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**Measuring and  
modelling SOM  
quality distributions**

S. Bruun et al.

# Measuring and modelling continuous quality distributions of soil organic matter

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## Abstract

An understanding of the dynamics of soil organic matter (SOM) is important for our ability to develop management practices that preserve soil quality and sequester carbon. Most SOM decomposition models represent the heterogeneity of organic matter by a few discrete compartments with different turnover rates, while other models employ a continuous quality distribution. To make the multi-compartment models more mechanistic in nature, it has been argued that the compartments should be related to soil fractions actually occurring and having a functional role in the soil. In this paper, we make the case that fractionation methods that can measure continuous quality distributions should be developed, and that the temporal development of these distributions should be incorporated into SOM models. The measured continuous SOM quality distributions should hold valuable information not only for model development, but also for direct interpretation. Measuring continuous distributions requires that the measurements along the quality variable are so frequent that the distribution is approaching the underlying continuum. Continuous distributions leads to possible simplifications of the model formulations, which considerably reduce the number of parameters needed to describe SOM turnover. A general framework for SOM models representing SOM across measurable quality distributions is presented and simplifications for specific situations are discussed. Finally, methods that have been used or have the potential to be used to measure continuous quality SOM distributions are reviewed. Generally, existing fractionation methods have to be modified to allow measurement of distributions or new fractionation techniques will have to be developed. Developing the distributional models in concert with the fractionation methods to measure the distributions will be a major task. We hope the current paper will help spawning the interest needed to accommodate this.

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## 1 Introduction

The carbon stored as soil organic matter (SOM) in soils has been estimated to be around 1500 Gt to a depth of 1 m and 2300 Gt to 3 m, which is 2 to 3 times more than the amount of carbon in the atmosphere (Jobbágy and Jackson, 2000). This offers the possibility for carbon sequestration by increasing the amount of SOM in the soils of the world (Lal, 2007). Other reasons to increase the amount of SOM stored in soil is that it affects many aspects related to soil quality positively. To achieve this, it is essential to have an understanding of the dynamics of SOM and the factors that may influence it such as, land use changes, land management practices and climate. However, the dynamics of SOM is very complex and therefore soil organic matter models are often applied to understand and predict the consequences of imposed changes.

Most soil organic matter models are multi-compartment models describing organic matter (OM) turnover as the consequence of transformations between different compartments of different decomposability or biological quality (McGill, 1996; Coleman and Jenkinson, 1996; Parton et al., 1987; Reichstein et al., 2009). However, these model compartments are unrelated to measurable entities. This means that the pools and flows between them are largely theoretical constructs introduced to mimic the heterogeneity of SOM and not inferred from direct evidence of their existence. To make multi-compartment models more mechanistic, it has been argued that their pools should correspond to measurable SOM fractions having a functional role in the soil (Hassink, 1995; Christensen, 1996; Elliott et al., 1996; Balesdent, 1996; Arah and Gaunt, 2001; Smith et al., 2002; von Lützow et al., 2007). The basis for validating a multi-compartment model is much improved when it is based on measurable SOM fractions because the models can be tested for their ability to simulate the amount of C and isotopic ratios in each SOM fraction. Following these publications, schemes to obtain fractions that are more uniform with respect to molecular composition or physical protection and, therefore, more suitable as model pools have been developed (Hassink, 1995; Trumbore and Zheng, 1996; Magid et al., 1996; Six et al., 1998; Sohi et al.,

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2001; Christensen, 2001). Attempts to base models on measurable SOM fractions have been advanced (Buyanovsky et al., 1994; Hassink and Dalenberg, 1996; Bird et al., 2002; Skjemstad et al., 2004; Zimmermann et al., 2007). However, the envisaged impact of measurable SOM fractions on SOM models has as yet only materialized to a  
5 modest degree.

The number of different chemical constituents in SOM found in soil is extremely large and the SOM is subjected to protection by a multitude of mechanisms (Sollins et al., 1996; von Lütow et al., 2006). Therefore, the decomposability or quality of SOM is better described as a continuum than as a number of separate compartments. Even a  
10 relatively well defined SOM fraction, such as black carbon, is more appropriately characterized as a continuum, ranging from slightly charred biomass to sod and graphite (Goldberg, 1985; Masiello, 2004). Therefore, the idea of representing the quality of SOM as a continuous quality distribution is obvious, and several models have been developed, based on this concept (Bosatta and Ågren, 1985; Ågren et al., 1996b). In their  
15 general form, they make very few simplifying assumptions. However, the definitions of the quality distributions are as unrelated to anything measurable as the compartments of the multi-compartment models.

We argue that rather than fractionating the SOM into a few operationally defined fractions or defining quality distributions that are not related to anything measurable, it may be feasible to develop methods to measure the continuous quality distributions of SOM and incorporate these into continuous quality distribution SOM models. The quality will then be represented by some measurable variable such as particle size, particle density or resistance of SOM to oxidation. Generally, the methods used to measure SOM fractions in soil will have to be modified to enable measurement of  
20 continuous quality distributions, or rather, new techniques will need to be developed and applied. We discuss the implications of characterizing SOM by continuous quality distributions, present possible model formulations and briefly review methods that may be employed to measure the distributions.  
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## 2 Models of measurable continuous quality distributions of SOM

SOM models with continuous quality distributions were originally suggested by Carpenter (1981). Later, the models and concepts upon which they are based were greatly expanded (Bosatta and Ågren, 1985, 1991, 2003; Ågren and Bosatta, 1996a, b). Boudreau (1992) developed a model based on similar arguments for organic matter in marine sediments.

Several model formulations incorporating measurable continuous quality distributions can be envisaged. In this paper we present an example of a one-dimensional continuous distribution model and suggest possible simplifications, extensions and generalizations that could be appropriate in different situations.

### 2.1 One-dimensional continuous distribution model

To obtain a model that represents the soil organic carbon (SOC) by a one-dimensional quality distribution, we introduce a variable that represents the quality of SOC,  $q$ . This variable is determined by the fractionation method used to measure the distribution of SOM qualities across that variable. It may be any of the variables suggested later such as size, density or resistance to oxidation. At time  $t$ , we assume that a continuous distribution of SOC,  $\rho(q,t)$  exists, defined such that  $\rho(q,t)dq$  is the amount of SOC in the quality interval  $q$  to  $q+dq$ . The total amount of SOC in the soil can thus be found by:

$$C(t) = \int_{-\infty}^{\infty} \rho(q,t) dq \quad (1)$$

If we assume that this distribution changes in time as a consequence of external inputs ( $I(q,t)$ ), respiration ( $R(q,t)$ ), and modifications of the quality in time ( $M(q,q',t)$ ), the

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time derivative is:

$$\frac{\partial \rho(q, t)}{\partial t} = I(q, t) - R(q, t) + \int_{-\infty}^{\infty} M(q, q', t) dq' \quad (2)$$

$M(q, q', t)$  is a distributional kernel which defines the rate with which SOC is moved from quality  $q'$  to  $q$ . Conservation of mass dictates that  $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} M(q, q') dq' dq = 0$ . The

temporal development of the distribution from time  $t$  to  $t+dt$  is illustrated in Fig. 1.

What remains to make the model functional is to assume some dependencies and functional forms of  $I(q, t)$ ,  $R(q, t)$  and  $M(q, q', t)$ . If the model is to be useful, these functions should be continuous and relatively simple with a small limited number of parameters. If this is not possible, the parameters will be impossible to estimate and the measurable entity chosen to represent  $q$  is not very useful. We assume that respiration is proportional to the amounts of carbon of different qualities, i.e. the respiration rate is equal to  $k(q, t)\rho(q, t)$ , where  $k(q, t)$  is a specific respiration function dependent on the quality  $q$ . Then, in the simple case where SOC can only move along the  $q$  axis, the model reduces to:

$$\frac{\partial \rho(q, t)}{\partial t} = I(q, t) - k(q, t)\rho(q, t) + \frac{\partial F(q, t)}{\partial q} \quad (3)$$

where  $F(q, t)$  is the rate of movement of SOC along the  $q$  axis. The initial quality distributions  $\rho(q, 0) = \rho_0(q)$  and two boundary conditions are also needed. Usually,  $F(q_1, t) = 0$  and  $F(q_2, t) = 0$  will be appropriate as boundary conditions. Now the problem reduces to choosing functional forms of  $I(q, t)$ ,  $k(q, t)$  and  $F(q, t)$ .

A simple way to describe movement along the  $q$ -axis is by analogy with either dispersion or convection or a combination of the two where the dispersion constant,  $D(q)$ , or the convection constant,  $v(q)$ , are dependent on the quality, i.e.

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$F(q, t) = -D(q) \frac{\partial \rho(q, t)}{\partial q} + v(q) \rho(q, t)$ . This means that Eq. (3) becomes:

$$\frac{\partial \rho(q, t)}{\partial t} = I(q, t) - k(q) \rho(q, t) - \frac{\partial \left( D(q) \frac{\partial \rho(q, t)}{\partial q} \right)}{\partial q} + \frac{\partial v(q) \rho(q, t)}{\partial q} \quad (4)$$

or:

$$\frac{\partial \rho(q, t)}{\partial t} = I(q, t) - k(q) \rho(q, t) - D(q) \frac{\partial^2 \rho(q, t)}{\partial q^2} + \left( v(q) - \frac{\partial D(q)}{\partial q} \right) \frac{\partial \rho(q, t)}{\partial q} + \frac{\partial v(q)}{\partial q} \rho(q, t) \quad (5)$$

In those cases where  $k(q)$ ,  $D(q)$ , and  $v(q)$  do not depend on  $\rho(q, t)$ , Eq. (5) is linear in  $\rho(q, t)$  and the principle of superposition applies. We can then solve the equation for the input of material with a single quality,  $I(q) = i_0 \delta(q - q_0)$  and follow how this is transmitted through the system. This can considerably simplify the interpretation of the properties of the equation. More complex inputs, consisting of a mixture of qualities, are obtained simply by summation of the individual inputs.

In labeling experiments or experiments with changes from vegetation with different photosynthetic systems (C4 and C3), the effects of isotopic fractionation during decomposition can be negligible. Assuming no isotopic fractionation, the processes described by  $k(q)$ ,  $D(q)$ ,  $v(q)$  will be the same for all isotopes and the Eq. (5) can be modified to describe the distribution of an isotope of C,  $\rho^*(q, t)$ :

$$\frac{\partial \rho^*(q, t)}{\partial t} = I^*(q, t) - k(q) \rho^*(q, t) - D(q) \frac{\partial^2 \rho^*(q, t)}{\partial q^2} + \left( v(q) - \frac{\partial D(q)}{\partial q} \right) \frac{\partial \rho^*(q, t)}{\partial q} + \frac{\partial v(q)}{\partial q} \rho^*(q, t) \quad (6)$$

Where  $I^*(q, t)$  is the input distribution of the isotope in question. Such equations for different isotopes can then be combined to produce equations for the isotope ratios.

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However, there is in principle no problem of extending Eq. (6) to cover isotopic fractionation, although the estimation of fractionation in the different processes can be difficult (Ågren et al., 1996a)

## 2.2 Other simplifying assumptions, modifications and possible extensions of the models

Different simplifications of Eq. (2) may be needed from the ones suggested above. Priming effects (Kuzyakov et al., 2000; Fontaine et al., 2003), where the addition of labile materials stimulates decomposition of recalcitrant materials, and decomposer controlled decomposition (Schimel and Weintraub, 2003; Manzoni and Porporato, 2007) invalidates the assumption that  $R(q,t)$  is proportional to  $\rho(q,t)$ . This leads to breakdown of the linearity, necessitating the use of numerical methods (see however Neill and Gignoux, 2006).

In some situations, it may be useful to introduce a theoretical quality variable,  $Q$ , and model the theoretical distribution of SOM across this variable,  $\Theta(Q)$ . This is what has been done in continuous quality models so far (Ågren and Bosatta, 1996b). The reason for introducing  $Q$  instead of using the measured variable,  $q$ , is to simplify the models. This can be achieved if the functions describing respiration as a function of  $Q$  and movement along the  $Q$  axis are simpler than the corresponding functions depending on  $q$ . Subsequently, relationships between  $Q$  and  $q$  can be pursued. When a theoretical quality variable is introduced, one should also consider the possibility of not aiming at solving the complete model, but instead use it to derive equations for simpler properties like the total SOM, or average qualities etc. (see Ågren and Bosatta, 1996a). It is worth pointing out the analogue with the fundamental equation of quantum mechanics, the wave function, which in principle is unobservable and only projections of it represent observables (momentum, velocity etc.).

The basic model presented in Eq. (2) can be extended in several ways. An obvious extension is to use several different distributions each corresponding to a SOM fraction. For example, it may be useful to separate microbial biomass from the rest of SOM as it

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has very different characteristics. In that case a transfer function from one distribution to the other is needed and the models becomes similar to the one presented by Bosatta and Ågren (1985). Another way to extend the model is to allow multidimensional distributions, this may in fact be necessary to obtain an adequate characterization of the SOM. The formalism presented in Eqs. (2) and (3) is easily generalized to accommodate this.

### 3 Linking model and measurable distributions

#### 3.1 Model application

An application of Eq. (4) requires the functional form of  $k(q)$ ,  $D(q)$  and  $v(q)$  to be chosen. In natural ecosystems, the input consists of plant litter and rhizodeposition, and therefore the function  $I(q, t)$  can be measured at least on part of the input. The dependence of the respiration is case specific. In the case where  $q$  represents size, respiration is expected to decrease as  $q$  gets smaller and perhaps some kind of hyperbolic or power function may describe this. The function should intercept (0,0) to allow respiration to approach zero as size approaches zero. In the case where size is used as the quality measure,  $D(q)$  and  $v(q)$  must also decrease with  $q$  and intercept at (0,0) to completely stop movement along the  $q$  axis as soon as size approaches zero. The way in which the functions  $D(q)$  and  $v(q)$  approach zero may have large implications (Bosatta and Ågren, 1985).

#### 3.2 Model parameterization

When functional forms for the functions  $k(q)$ ,  $D(q)$ , and  $v(q)$  have been chosen, the parameters will have to be estimated. Some parameters may be deduced from theoretical considerations, but most will have to be estimated from field or laboratory experiments. To be able to estimate the parameters, we need experiments with different treatments,

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for example experiments with different inputs similarly to the parameterization of the models with SOM pools. The process of parameterization is illustrated in Fig. 2. In the beginning of the experiment (at time  $t_0$ ) the distribution on the left hand side of Fig. 2 is measured. In some cases it may also be measured on an archived soil if the storage conditions can be trusted not to have altered the distribution. Then different treatments are applied and at a later stage (at time  $t_1$ ) the distributions are measured under the different treatments as shown on the right hand side of Fig. 2. The changes in the distributions under the different treatments are then used to estimate the parameters of the functions  $k(q)$ ,  $D(q)$ , and  $v(q)$  with an appropriate optimization routine. As the number of parameters of these functions is limited, this may actually be achieved. Iso-  
tope measurements at different points along the distribution will allow for distributions of the other carbon isotopes or isotope ratios along the quality axis to be concatenated. These will constitute an additional source of data that would be highly valuable for parameter estimation.

When the measured quality variable makes the simplifying assumptions inappropriate, the more general Eq. (2) may have to be applied. In these cases,  $M(q, q', t)$  and  $R(q, t)$  can be complicated functions, for example in the case of  $^{13}\text{C}$  nuclear magnetic resonance (NMR) spectra to be discussed later. In these cases, it may be advantageous to use a model introducing a theoretical quality variable,  $Q$ . There is not likely to be a monotonous relationship between the measured quality variable,  $q$ , and  $Q$ . Nevertheless, estimation of the relationship between  $q$  and  $Q$  could be achieved through multivariate calibrations (Martens and Naes, 1989). First, the theoretical distribution is established by model fitting to experimental data with different treatments. This gives rise to theoretical distributions across the theoretical quality variable,  $\Theta(Q)$ . The multivariate calibrations are used to establish a relationship between measurements,  $\rho(q_i)$ , and the theoretical distribution,  $\Theta(Q_j) = f(\rho(q_i))$ . Another possibility is to attempt to predict other properties of the theoretical distribution such as the average quality (i.e.  $\bar{Q} = \int Q\Theta(Q, t)dQ / \int \Theta(Q, t)dQ$ ). The multivariate approaches however require data from experiments with many different treatments influencing the distributions.

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## 4 The difference between continuous distributions and fractions

As carbon and isotopes of carbon can only be measured on a finite sample, a continuous quality distribution of SOC can only be measured by concatenating or merging the finite samples into a distribution. Therefore, measuring a distribution may be viewed as measuring a large number of fractions along the same separation axis, and one might ask what the difference is between measuring fractions and measuring a continuous distribution. The difference is both in terms of model formulation and in terms of requirement for the measurements. The requirement for the measurements is that the obtained distribution is approaching a continuum. This is illustrated in Fig. 3. If there is an underlying continuous distribution, then the resolution of the measurements should be so small that the measured distribution is approaching the underlying continuum. This is hardly possible with two or three fractions, especially if more or less arbitrary demarcations between the fractions or model pools are chosen. As we do not know the underlying distribution there is no way to ensure that the resolution of the measured distribution is actually fine enough to approach the underlying continuous distribution with the desired certainty. However, a requirement that must be fulfilled is that measurements next to each other have values closer to each other than measurements longer from each other. This means that the distribution can be viewed as continuous and that it is independent of the more or less arbitrary choices of demarcations between the fractions. Another requirement could be that changing the demarcations between the different fractions constituting the distribution or increasing the number of fractions does not markedly change the distribution. The measured continuous SOM quality distributions provide much information about the underlying distribution which should be valuable not only for model development, but also for direct interpretations. Once the underlying distribution has been revealed and possible peaks have been found and identified, it may again be possible to measure a smaller number of fractions where the demarcation between them is determined by the underlying continuum.

The important difference in model formulation can be seen from Eq. (3) where a

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single function  $F(q,t)$  is used to describe the movement of SOM along the  $q$  axis, a single function  $k(q,t)$  is used to describe respiration. If we are measuring a continuous distribution, these functions are also more likely to be continuous. This means that these processes can be described by a very limited number of parameters. In contrast, an equivalent multi-compartment formulation would require a large number of compartments and an immense number of parameters to describe these processes from all of the compartments. Thus, the requirement that the functions  $F(q,t)$  and  $k(q,t)$  are continuous, considerably constrains the shape of functions, whereas for the multi-compartment formulation even large differences in parameter combinations will result in nearly equally good fits between data and model (Hyvönen et al., 2005). This means that the resulting parameter combinations are unlikely to have a meaningful biological interpretation. The reduced number of parameters and large number of measurements used for model parameterization of the continuous quality distributions mean that the number of parameters combinations that will allow the model to fit the experimental data is reduced. This is likely to increase the possibility for meaningful interpretations of the parameters and the validity outside the range of conditions tested in the experiments.

## 5 Measuring continuous quality distributions of SOM

Theoretically the methods that have been used to fractionate SOM into a small number of fractions can be modified by increasing the number of fractions to constitute a virtual continuum. Often, however, this will result in too laborious methods and therefore the application of continuous quality distribution models involves developing new fractionation methods and employing new technologies that are based on similar principles. Fractionation methods can be divided into physical, chemical and biological fractionation methods and we will adopt the same categories here.

Isotope techniques including measurements of isotope ratios in experiments with vegetation changes between C4 and C3 plants, natural abundance of  $^{14}\text{C}$  and isotope

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labeling experiments can be used to understand the dynamics of the different SOM fractions (Saggar et al., 1996; Balesdent and Mariotti, 1996; Bernaux et al., 1998; Bruun et al., 2004, 2005a). In a similar way, measuring isotope ratios along the quality distributions of SOM from similar experiments will undoubtedly greatly help interpretations and model development of continuous quality distribution models of SOM. This requires that the isotopes are measured frequently enough along the quality axis to produce a distribution of the other isotopes or the isotope ratio.

## 5.1 Physical fractionation methods

### 5.1.1 Particle size

Fractionation according to particle size is based on the fact that mineral particles of different sizes are also of different mineralogical origin and composition and therefore interact with SOM in different ways (Christensen, 1992). The sand fraction which is dominated by quartz only exhibits weak interactions with SOM while clay provide a large negatively charged surface area for sorption of SOM. This provides different degrees of protection from microbial degradation. However, the transition from quartz to clay minerals is more likely to be continuous rather than discrete.

Methods used to separate SOM according to particle sizes include sieving and sedimentation and more advanced fractionation methods after dispersion treatments such as treatment by ultrasonic vibrations or application of a chemical dispersant (Christensen, 1992). However, in their extensive review von Lützow et al. (2007) found very variable estimates of turnover times for SOM in different fractions. The lack of an unequivocal relationship between particle size and turnover time may be improved by separating a size continuum to resolve the distribution better, but may also require separation according to other quality variables as well.

A range of methods have been used to separate colloids according to size (Buffle and Leppard, 1995; Kretzschmar et al., 1999). Some of these methods may be adapted to continuous size distributions of SOM in clay and silt fractions of soils. To measure the

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whole range of the SOM size distribution relevant for SOM models requires application of a combination of these methods in different size ranges.

Sieves can be used to measure a size distribution of particles larger than 20–40  $\mu\text{m}$  depending on the soil type. However, most carbon is present in smaller sized fractions (Christensen, 1992). In theory, the resolution can always be improved by including more sieves, but the number will be limited in practice. Filtration and ultrafiltration can be used to isolate smaller sized particles and has been used to separate aquatic colloids in the range of 1 nm to 100  $\mu\text{m}$  (Buffle and Leppard, 1995). To avoid artifacts especially colloid interactions with the membrane and colloid coagulation at the membrane surface, tangential flow filtration may be used to reduce the last artifact.

Sedimentation in water by gravity, centrifugation or ultracentrifugation can be used on smaller particle sizes; however, it suffers from the problem that it separates on the basis of both size and density. Traditionally, sedimentation has been performed by repeatedly suspending soil particles in a water column and waiting for a specific time (calculated according to Stokes law) before removing the upper part of the column (Christensen, 1992). Obtaining a distribution of sufficient resolution probably requires application of new techniques.

Split flow thin cell (SPLITT) fractionation is a technique developed to separate mixtures of materials into fractions of homogeneous materials (Giddings, 1985) and it has already been employed for SOM fractions (Kiem et al., 2002). Size exclusion chromatography and capillary hydrodynamic fractionation (DosRamos and Silebi, 1990) can generally only be used to fractionate particles smaller than 0.1  $\mu\text{m}$  without serious artifacts. A very promising technique to separate on the basis of particle size, is field flow fractionation (FFF) (Fraunhofer and Winter, 2004). The technique employs a flat channel through which a carrier liquid is pumped establishing a parabolic laminar flow profile. The sample is propelled through this channel while a physical field is applied across it making the particles accumulate at one flank of the channel. Small particles exercise faster Brownian motions and can therefore diffuse against the physical field to where the laminar flow is faster and are thus eluded faster. Several physical fields

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can be applied across the membrane giving rise to different sub-techniques. The most important sub-techniques in connection with colloids are sedimentation FFF where the channel is rotated in a centrifuge and flow FFF where a cross-flow is established through permeable channel walls. The technique has been applied to study colloid transport in soils (Ranville et al., 2005), but there seems to be a great potential for using the technique on the clay fractions after removing the larger fractions by SPLITT fractionation or some other method.

### 5.1.2 Density

Density fractionations have most often consisted of separating SOM from heavy and light fractions (Christensen, 1992). The heavy fraction is assumed to consist of organomineral complexes and the SOM of this fraction to be stabilized by the interaction with the mineral phase. The light fraction is assumed to be free of mineral associations and is therefore more susceptible to microbial decay. Other more complex fractionation schemes have been proposed. Shaymukhametov et al. (1984) separated the soil into three fractions: a light fraction with no mineral associations, and medium density fraction consisting of organomineral complexes and a heavy fraction consisting of minerals coated with SOM. Other studies have fractionated the soil into even more density fractions (e.g. Dalal and Mayer, 1986; Essington and Mattigod, 1990; Cambardella and Elliott, 1994; Six et al., 2000). In reviewing the literature, Christensen (1992) recognized that the bonding strengths between SOM and mineral particles varies continuously. Therefore, there does not seem to be a specific density at which mineral associated organic matter is separated from free organic matter. Rather, the ash content, which indicates presence of mineral soil, seems to increase as density increases, displaying a continuum rather than fixed cutoff.

The usual method used to fractionate soil according to density is by centrifugation of the sample in a heavy density liquid, to obtain a fraction heavier and lighter than the density of the liquid (Christensen, 1992). In recent years, polytungstate has been the preferred substance. This can be generalized by using a range of different densities to

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obtain a distribution with the desired resolution. However, this is a very tedious procedure and a potentially more powerful approach is to use density gradient centrifugation (DGC). DGC has not been widely used for this purpose, but is being applied routinely for separating microorganisms from soil or other media (Lindahl and Bakken, 1995; Stevens and Jaykus, 2004). After centrifugation in a density gradient a density distribution of particles will have settled in the gradient and samples could be taken out at different positions for determination of C content and isotope ratios.

### 5.1.3 Aggregate size

OM seems to turn over more slowly within microaggregates (Six et al., 2002). This has been ascribed to protection involving several mechanisms including seclusion from microbes (Veen and Kuikman, 1990), reduced oxygen diffusion (Sexstone et al., 1985; Vor et al., 2003) and prevention of microbial predation within aggregates (England et al., 1993). Small aggregates (i.e. microaggregates) seem to offer better protection than larger aggregates. A distribution of aggregate sizes can be obtained by applying either sieving or sedimentation without a preceding dispersion treatment. For the separation of aggregates into a virtual continuum of different sizes, the SPLITT technique described earlier may be applicable. The separation of aggregates is complicated by the fact that a hierarchy of aggregates seems to exist, where smaller first order aggregates are found within larger second order aggregates, which again are collected into larger third order aggregates (Tisdall and Oades, 1982; Oades and Waters, 1991).

### 5.1.4 Association with iron oxides

Iron oxides provides a large surface area in many soils and a strong bonding with SOM by ligand exchange providing protection against microbial decay (Torn et al., 1997; von Lützow et al., 2007). This means that amount of and crystallinity of iron oxides influences the turnover of the SOM associated with it. Some studies have indicated that clay fractions of intermediate magnetic susceptibility were most stable (Shang and

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Tiessen, 1997) while other studies have indicated that the fraction of highest magnetic susceptibility was most stable (Shang and Tiessen, 2000). As the transition from SOM with a low degree of association with iron oxides to a high association or from particles with low magnetic susceptibility to high is likely to be continuous, separating a continuous distribution also appears to be relevant.

Particles of different magnetic susceptibility have been separated using high-gradient magnetic separation (Shang and Tiessen, 1997). In this technique a soil suspension is passed through tubes fitted with stainless steel wool placed in a magnetic field. The material of a high magnetic susceptibility is trapped while the less susceptible passes through the tubes. By gradually increasing the magnetic field density is should be possible to separate a virtual continuum of particles of different magnetic susceptibility. Despite promising results, the number of studies using high-gradient magnetic separation is still limited and restricted to tropical soils (von Lützow et al., 2007). Therefore separation into a virtual continuum using this technique could prove interesting.

### 5.1.5 Surface charge

OM adsorbed on soil particles changes the charge of the particles (Tipping and Cooke, 1982; Saito et al., 2004). Whether resistant SOM adsorbed on the surfaces changes surface charge more or less than more labile SOM is unknown. However, as the functional groups on the surface of the SOM changes as it decomposes, the effect on surface charge is also likely to change. Therefore, it may be worth attempting to separate soil particles according to surface charge to obtain a quality distribution of SOM. Electrophoresis is a technique where an electrical field is applied across a cell and the particles start moving according to their electrophoretic mobility which is related to zeta potential and surface charge (Hunter, 1981). The technique has been used to separate soil clays according to electrophoretic mobility (e.g. Arshad et al., 1971).

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## 5.2 Chemical fractionation methods

The chemical fractionation methods involve some kind of chemical treatment that is applied to hydrolyze or oxidize labile organic matter more susceptible to the treatments. These methods can be generalized by applying successively higher concentrations or successively longer treatment time. We suggest that fractionation methods using different concentrations and allowing the process to attain steady-state before the measurements are carried out is better than methods employing different treatment times for the following reason. Under the non steady-state conditions the labile SOM will supposedly be removed faster than more resistant SOM. However, since steady-state has not been attained all of the labile material will not have been removed and a small part of the resistant SOM will also be affected right from the beginning of the treatment.

### 5.2.1 Chemical Oxidation

A range of different chemical treatments (e.g.  $\text{H}_2\text{O}_2$ ,  $\text{Na}_2\text{S}_2\text{O}_8$  and  $\text{NaOCl}$ ) has been adopted to remove labile SOM from soil leaving behind a more resistant fraction (Mikutta et al., 2005). Different kinds of chemical oxidation methods have also been proposed to isolate black carbon (Schmidt et al., 2001; Simpson and Hatcher, 2004), which is believed to be resistant to biodegradation (Bruun et al., 2008a). Several studies have found the fractions left behind after oxidation to be of higher radiocarbon ages than those removed (Kleber et al., 2005; Eusterhues et al., 2005; Helfrich et al., 2007). However, attempts to verify that the fraction left behind changes in response to organic matter inputs and other aspects of management history are scarce and not very successful (Balesdent, 1996; Plante et al., 2004; Bruun et al., 2008b). This may mean that the chemical oxidation agents may not fractionate the soil in a meaningful way in terms of SOM turnover, but it may also reflect the fact that a stable fraction cannot be resolved by a few fractions with different susceptibility to oxidation, which may possibly be alleviated by measuring a continuous distribution of oxidizability.

Continuous distributions could be achieved by modifying oxidation methods using

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different concentrations of oxidants or oxidation times with the results concatenated into a distribution. An example of the later can be found in Plante et al. (2004) who oxidized soils supposed to have different amounts of resistant SOM using  $H_2O_2$  and took out aliquots by syringe after different oxidation times and analyzed it for organic carbon.

5 The resulting distribution seemed to differ between the soils, with soils containing more labile carbon losing carbon faster during the first 3–8 h.

### 5.2.2 UV oxidation

UV oxidation was proposed as a method to isolate an inactive fraction of SOM because the oxidizing agents produced by the light were believed to be unable to penetrate into aggregates (Skjemstad et al., 1993). Later, UV oxidation was developed into a method to reduce SOM fractions other than black carbon before determination of the black carbon content (Skjemstad et al., 1999). UV oxidation offers opportunities for measuring quality distributions by varying either the effect of the UV lamp or the oxidation time. Skjemstad et al. (1993) observed the disappearance of organic C during the first 8 h of oxidation and found that C disappeared faster in some soils than other soils. In contrast, Bruun (2008b) observed a faster removal of old SOM than litter, possibly because of the lignin in the litter that is resistant to UV oxidation, and thus did not find any evidence that old SOM is more protected from UV oxidation. The method is rather laborious and fractionating the complete quality continuum may therefore be difficult unless modifications of the procedure are implemented. For example, it may be possible to sub-sample after different oxidation times or measure  $CO_2$  evolution and the isotopic composition of the evolved  $CO_2$ .

### 5.2.3 Thermal treatment

25 Thermal treatment will, through oxidation and/or production of pyrolysis products, remove some SOM and leave other SOM behind. A distribution, known as a thermogram can be produced by following a set heating program usually with a constant heating

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rate. The rate of oxidation/pyrolysis can be determined by weight loss (thermogravimetry), carbon dioxide production or the pyrolysis products can be analyzed by different kinds of ionization mass spectrometry (David, 1975; Schulten, 1993). Either method offers an easy way to measure the amount of carbon or mass lost at different temperatures producing a thermogram. Thermal treatments often exhibit different peaks for labile and more resistant SOM (Kristensen, 1990; Schulten and Leinweber, 1999; Siewert, 2004; Lopez-Capel et al., 2005b; Bruun et al., 2008b). Thermal treatments have also been used to isolate black carbon from soil (Gustafsson et al., 1997, 2001; Gelinas et al., 2001). If a strong relationship between the thermogram and the degradability of SOM can be established, the use of a thermogram to characterize a continuous distribution of SOM in a distributional model, would be a straight-forward procedure.

Lopez-Capel et al. (2005a) analyzed the evolved gasses during the thermal treatment by coupling a thermo-gravimetric system with an isotope ratio mass spectrometer. This appears to be a very powerful setup because it enables measurement of isotope ratios along the quality distribution of SOM.

Mass spectrometry of the pyrolysis products can be used to construct thermograms with the total ion intensity, but can further be used to make thermograms of compound classes such as carbohydrates, lignin monomers, lignin dimers, alkyl aromatics, lipids and N-containing compounds, thus, giving rise to a different distribution for the each compound class (Schulten and Leinweber, 1999, 2000). To apply the proposed distributional models to these distributions therefore also requires a model with several distributions and assumptions about their formation.

#### 5.2.4 Hydrolysis

Acid hydrolysis is one of the most widely used methods for isolation of an inactive fraction of SOM (e.g. Laevitt et al., 1996; Trumbore et al., 1996). Usually hot 6 M HCl is refluxed for 18 h and the supernatant is removed after centrifugation. Subsequently, the remaining amount of C is measured. A distribution of hydrolyzability can be produced

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by employing different concentrations of acid or different reaction times. As requires a large number of treatments to get a sufficient resolution on the measured distribution, samples of the supernatant may instead be taken and analyzed for dissolved SOM by different methodologies. Acid hydrolysis has been widely applied to isolate an inactive fraction and seems to isolate old SOM (Martel and Paul, 1974; Laevitt et al., 1996; Paul et al., 1997). However, as for the chemical oxidations the fraction of hydrolysable C seems to be relatively independent of the management in field trials (Balesdent, 1996; Plante et al., 2006). Some of these problems may be solved by measuring a continuous distribution instead of just using a predetermined acid concentration or treatment time.

### 5.3 Spectroscopic methods

Several spectroscopic methods including py-GC/MS, near-infrared spectroscopy (NIR), mid-infrared spectroscopy (MIR) and nuclear magnetic resonance spectroscopy (NMR) and others have the potential to generate spectra that are related to quality of SOM. Generally there is not likely to be a simple relationship between the spectra and  $R(q,t)$  and  $M(q,q',t)$ . However, it may still be possible to establish the relationships by multivariate calibrations as described above. Therefore we will briefly describe the possibilities of using NMR and NIR.

#### 5.3.1 Nuclear magnetic resonance spectroscopy (NMR)

NMR measures the shifts in the frequency at which atomic nuclei resonate relative to a reference compound when subjected to a magnetic field. The chemical shift is influenced by the electron clouds around the nucleus and therefore provides information about the chemical environment in which it exists (Veeman, 1997). The chemical composition of SOM has been characterized by solid state  $^{13}\text{C}$  NMR (e.g. Skjemstad et al., 1997; Kögel-Knabner, 2002). The spectrum that is obtained by  $^{13}\text{C}$  NMR is generally split into four main regions (carbonyl, aromatic, O alkyl, and alkyl) and the area

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of a given region is proportional to the frequency of that group. During decomposition the spectra of SOM change in characteristic ways (Skjemstad et al., 1997) with alkyl carbon being lost initially.

In the case of NMR spectra, the measured quality variable across which the carbon distribution is measured is the chemical shift. A specific chemical shift corresponds to a C atom in a specific chemical constellation and therefore should also correspond to a specific respiration rate and a specific rate of transformation to other chemical constellations. Unfortunately, as for most spectroscopic methods, there is not likely to be a simple relationship between chemical shift and  $R(q,t)$  and  $M(q,q',t)$ .

### 5.3.2 Near-infrared spectroscopy (NIR)

The detailed chemical structure of SOM can also be revealed by near-infrared spectroscopy (NIR), which measures absorbance or reflectance of electromagnetic radiation in the near infrared range. This is related to vibrational and rotational movements of important biochemical functional groups such as -CH, -OH, and -NH chemical bonds (Shenk et al., 2001). During the course of decomposition, the NIR spectra is modified in a regular way (Joffre et al., 1992; Gillon et al., 1999) and the pattern of decomposition can be predicted from the NIR spectra (Bruun et al., 2005b). However, no monotonous relationship is likely to exist between the frequency at which light is absorbed and resistance to biodegradation. However, using multivariate analysis, these modifications in spectra have been correlated with the change in the average theoretical quality of the carbon compounds in a model for litter decomposition (Joffre et al., 2001).

### 5.4 Biological fractionation methods

The advantage of biological fractionation methods is that they are related directly to the mechanisms responsible for the decomposition in the soil. Soil incubations under constant favorable conditions have been used to isolate labile and more resistant fractions of SOM (Paul et al., 2006). This can be generalized to measure a continuous

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quality distribution by continuously measuring CO<sub>2</sub> evolution. However, analogous to the chemical treatments of different time, the incubations will not start by removing the labile material but also remove resistant SOM, albeit more slowly right from the beginning. If a whole continuum of SOM qualities exists, the data produced in the incubations are not likely to be enough to restrain the quality distribution (Bruun and Luxhøi, 2006). Furthermore, by the very nature of resistant SOM, incubations cannot be used to measure the distribution covering the SOM of lower quality. Another problem with soil incubations is that the soil is often disturbed during sampling so the observed flux of CO<sub>2</sub> is due to mineralization of organic matter liberated from protection rather than a labile fraction occurring in the soil.

A possible alternative would be to use enzyme digestion. A range of enzymes designed to dissolve different organic compounds very fast at high temperatures has been developed. This type of enzymatic digestion could also be used to estimate a quality distribution by repeated measurements of the amount of dissolved SOM. To our knowledge enzyme digestion has not been used to fractionate SOM before and require development and their usefulness needs to be proved. A potential problem with this approach is that lignolytic enzymes seem to be unable to digest all lignin in fresh plant material although it is not considered to be highly resistant to decay (Kiem and Kögel-Knabner, 2003). As the addition of enzymes also results in the addition of organic matter, these techniques would require some form of labeling experiment to distinguish C from enzymes and SOM.

## 5.5 Measuring several distributions

As suggested in the model formulation it may be useful to determine quality distributions for several fractions. For example, it could be useful to measure the quality of the microbial biomass separately because of the very different role of this fraction of SOM. However, there is no obvious way to separate microbial biomass from the rest of the SOM. More generally the approach of separating the SOM into fractions with different distributions, suffers from the same shortcomings as the models of measurable frac-

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tions. Usually there will be no well defined thresholds between the fractions making the choice of a threshold more or less arbitrary. Therefore, it is doubtful that this can be made operational.

## 5.6 Distributions in more dimensions

5 Measuring distributions in several dimensions is probably necessarily because a single quality variable as defined above is not likely to capture all the different mechanisms that will affect the decomposition of SOM. Essentially what it requires to apply continuous quality SOM models in two dimensions is two different ways of measuring quality, say  $q_1$  and  $q_2$ . For example, first a distribution of particle sizes may be separated and  
10 then samples along this distribution could be separated by thermal analysis. Such a combination of fractionation methods may provide very valuable information, because it leads to a characterization of SOM quality of a much higher resolution and may capture different mechanisms of stabilization.

## 6 Discussion and conclusions

15 Generally two different approaches have been taken to represent the heterogeneity of SOM in SOM models. Either multi-compartment models that represent SOM as number of pools or distributional models representing SOM by a quality distribution have been employed. To increase the number of criteria that the multi-compartment models can be validated against and make the models more mechanistic several authors have  
20 advocated that the pools of these models should correspond to the fractions that can be measured and have a functional role in the soil. Similar arguments can also be used to argue that distributional models should be based on measurable quality distributions and this is the point we are trying to advance in this paper.

25 We introduce a quality variable,  $q$ , which can be any measurable variable (e.g. particle size density or resistance to chemical treatment) related to quality and a distribution

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of carbon,  $\rho(q,t)$ , across that variable, which is the distribution we will attempt to measure. A distribution will always be measured with a certain resolution and therefore it may be argued that measuring a distribution is merely a case of measuring many fractions. This is partially true, however, measuring a distribution requires that the fractions are so close to each other that the distribution approaches the underlying continuum so much that the continuum can be estimated. This allows the models to be formulated as distributional models instead of multi-compartment models which can reduce the number of parameters that have to be estimated considerably. The reduced number of parameters and large number of measurements used for parameterization mean that the number of parameter combinations that will allow the model to fit the experimental data is reduced, increasing the possibility for meaningful interpretations of the parameters and the validity outside the range of conditions tested by experimentation. Fractionation according to more quality variables giving rise to continuous quality SOM distribution in two or more dimensions may be necessary to get a characterization of the SOM distribution which is sufficient to capture all the aspects of SOM quality.

Many methods have already proven their merits for measuring SOM fractions. These fractionation methods have to be modified to enable measurement of continuous quality distributions, and most often, new techniques need to be developed. The measured continuous quality SOM distribution should also be useful for direct interpretations and knowledge about the underlying continuous distribution may help directing useful discrete fractionations schemes.

Physical fractionation methods that appear promising for measuring continuous quality distributions of SOM according to particle size include sieving, sedimentation and some more advanced methods such as split flow thin cell fraction (SPLITT) and field flow fractionation (FFF). Sieving, sedimentation and SPLITT can also be used to measure distributions of aggregate sizes. Density gradient centrifugation is a potential method to measure density distributions of SOM. Surface charge is a large unexplored variable for fractionating soil for measurement of SOM quality distributions. Different electrophoretic methods can be used to fractionate soil according to surface charge. A

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number of oxidation methods have been used to isolate discrete fractions of SOM and can potentially be used to isolate distributions as well. Isolation of a whole distribution using these methods may result in useful information increasing the applicability of these methods. Methods include oxidation by UV light, thermal treatment and chemical agents such as  $H_2O_2$ ,  $Na_2S_2O_8$  and  $NaOCl$ . Hydrolysis using different acids is also a possibility for measuring quality distributions for SOM models. Finally, biological fractionation methods including incubations and enzyme digestion may hold some potential while a number of spectroscopic methods offer more advanced opportunities.

In conclusion, there seems to be a range of potential methodologies that can be employed to measure distributions to represent quality distributions in SOM models. Based on the evidence available, we believe that fractionation according to size and density and thermal treatment is the most promising methods to be used for the fractionation of continuous quality SOM distributions. The fractionation methods presented here, offers new opportunities for improving SOM models in terms of predictive power and mechanistic understanding. Developing the distributional models in concert with the fractionation methods to measure the distributions will be a major task. New fractionation techniques will have to be developed and the methods can be combined in a large number of different ways. Therefore, this task requires the effort of a large research community. The improvements in terms of predictive capability of the SOM models as well as conceptual and mechanistic understanding of SOM dynamics that this approach has to offer, remains to be shown. We hope that the current paper will spawn interest in the approach and entice enough researchers to explore the possibilities to prove its merits.

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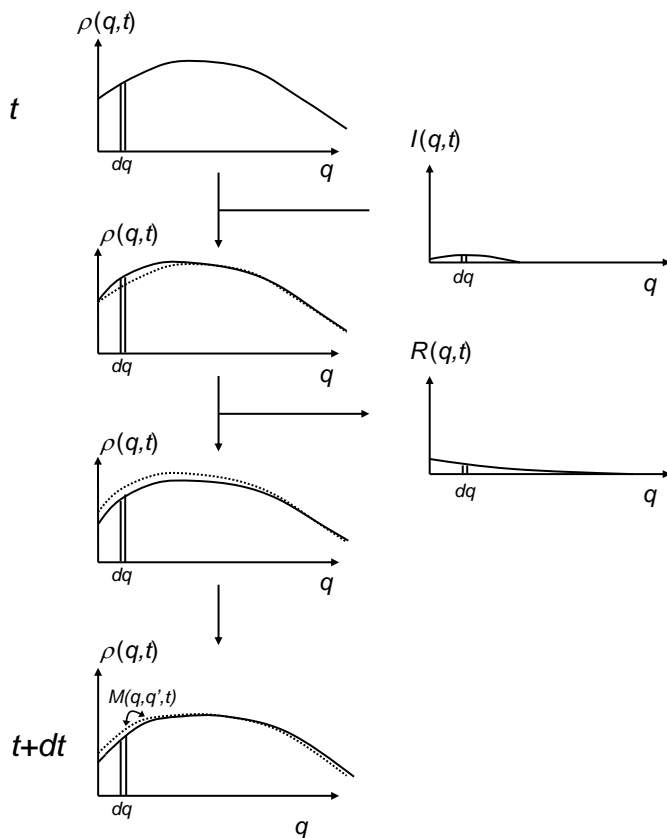
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**Fig. 1.** Changes to the quality distribution of the model in Eq. (2) during a time step. The distribution,  $\rho(q, t)$ , occurring at time  $t$  received carbon from inputs in the form of the distributions  $I(q, t)$  and loses carbon due to respiration in the form of the distribution  $R(q, t)$ . Finally the distribution is modified by changes in quality or movement of material from quality  $q$  to  $q'$ ,  $M(q, q', t)$ .

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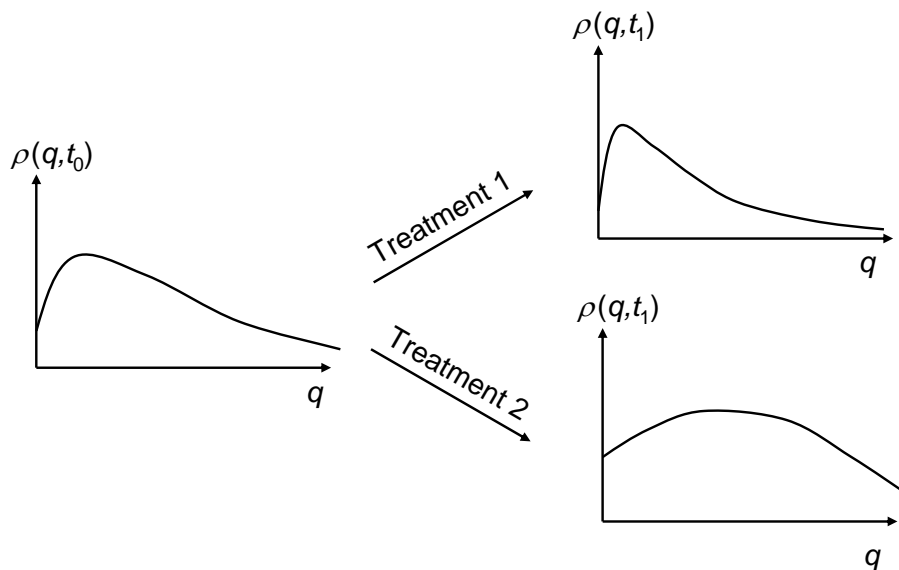
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**Fig. 2.** Changes to a quality distribution induced by different treatments of an experiment applied from time  $t_0$  to  $t_1$ . These changes are used to estimate the parameters of the distributional models advocated here.

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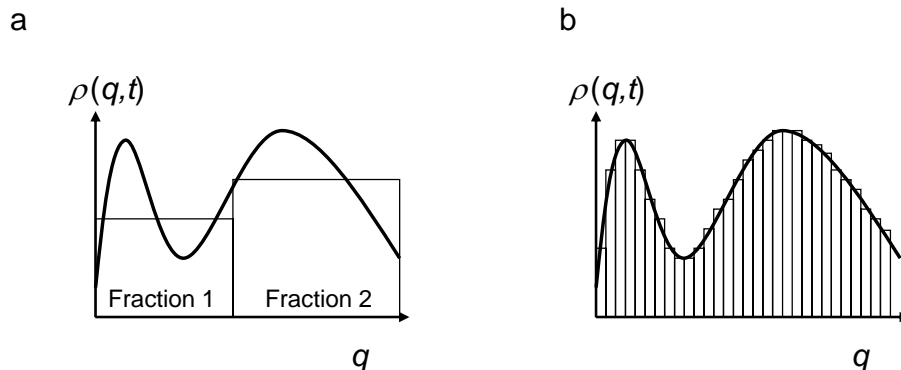
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**Fig. 3.** Illustration of the way an underlying continuous distribution is approximated by concatenating a large number of measurements along the axis of measurement. In (a) the underlying distribution is fractionated into two arbitrary fractions that is difficult to relate to the underlying distribution, whereas in (b) the number of fractions has been increased so that the distribution approaches the underlying continuous distribution.

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