

Parameter variable	Y[A]	Y[G]	<i>k</i> (year ⁻¹)	r ²	<i>t</i> _{1/2} (years)
C _{org}	0.85	1.72	0.0217	0.887	32
(g 100 g ⁻¹)	(0.05)	(0.11)	(0.004)		
N _t	0.93	1.57	0.0306	0.884	22
(g kg ⁻¹)	(0.11)	(0.11)	(0.006)		
N ₀	125	192	0.071	0.771	10
(mg kg ⁻¹)	(16)	(25)	(0.020)		

 N_0 , which may be derived from microbial N, decreased by 35% and had a half-life of ~10 years. This is longer than predicted for N_{mic} in the SUNDIAL model (Bradbury *et al.*, 1993).

Simulations

The SUNDIAL simulation results presented here include the active organic matter fractions, humus and biomass, and net mineralization. Nitrogen in the active humus fraction initially is underestimated by ~1000 kg N ha⁻¹ (Fig. 2.3.2a; humus N + N_{mic}). Depending on the C/N ratio, this corresponds to ~10–15 t C ha⁻¹, which can be attributed to the

grass sod being ploughed in. In permanent grassland, Garwood *et al.* (1977) found 22.8 t ha⁻¹ of macroorganic matter in the top 15 cm which corresponds to 13 t C ha⁻¹. The rate of N loss in the first 30 years of arable cultivation is underestimated in the simulation by > 1000 kg N ha⁻¹, corresponding to 40 kg N ha⁻¹ annually. The differences in arable management



Fig. 2.3.2. Comparison of simulated and observed course of N in the soil after grassland ploughing (GP): (a) total N (humus + N_{mic}) related to management as rape rotation, residues returned (Y/N) and yield potential (maX/miN) and (b) N_{mic} (G/GP •; A \odot) related to model parameterization.

(straw incorporation; yield potential) accounts for a variation in N_t of ~500 kg N ha⁻¹, about half the spread observed in the catchment values.

The fraction of N_{mic} in the soil is quickly decreasing after ploughing grassland by ~200 kg N ha⁻¹ to a value fairly stable over the next 30 years (Fig. 2.3.2b). Increasing the fraction of microbial carbon (C_{mic}/C_{org}) in the simulation to values measured in soils could not explain the absolute height of microbial N observed for grassland, $N_{mic}(G)$. To fit the value $N_{mic}(G)$, the C_{mic} fraction needed to be increased to 0.06, which is 70% higher than before. The difference between model predictions and observations may be caused by the distribution assumed for SOM and biomass. In arable soils, it is assumed that SOM and biomass are distributed 80% in the top 25 cm and 20% in the horizon below. Lavahun et al. (1996) found only minor differences for the distribution of C_{mic} in profiles of grassland and arable soils. However, grassland contains a higher proportion of Corg in the top 25 cm. This could be attributed to grass sod incorporated initially, and the microbial biomass associated with it. Joergensen (2000) found that considerable C_{mic} in rhizosphere material and on grass roots was ignored in standard CFE. Finally, the protective power of these silt-loam soils is underestimated, and the model reaches the equilibrium content, N_{mic}(A), too quickly. Net mineralization is predicted as a quasi-linear process during the first 30 years of simulation; however, with 150 kg N ha⁻¹ year⁻¹, it is twice as high as estimated for continuous arable (65 kg N ha⁻¹ year⁻¹).

Conclusions

The static model predicts different equilibria and half-lives for the total and active N fraction. Dynamic simulation proved to be a valuable tool in detecting missing links: fitting a single parameter, we could quantify microbial activity. The concept of 'microbial biomass' in the soil needs to account for N_{mic} and C_{mic} associated with litter and crop debris, possibly by regarding two different biomass fractions (bacteria and fungi) as explaining flush and protection in ploughed-up grassland. Further improvements to SUNDIAL should allow the model to be used explicitly to simulate ley-arable rotations.

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Modelling Decomposition of 2.4 Sugarcane Surface Residues and the Impact on Simulated Yields

P.J. THORBURN¹, F.A. ROBERTSON², S.N. LISSON³ AND J.S. BIGGS¹

¹CSIRO Tropical Agriculture, 306 Carmody Rd, St Lucia Qld 4067; ²CRC for Sustainable Sugar Production, BSES, PMB 57, Mackay MC, Qld 4740; and ³CRC for Sustainable Sugar Production and CSIRO Tropical Agriculture, PMB, PO Aitkenvale, Queensland 4814, Australia

Introduction

The Agricultural Productions Systems Simulator (APSIM; McCown *et al.*, 1996) describes the dynamics of crop growth (for various crops), soil water, soil nitrogen (N) and carbon (C), and plant residues as a function of climate, cropping history (e.g. crop type, sowing date) and soil management (e.g. tillage, fertilizer application). APSIM's linking of crop growth with soil water and N/C dynamics makes it particularly suited for extrapolating the results of agronomic experiments to different soil, management and/or climatic conditions (Probert *et al.*, 1995, 1998b; McCown *et al.*, 1996; Keating *et al.*, 1997). Despite its wide application for this purpose, to date some APSIM modules have been developed and tested in grain and legumes systems in semiarid, rain-fed areas (Probert *et al.*, 1995, 1998a,b; Carberry *et al.*, 1996) and so could benefit from wider testing. This is particularly so of the APSIM-Residue module that describes the decomposition of surface residues.

Recently, increasing attention has been paid to the impact of crop residue retention on soil water and N dynamics of sugarcane systems in the environmentally sensitive humid coastal areas of Australia. APSIM provides a means of modelling these systems (Keating *et al.*, 1997; Thorburn *et al.*, 1999). While the overall agreement between measured and modelled data has been good (Thorburn *et al.*, 1999), the climate, soils and agronomic characteristics (e.g. residue mass, N fertilizer application rates, frequency of fallows) are markedly different from those where the APSIM-Residue module was developed and most widely used. So it is appropriate that the performance of that module is examined in more detail in this environment.

This study contained three elements: the APSIM-Residue module was parameterized using experimental data (Robertson and Thorburn, Chapter 3.1) from two sites. The applicability of the parameter values to other sugarcane systems was then assessed against independent measurements of decomposition at another site. Finally, the impact of different residue decomposition rates, resulting from the different parameterizations, on simulated yield was assessed from longer term systems simulations for two of the sugarcane residue management experiments.

Methods

Field experiments

Sugarcane residue decomposition was measured over 1 year within three longer-term residue management field experiments, referred to as Mackay Early (harvested in July each year), Mackay Late (harvested in November) and Harwood Early (harvested in July) by Robertson and Thorburn (Chapter 3.1), who fully describe the methods employed. Harwood is located approximately 1500 km south of Mackay, and has a temperate climate compared with the tropical climate at Mackay (Robertson and Thorburn, Chapter 3.1). After harvest of a sugarcane crop, crop residues were left on the soil surface (as is common practice in the Australian sugar industry) and 8–10 quadrats, 1.5 m × 0.75 m in area, were established in each replicate plot of each experiment. A known mass of residue was enclosed within each quadrat. Residue in the quadrats was in direct contact with the soil, but enclosed over the top with fine nylon mesh ~20 mm in diameter. The mass of residue in individual quadrats was measured destructively over 12 months. Daily weather was measured at each site.

In addition to these measurements, soil moisture was logged hourly with Campbell CR10X dataloggers and CS615 water content reflectometers in one replicate plot of the experiments. Measurements were made over the 0–50 mm soil depth interval, and at 75 and 175 mm depth. Daily average values were calculated from the data.

The APSIM Model

The APSIM model configuration used in this study consisted of modules for soil N and C (APSIM-SoilN), soil water (APSIM-SoilWat) and surface residue (APSIM-Residue) dynamics (Probert et al., 1998b), and sugarcane growth (APSIM-Sugarcane; Keating et al., 1999). These modules have been fully described in the aforementioned papers, but a short description of them follows. The modules are one-dimensional and driven by daily climatic data. The dynamics of water, N, C and roots are simulated in soil layers, with water (and associated nitrate) moving between layers where gradients exist. The soil organic matter is divided into three 'pools', with fom representing the fresh organic matter (i.e. roots and incorporated plant residues), biom representing the active biomass in the soil, and hum representing the humified material. Part of the hum pool is considered inert. The soil water module is a 'cascading bucket' water balance model, with water between the drained upper limit (dul) and saturation draining to the layer below. The drainage rate is controlled by the parameter *swcon*. The lower limit of plant available water is defined by the parameter ll15. Evaporation from the soil follows Ritchie's (1972) two-stage evaporation model. The presence of plant residues on the soil surface affects runoff (and hence infiltration) and evaporation. The sugarcane module uses intercepted radiation to produce assimilates, which are partitioned into leaf, structural stalk, roots and sugar. The processes represented in the module are responsive to radiation and temperature, as well as water and N supply. Farming operations (such as fertilization, planting, incorporation of crop residues through cultivation or burning of crop residues) can be specified through the APSIM-Manager module to represent actual or hypothetical conditions.

APSIM-Residue and its Parameterization

In APSIM, plant residue on the soil surface is considered separately from soil organic matter. C in the residues is transferred into the soil organic matter pools upon tillage, which results in incorporation of residue into the *fom* pool, or decomposition, which transfers C into the *biom* and *hum* pools. The rate of residue decomposition is controlled by first order kinetics;

$$dR/dt = -kR \tag{1}$$

where R is the mass of residue per unit area, t is time and k is the rate coefficient given by

$$k = r_{\text{max}} \cdot F_{\text{C}:\text{N}} \cdot F_{\text{temp}} \cdot F_{\text{moist}} \cdot F_{\text{contact}}$$
(2)

where r_{max} is the maximum (or potential) decomposition rate and $F_{\text{C}:N}$, F_{temp} , F_{moist} and F_{contact} are factors, scaled from 0 to 1, accounting for the limitations to decomposition of residue C:N, temperature, moisture and residue–soil contact, respectively. The functions defining the factors are,

$$F_{C:N} = \exp[j(1 - C: N/C: N_{opt})], \quad C: N > C: N_{opt}$$
 (3a)

$$F_{\text{temp}} = (T/T_{\text{opt}})^2, \qquad T \le T_{\text{opt}}$$
(3b)

 $F_{\text{moist}} = 1 - (\Sigma E_{\text{os}})/E_{\text{os, max}}, \qquad (\Sigma E_{\text{os}}) < E_{\text{os, max}} \qquad (3c)$

$$F_{\text{contact}} = 1.54 - 0.36 R,$$
 $1.5 < R \le 3$ (3d)

where *j* is the coefficient determining the slope of Equation 3a, *T* is the average daily air temperature, E_{os} is the potential daily soil evaporation and the subscripts 'opt' and 'max' refer to the optimum and maximum parameter values, respectively. Outside the given limits, the factor values are set equal to 1 or 0, except for $F_{contact}$ which has a minimum ($F_{contact, min}$) of 0.46 in the default values (Table 2.4.1).

For parameterization, APSIM-Residue was programmed into a spreadsheet and the inputs for calculating the factors from Equation 3, i.e. residue C : N, daily air temperature and soil evaporation, were taken from measured data. Soil evaporation data were derived from daily water balance calculations performed on the soil moisture data from the experiments. Using the input data, daily values of k were calculated from Equation 2, and daily residue mass from Equation 1. Optimal values of r_{max} , T_{opt} , $E_{os, max}$, $F_{contact, min}$ were determined by the generalized reduced gradient optimization method of Fylstra *et al.* (1998) to minimize an objective function, D (Table 2.4.1). F_{C : N} was not considered explicitly (i.e. was not included in Equation 2) in the optimization since it is constant once calculated from initial residue C : N, which did not vary greatly (75–95) between the three sites. Instead, the optimal value of r_{max} included the C : N limitations to decomposition, which were assumed to be uniform across the experiments.

To derive more general parameter values from the optimization, values of r_{max} , T_{opt} , $E_{\text{os, max}}$ and $F_{\text{contact, min}}$ were optimized for both the Mackay Early and Mackay Late experiments, i.e. to minimize the sum of the objective function from the two experiments. To provide some test of their generality, the optimal parameter values were used to predict residue decomposition at the third site, Harwood Early.

Table 2.4.1. Parameter values and resultant values of the objective function (D) in each experiment for two parameterization schemes, the default parameters (Probert *et al.*, 1998b; which included those for $F_{C:N}$, not shown here) and the result of the optimization.

		-				-	
	Parameter value			Values of D ^a			
Scheme	r _{max}	E _{os, max}	$T_{\rm opt}$	F _{contact, min}	Mackay Early	Mackay Late	Harwood Early
Default	0.100	20	20	0.46	100.3	384.9	129.0
Optimal	0.007	9	23	1	10.2	21.4	18.8

 ${}^{a}D = \Sigma (|R_{p} - R_{o}| + 1)^{2}$, where the subscripts p and o refer to predicted and observed values, respectively.

Parameterization of APSIM for Systems Simulations

The systems simulations were performed on the residue retention treatments of the Mackay Late and Mackay Early experiments. The experiments commenced with planting in July 1992 for the Early experiment and November 1992 for the Late experiment. The sites were managed similarly, differing only in the harvest date. Crops were grown for 12 months then harvested and allowed to ratoon (i.e. regrow), four and five times for the Early and Late experiments, respectively. Information on fertilization and tillage practices was used to specify crop management in the model. Model parameters were based, wherever possible, on measured data. The soil profile was sampled to 1.5 m depth in 1997, following the residue decomposition measurements, and soil total C and N, mineral N and bulk density measured to initialize N and C in APSIM-SoilN. Measurements of microbial biomass (Robertson and Thorburn, Chapter 3.1) were used to set the *biom* pool size. All other pools were set equal to values used in previous APSIM simulations of soil N dynamics in sugarcane residue retention experiments (Thorburn et al., 1999). The soil water parameters (saturation, dul and ll15) were estimated from the daily soil moisture data. Default parameter values (Keating et al., 1999) for the sugarcane variety grown in the experiments (Q124) were used.

Results and Discussion

Optimization of decomposition parameters

The optimal APSIM-Residue parameter values differed from the default values (Table 2.4.1) and gave predictions of residue mass much closer to measured values (Fig. 2.4.1a) with consequently lower D values (Table 2.4.1). When the optimal values were used to predict residue mass at the third experiment, Harwood Early, predictions of residue mass were also much closer to measured values than those resultant from the default parameters (Fig. 2.4.1b).

The optimal value of $E_{os, max}$ was lower than the default (Table 2.4.1), indicating a greater moisture limitation to decomposition, whereas the value of $F_{contact, min}$ indicated no residue-soil contact limitation. This latter difference was unexpected as initial residue masses were large (10–20 t ha⁻¹) in the field experiments, a condition under which residuesoil contact should be a limit to decomposition. It may be that a more appropriate function is required to describe the contact limitation properly.

Another substantial change in the parameter values was the value of r_{max} , which was reduced from the default value of 0.1 to 0.007 in the optimization (Table 2.4.1). Since the limitation to decomposition imposed



Fig. 2.4.1. Comparison of measured (symbols; bars represent ± 1 sp about the measured values) and predicted (lines) decomposition of sugarcane residue following harvest of a crop. The solid lines are the predictions using the parameter values optimized on the data from the two experiments shown in (a) (\bullet – Mackay Late, \bullet – Mackay Early), while independent predictions for the third experiment (Harwood Early) are shown in (b). The dashed lines are the predictions using the default parameter values (Probert *et al.*, 1998b).

by the high C : N of the sugarcane residue was implicit in the optimal value of r_{max} , the optimal value is not directly comparable with the default. However, the value of $F_{C:N}$ (from Equation 3a) was ~0.5 at both the Mackay experiments, implying an r_{max} value of ~0.014 without the C : N limitation, a value that is still substantially lower than the default. Snow *et al.* (1998) also had to reduce the default value of r_{max} (to 0.025) to simulate the decomposition of litter in a *Eucalyptus* plantation accurately. These experiences suggest that the value of r_{max} and other parameters in Equation 2 are not yet generic across the wide range of environments (e.g. semiarid temperate areas to the humid tropics) and agricultural systems (cereals, legumes, sugarcane and forests; both rain-fed and irrigated) where APSIM is being applied.

Impact of different decomposition rates on cropping system simulations

In simulation of the Mackay Early experiment, the different residue decomposition rates produced by the different parameterization schemes substantially affected simulated sugarcane yield (Fig. 2.4.2a). In all but the first crop, the simulation with the optimized parameter scheme gave higher yields, closer to those measured in the experiment. The effect of

decomposition on yield was likely to have been caused by impacts of decomposition on the water balance in the simulation (Table 2.4.2). The simulations with the optimal decomposition parameters averaged lower runoff and soil evaporation, and higher deep drainage as would be expected with the greater residue mass throughout the season (e.g. Fig. 2.4.1). These differences were not present in the first crop (data not shown) that was planted into a bare field. Average simulated nitrate leaching from the soil was higher with the optimal parameter scheme (Table 2.4.2) due to increased deep drainage and changes in the patterns of N mineralization (i.e. reduced immobilization of N with the slower decomposition) in the simulation. However, there was little difference in denitrification. Overall, the differences in simulated loss of N were not great enough to affect the crop.



Fig. 2.4.2. Comparison of measured (\blacksquare ; bars represent ± 1 sp about the measured values) and simulated (\bullet) sugarcane yields at two experiments; (a) Mackay Early and (b) Mackay Late. Simulations were performed with two parameterization schemes, the default parameters (Probert *et al.*, 1998b; dashed lines) and the result of the optimization (solid lines).

 Table 2.4.2.
 Effect of different residue decomposition parameter schemes on simulated components of the water balance and nitrogen losses, averaged across all seasons, at the two Mackay field experiments.

Experiment/	Water bal	ance (% d	Nitrogen losses (kg ha ⁻¹)		
scheme	Deep drainage ^a	Runoff	Soil evaporation	Nitrate leached	Denitrification
Early/default	11	13	22	1	26
Early/optimized	14	11	12	5	24
Late/default	18	12	21	8	61
Late/optimized	19	11	20	14	60

^aBelow the active rooting depth.

Contrary to the situation in the Mackay Early experiment, simulated yields (Fig. 2.4.2b) and water balance (Table 2.4.2) in the Mackay Late experiment were little affected by the different decomposition of residues. The difference in the impact of the parameter schemes between the two experiments can be attributed to the timing of residue decomposition in relation to climate at the sites and, primarily, its impact on soil evaporation. Differences in residue mass simulated with the two parameter schemes were greatest from ~ 100 days after harvest (Fig. 2.4.1). In the Mackay Late experiment (harvested in November each year), this time occurred in the cooler, drier months of late autumn and winter, when potential soil evaporation was low in the Mackay Late experiment, and so the presence (or absence) of residue would have the least impact on soil evaporation. However, the situation was reversed in the Mackay Early experiment (harvested in July each year). There the greatest differences in simulated residue mass occurred in the hotter, wetter months of late spring and summer when potential soil evaporation was high. It is under these conditions that the presence of residue has the greatest impact on soil water balances, and hence yields.

The difference in the simulation results between the two experiments highlights the interactions between climate, crops and soil processes and their impact on cropping system characteristics. Successful use of cropping system models to extrapolate the results of agronomic experiments to different soil, management and/or climatic conditions requires that all these interactions are captured and described adequately.

Acknowledgements

The authors thank Drs Merv Probert and Brian Keating for their advice and constructive comments during the study, members of the Bureau of Sugar Experimental Stations, Mackay, for access to information on the long-term experiments, and Dr Graham Kingston for facilitating the experimental work at Harwood. This study was partially funded by the Sugar Research and Development Corporation, Australia.

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Questionable Assumptions in 2.5 Current Soil Organic Matter Transformation Models

J.R.M. ARAH¹ AND J.L. GAUNT²

¹AAT Consultants, 15 Clerk Street, Edinburgh EH8 9JH; and ²IACR-Rothamsted Experimental Station, Harpenden, Hertfordshire AL5 2JQ, UK

Introduction

Cycling of soil organic matter (SOM) lies at the heart of all terrestrial (agro)ecosystems, controlling the direction and nature of soil–atmosphere trace gas exchange, modulating nutrient availability, and thereby influencing productivity. Current SOM transformation models, especially those designed for incorporation within larger ecosystem-scale models, almost universally assume (i) a soil which is areally homogeneous with respect to all relevant processes and (ii) first-order decomposition kinetics. In this chapter, we analyse these assumptions and examine the conditions which must be satisfied for them to hold. We go on to suggest that in order to test these assumptions it is necessary to depart from a third universal supposition, that (iii) of the existence within the soil of well-defined and functionally discrete SOM pools. Measurements of the transformations of measurable (extractable) SOM fractions are essential in order to secure the foundations on which existing transformation models are built.

It will be clear from the notation that Fig. 2.5.1 represents no published model. It is a caricature, intended to highlight the arbitrary and questionable aspects of the type of model it portrays. Allowing for a few pools more or less, and a little more sophisticated treatment of flux partitioning, nearly all existing SOM transformation models can be represented by a diagram similar to Fig. 2.5.1. We have no space here to mention all the major current contenders; the reader is referred to Powlson *et al.* (1996) for a review. The major apparent exception is the cohort model of Ågren and Bosatta (1987), in which individual additions of organic matter are tracked

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Typical SOM model



Fig. 2.5.1. A typical SOM transformation model. Pool decomposition rates are determined by intrinsic rate constants K_i and extrinsic rate modifiers F; partition functions Φ_{ij} are shown where required by the reaction network.

through time as their reactivity declines according to a pre-defined pattern. This model, however, becomes mathematically equivalent to the others wherever a sufficient range of (usually geometrically distributed) pool reactivities (K_i) is considered. It is conceptually distinct but, given enough pools, functionally equivalent to the majority. It too assumes areal homogeneity and effective first-order kinetics.

Transformation processes within these models are typically represented by some form of Equation 1:

$$V_{i} = K_{i}F_{i}(T, \Theta, C)Y_{i}$$
⁽¹⁾

with partitioning between products being handled by some form of equation [2]:

$$\mathcal{J}_{ij} = \Phi_{ij}(T, \Theta, C); \sum_{j \neq 1} \Phi_{ij}(T, \Theta, C) = 1$$
(2)

In these equations, V_i is the decomposition rate of substrate Y_i , Y_i is its concentration and K_i its effective first-order decomposition rate constant; $F_i(T, \Theta, C)$ is a modifier function representing the effects on Y_i decomposition of temperature (T), volumetric moisture content (Θ) and clay fraction (C); \mathcal{J}_{ij} is the flux from source pool *i* to target pool *j*, and $\Phi_{ij}(T, \Theta, C)$ is the corresponding partition function. Upper case symbols $(T, \Theta, C, Y_i, F_i, V_i)$

 $\Phi_{ij}, \mathcal{J}_{ij}$ denote properties and functions of depth z and time t integrated over the unitary area of the model (usually at least 1 m², commonly as much as 10⁴ m²). In most models, K_i is an invariant property of SOM pool i; in the cohort model, it is a function of the age of the cohort. Equations 1 and 2 are actually over-generous in the degree of flexibility they accord to most existing SOM transformation models. Rate modifier functions F_i (T, Θ, C) are almost universally assumed to be simple products of individual modifier functions $F_T(T), F_\Theta(\Theta)$ and $F_C(C)$ equally applicable to all reactions, while partition functions $\Phi_{ij}(T, \Theta, C)$ are generally taken to depend only on the clay content C.

Underlying assumptions

Equations 1 and 2 invoke soil properties, concentrations and reaction rates averaged over areas of 1 m^2 or more. Microbial biomass does not feature in the formulae. Yet (i) SOM decomposition is known to be microbially mediated and (ii) microbial populations and metabolic reaction rates are known to be markedly heterogeneous over distances considerably smaller than 1 m. How are these apparent contradictions to be resolved?

Spatial variability and reaction kinetics

Consider a microsite small enough to be treated as homogeneous. Let T, θ , c and y_i represent microsite temperature, moisture content, clay fraction and substrate concentration (and T, Θ , C and Y_i , as before, their macroscale equivalents). Let μ_i represent the microbial biomass responsible for bringing about Y_i -decomposition, with local (microsite) rate v_i . In general:

$$v_{i} = v_{i}(T, \theta, c, y_{i}, \mu_{i})$$
(3)

(i.e. v_i is a function of T, θ , c, y_i and μ_i) and the corresponding macroscopic rate V_i is:

$$V_{i} = \int v_{i}(T, \theta, c, y_{i}, \mu_{i}) p(T, \theta, c, y_{i}, \mu_{i}) d(T, \theta, c, y_{i}, \mu_{i})$$

$$\tag{4}$$

where $p(T, \theta, c, y_i, \mu_i)$ is the probability of an individual microsite having the particular set of controlling properties T, θ, c, y_i and μ_i . Assuming – and it is quite a big assumption – that the microsite-scale influences of temperature, moisture content and clay fraction can be disentangled from those of biomass and substrate supply, Equation 3 may be written:

$$v_{i} = f_{i}(T, \theta, c)g_{i}(y_{i}, \mu_{i})$$
(5)

and Equation 4 becomes:

$$V_{i} = \int f_{i}(T, \theta, c)p(T, \theta, c)d(T, \theta, c) \int g_{i}(y_{i}, \mu_{i})p(y_{i}, \mu_{i})d(y_{i}, \mu_{i})$$
(6)

or, equivalently:

$$V_{i} = f_{i}(T, \theta, c)g_{i}(y_{i}, \mu_{i})$$

$$(7)$$

where the macron (over-line) denotes integration over the appropriate probability distribution (area averaging). Equating the two macroscale Equations 1 and 6–7 reveals the following assumptions implicit in Equation 1:

$$F_{i}(T, \Theta, C) \equiv F_{i}(\overline{T}, \overline{\theta}, \overline{c}) = \overline{f_{i}(T, \theta, c)} \equiv \int f_{i}(T, \theta, c)p(T, \theta, c)d(T, \theta, c)$$
(A1)
and:

$$K_{i}Y_{i} \equiv \overline{K_{i}y_{i}} = \overline{g_{i}(y_{i},\mu_{i})} \equiv \int g_{i}(y_{i},\mu_{i})p(y_{i},\mu_{i})d(y_{i},\mu_{i})$$
(A2)

Assumption A1 can be true only where microsite temperature, moisture content and clay fraction are homogeneous, in which case F_i is by definition equal to f_i . Under any other circumstances (e.g. in particular, where physical aggregation leads to higher clay fractions and moisture contents in some microsites than in others), there is no simple relationship between F_i and f_i . Instead, the macroscale function depends on the probability distributions of the microsite properties T, θ and c. Macroscale functions F_i appropriate for one particular distribution of microsite properties may therefore be inappropriate for another. Macroscale partition functions Φ_{ij} are similarly vulnerable.

The assumption that there is one set of rate modifier functions F_i (and partition functions Φ_{ij}) appropriate for all soils under all climatic and cultivation regimes amounts to an assumption that the probability distributions of the microsite properties T, θ and c are always and everywhere roughly the same.

Similar considerations apply with regard to the microscale distribution of substrate concentration y_i in assumption A2. An additional difficulty concerns the elimination of microbial biomass μ_i from the macroscale formula. Two possible scenarios (pictures of microbial life in soil) can be invoked to justify this first-order approximation. The first – probably the most general where the assumption is questioned at all – is of a universal and diffuse war of all against all; all possible microbial life strategies are everywhere present, the most efficient inevitably prevails, successful microbial populations expand until their substrate becomes limiting. The longer the model time step and the larger the simulated area, the more credible such a picture becomes.

What if we want to model short-term SOM dynamics on a time scale of days or weeks (relevant to the crop, but also within the range of microbial population fluctuations)? Can we then make the assumption that potential microbial strategies are universally distributed, and that – basically – whatever makes thermodynamic sense will occur? The evidence seems to be against it (J.M. Tiedje, Los Baños, Philippines, 1999, personal communication). Spot measurements of microbial DNA point to widely different populations (with, presumably, widely different life strategies) occupying adjacent microsites and exhibiting little short-term mobility. This scenario may lead to first-order kinetics provided that microbial microsites (i.e. population nodes) are sufficiently small and sufficiently diverse that an adequate range of life strategies is represented even within the larger physicochemical microsites defined by approximately uniform y_i . Most of the microsite volume will then effectively be inert, activity being confined to, and substrate-limited within, those population nodes fortunate enough to be equipped with the relevant enzymes. A corollary of the second scenario is that macroscopic reaction rates must be very much smaller than incubation optima.

Whichever is the case, it should be noted that the first-order assumption is only that: an assumption the validity of which depends on the time and space scales of the model within which it is employed.

Functionally Defined SOM Pools

Figure 2.5.1 is a caricature. It nevertheless captures one essential feature of the type of model discussed so far: model SOM pools are defined arbitrarily in terms of their effective (macroscale) first-order reaction constants K_i . These parameters are not amenable to measurement or optimization; they are simply defined as part of the definition of the model. Equally, model pool names – while generally indicative of model pool function – provide no clue for quantification (try to imagine an extraction procedure which reliably isolates all and only that fraction of the soil organic matter with an effective turnover time of 1 day). We have seen that the macroscopic rate modifiers F_i and partition functions Φ_{ij} could not in general be deduced from microscale measurements even were the microscale properties T, θ , c, y_i and μ_i measurable, and that y_i cannot be measured even in principle.

How then is such a model to be evaluated? Its primary predicands (the various SOM pool concentrations Y_i) cannot even be measured.

The answer is that SOM transformation models are typically designed to be incorporated into larger models with components representing energy, water, plants, even animals, and driven by various climatic and anthropogenic inputs. They are evaluated not by reference to their primary predicands but in terms of the overall behaviour of the system-level model within which they are embedded. It should be obvious that this provides plenty of scope for fortuitous fits. In view of the load they are expected to bear – forecasts of C sequestration and release over hundreds of years, predictions of indigenous N supply and sustainability under different management regimes – it is clearly desirable that the assumptions which underlie most SOM transformation models should be tested and shored up wherever possible. How is this to be done?

Prognosis

Isotope tracing offers the potential for tracking C and N fluxes between measurable (i.e. real) SOM fractions. Where ¹⁵N and ¹³C are employed in tandem, it should be possible in theory to measure the fluxes between up to five fractions including the gaseous and solution phases (Arah, 2000a). This in turn should allow the assumptions (approximations) of effective spatial homogeneity and first-order reaction kinetics to be examined in detail. Such work seems to us to be essential.

It calls for the following: (i) development of a fractionation procedure which partitions soil organic matter into five routinely measurable fractions, the first gaseous, the second soluble and the other three defined solely by their method of extraction, such that fractions 1–5 add up to the total organic content of the sample, elemental and isotopic contents of each fraction can be determined, and, ideally, fractions 1–4 are reasonably dynamic over a typical cropping cycle; (ii) incubation of ¹⁵N- and ¹³C-labelled soil samples with SOM fractionation and fraction analysis at intervals; and (iii) interpretation of the results via some kind of a model in which ⁽¹³⁾C and ⁽¹⁵⁾N fluxes are linked, to derive the actual C and N fluxes between the measurable (indeed measured) SOM fractions of the incubation. Sohi *et al.* (2000) describe such a fractionation procedure; Arah (2000b) describes such an interpretative model.

Comparison of the results of such an exercise against the constant first-order-reactivity and effective spatial homogeneity assumptions implicit in all current SOM transformation models might do one of three things. It might reveal these assumptions to be unacceptable, necessitating the development of a new generation of models in which more attention is paid to soil structural and microbial kinetic parameters. It might throw up no major contradictions, allowing a relatively seamless shift from the dependence of existing models on functionally defined, unmeasurable SOM pools to a dependence on similarly uniform but procedurally defined, measurable SOM fractions and thereby permitting the development of predictive soil tests for SOM function. Or, most likely, it might fall somewhere between these extremes, suggesting circumstances in which either response is appropriate.

Acknowledgements

We thank the UK Department for International Development (DFID) Natural Resources Systems Programme (NRSP) project R6750 (Modelling soil organic matter transformations and nitrogen availability in periodically flooded soils) for financial support.

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A Procedure for Isolating Soil 2.6 Organic Matter Fractions Suitable for Modelling

J.L. GAUNT¹, S.P. SOHI¹, H. YANG^{1,2}, N. MAHIEU³ AND J.R.M. ARAH⁴

¹Department of Soil Science, IACR-Rothamsted, Harpenden, Hertfordshire AL5 2JQ, UK; ²International Rice Research Institute, PO Box 933 Manila, Philippines; ³Department of Chemistry, Queen Mary and Westfield College, University of London, London E1 4NS; and ⁴AAT Consultants, 15 Clerk Street, Edinburgh EH8 9JH, UK

Introduction

Jenkinson and Rayner (1977), and many others since, have modelled the turnover of soil organic matter (SOM) in terms of discrete conceptual pools, each with different characteristic properties and a measure of reactivity (e.g. the first-order reaction constant k). Although the decomposition of plant material in soil is a complex process, such simple models have successfully described the long-term dynamics of SOM.

If a SOM turnover model is to predict nitrogen (N) transformations as well as carbon (C) fluxes, it is necessary to include a functional characteristic of organic matter that determines N mineralized or immobilized during turnover of C. A typical example of such a functional characteristic is the C : N ratio of a conceptual pool. The application of models based on conceptual pools with a first-order reaction constant and a fixed definition of function make for easy modelling but parameters (e.g. initial pool sizes) which are unmeasurable. The overall performance can be optimized against system outputs such as soil C content.

There are drawbacks to such models. Parameterization against systemlevel outputs alone cannot guarantee process-level accuracy. Perhaps the most important drawback is that such models are not directly testable: it is impossible to devise a procedure that will reliably extract all and only that part of the SOM with a first-order reaction constant k. For the same reason, it is not possible to make a measurement in an unknown field and predict future SOM decomposition. Recognition of these limitations has fuelled a debate as to whether we should aim to 'model the measurable' rather than 'measure the modellable' (Elliot *et al.*, 1996; Magid *et al.*, 1997).

If a model is based on measurable fractions, SOM pools are defined as fractions isolated by a specified experimental procedure rather than their reactivity. This has the potential advantage that the size of a SOM pool can be measured in any soil at any time. It has the corresponding drawback that the reactivity of an SOM fraction cannot simply be assumed to be constant.

Requirements of the Extraction Protocol

If the C and N fluxes predicted by the model are to be verified, the number of pools that can be included in the model, and the associated extraction protocol, is determined by the number of tracers employed. Consider a fractionation procedure that divides SOM (including its mineral component) into *n* fractions. Over any given time period in a closed system, there are n (n - 1) carbon fluxes between these fractions, and the same number of nitrogen fluxes. These fluxes represent 2 n (n - 1) unknowns for each incubation period. If C is traced by ¹³C and N is traced by ¹⁵N, we have 4 n knowns at each stage of the incubation. Assume, finally, that C and N fluxes are interdependent. If this is the case, then at each stage of the incubation we have n (n - 1) unknown fluxes and 4 n known differences.

Therefore, if ¹³C and ¹⁵N tracers are used, it should be possible to infer the transformations, and hence derive the effective reactivity, of up to five SOM pools. Therefore, a key requirement of our extraction protocol was that a maximum of five pools should be isolated and that these should account for the total C and N in the system. It is also desirable that the fractionation process should be simple and quick and that the protocol/ modelling strategy should identify fractions which differ significantly in measured chemical properties. This difference in chemical properties is important because, as a first approximation, differing chemical properties infer likely differences in reactivity.

The Extraction Method

We developed an extraction protocol (Sohi *et al.*, 1998) and are currently developing and testing an associated model. In brief, the pools extracted are as follows; fraction 1 is the gaseous phase; fraction 2 is the soluble fraction; fraction 3 is isolated by suspending soil in dense liquid, with no prior energy input (other than swirling) referred to as free material herein; fraction 4, denoted intra-aggregate, comprises material that is released by ultrasonic disruption of aggregates and recovered by a second density separation and;

fraction 5 is the residual organomineral component. This can be divided further on the basis of particle size.

Chemical composition of solid fractions

Chemical characterization of the solid fractions (fractions 3, 4 and 5 above) was done by ¹³C cross-polarization magic angle spinning (CPMAS) NMR. Material in the organomineral component was divided further on the basis of size into sand, silt and clay fractions. Full experimental details are published elsewhere (Gaunt et al., 1999). Figure 2.6.1 shows the chemical composition of the solid organic matter fractions separated by our fractionation procedure and that of whole soil, using the ¹³C CPMAS NMR technique (Sohi et al., 1998). Carbon in free organic matter was located predominantly in O-alkyl structures. Intra-aggregate organic matter contained a lesser proportion of C in O-alkyl groups, and more in aromatic and alkyl groups. Lowering of O-alkyl to alkyl ratios is characteristic of the early stages of the degradative process (Preston, 1996). This is attributable to the transformation of readily metabolizable carbohydrates, and production and persistence of biomass- and plant-derived alkyl C. Our analysis suggests, therefore, that the free fraction represents less altered organic matter (i.e. closer to the composition of incoming plant material) as compared with the intra-aggregate.

The distribution of NMR-visible carbon for the clay organomineral fractions appears more similar to that of intra-aggregate rather than free organic matter (with slightly greater proportions of carbonyl C, less aromatic and phenolic C). The observed differences between the free and the intra-aggregate and organomineral fractions are potentially important, since the chemical properties of a particular fraction will affect its reactivity. We have found that these differences are consistent across soil type and climate in soils taken from seven long-term experiments, where cereals are grown under mineral fertilization (Gaunt *et al.*, 1999).

Isotope Tracing Through Fractions

If the proposed fractionation protocol and associated model is to be used to predict C and N fluxes over a single crop-growing season, we need to measure, and predict, fluxes of C and N over a period < 1 year. To establish the sensitivity of our fractionation protocol, we set up incubation studies using ¹³C and ¹⁵N tracers. To trace C, we used a ¹³C natural abundance technique. The stable isotope composition of plants differs depending on the type of photosynthetic pathway (C₃ and C₄) of the plant. This results in a difference in the ¹³C content of 12–14‰, with C₄ plants being more



Fig. 2.6.1. Chemical composition as seen by ¹³C NMR of whole soil and organic matter fractions for a clay texture arable soil from the UK.

enriched. Thus we added C₄ plant material (maize) at approximately -12% ¹³C labelled with ¹⁵N to a C₃ soil at approximately -26% ¹³C.

Figure 2.6.2 shows an example of the change in the δ^{13} C signal of the solid fractions defined by our protocol over a period of ~1 year after incorporation of maize material in pots (unplanted). The disappearance of maize-derived C from the free fraction due to decomposition was accompanied by a small, but detectable, increase of maize-derived material



Fig. 2.6.2. The δ^{13} C signal of soil organic matter recovered from a C₃ soil after addition of C₄ plant residues. Dashed lines represent the unamended control.

in the intra-aggregate. The appearance of maize-derived material in the organomineral fraction cannot be seen; this may be either because this fraction is less important to describe short-term turnover of C or because the large amount of C in this fraction masks the incorporation of maize-derived material. Results for ¹⁵N show similar patterns and thus are not shown here.

The difference between the δ^{13} C enrichment at natural abundance of the free and intra-aggregate fraction in the unamended control soil may reflect isotope discrimination during the decomposition of organic matter. The products of microbial transformation are generally enriched in the heavier isotope form when compared with the substrate. Thus the fact that the intra-aggregate material is less depleted in ¹³C than the free fraction, and therefore heavier, appears to confirm the results above that suggest that the free fraction represents less altered organic matter when compared with the intra-aggregate.

Conclusion

An extraction protocol that meets the basic requirements for a model based on measurable pools is presented. The solid organic fractions obtained by our physical fractionation procedure (i.e. free and intra-aggregate fractions) show strong contrast in chemical composition. These differences have been found to be consistent across environment and soil type.

Preliminary isotope data suggest that we can measure fluxes of added C through the pools defined in the model. Thus we can derive the reactivity,

in situ, of the organic matter in these pools. We plan to use the model to test the assumption of first-order reactivity used by most models. Further, the combined modelling and fractionation approach presented provides a unique opportunity to relate the chemical characteristics of soil organic matter to its *in situ* reactivity. Work to establish these relationships is planned.

Acknowledgements

This research was funded by the UK Ministry for Agriculture Fisheries and Food (MAFF), the Biotechnology and Biological Sciences Research Council (BBSRC) and the Department for International Development (DFID). The views expressed are not necessarily those of DFID. IACR receives grant-aided support from UK Biotechnology and Biological Sciences Research Council.

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