Anoxic conditions in a Douglas fir litter layer
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4 Simulating the anoxic volume of a Douglas fir litter layer

with C. Rappoldt, W. Bouten and J.M. Verstraten
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Abstract
Forest soils are the largest contributor to global N$_2$O production. An important source of N$_2$O is denitrification, which is associated with the occurrence of anoxic conditions. Anoxic conditions in soil result from an oxygen demand that is larger than the oxygen supply due to oxygen diffusion. Oxygen diffusion in mineral soils depends on air-filled porosity and soil structure. A simple but physically sound representation of forest soil structure is needed for a good parametrization of models, which predict the anoxic soil volume and accompanying production of nitrous oxide.

The aim of this study is to test the applicability of a method for the characterization of soil structure for a litter layer. In this method soil structure is represented by an equivalent cylinder system with cylinders of different radii and infinite length. Applicability of this method for litter layers would be advantageous in large-scale model applications as it is simple and fastworking.

The geometrical information of the structure that is needed for the calculations of the cylinder system is the frequency distribution of distances from points in the organic matter fabric to the nearest interparticle pore. This was derived from a soil thin section.

Testing the method involves the application of an oxygen diffusion-reaction model both to the equivalent cylinder system as well as to the organic matter fabric observed in a thin section. The model result to be evaluated is the relation between the anoxic fraction and the process length d, which depends on the diffusion coefficient, oxygen consumption rate and oxygen concentration in interparticle pores. The anoxic volume depends both on the process length d and shape. Deviations in the relation between anoxic volume and d for the cylinder system and the organic matter fabric are attributed to simplification of shape.

The absolute error introduced by simplification of shape was 0.022-0.029, which amounted to about 25% of the anoxic fraction. An error of this order is acceptable, since the uncertainties in factors determining the anoxic fraction in a litter layer are expected to be still larger, due to variations in diffusion coefficients and particle size distributions. Furthermore, with the cylinder system a correction can be made for the use of 2D cross-sectional distances instead of the true 3D distances, providing that the structure is isotropic. In practice however, cross-sectional distances may be used without a correction as the effects of simplification of shape and the use of cross-sectional distances partly compensate each other. For succesful application of the method, it is crucial that a clear distinction between inter- and intraparticle pores can be made.
4.1 Introduction

Soils are the largest source of global $\text{N}_2\text{O}$ production, with forest soils as the most important contributor (Davidson, 1991; Duxbury et al., 1993). A significant source of $\text{N}_2\text{O}$ is denitrification, which is associated with the occurrence of anoxic conditions in soil. The anoxic volume of soils can be estimated with diffusion-reaction models (Leffelaar, 1979; Smith, 1980; Rappoldt, 1990, Renault and Sierra, 1994). Estimates of anoxic volume fractions are also implemented in various models simulating nitrous oxide production (Arah and Vinten, 1995; Vinten et al., 1996; Li et al., 2000; Riley and Matson, 2000).

Anoxic conditions in soil result from an oxygen demand that is larger than the oxygen supply due to oxygen diffusion. Oxygen diffusion in mineral soils depends on air-filled porosity and soil structure. Estimates of the anoxic volume of a soil have been simulated with different approximations of soil structure: homogeneous soil layers (Cho et al., 1997; Freijer, 1994b), aggregate assemblies (Arah and Vinten, 1995; Vinten et al., 1996; Riley and Matson, 2000) or soil structural units divided by cylindrical pores (Rijtema and Kroes, 1991).

Simulated anoxic soil volumes appeared to be very sensitive to the precise representation of soil structure (Arah and Vinten, 1995). Therefore, a simple but physically sound representation of forest soil structure is needed for a good parametrization of models, which predict the anoxic soil volume and accompanying production of nitrous oxide. In forest soils, the structure of the mineral soil differs from that of the litter layer, which largely consists of organic matter. As the litter layer significantly contributes to total surface fluxes of nitrous oxide (Musacchio et al., 1996; Dong et al., 1998; Regina et al., 1998), it is relevant to specifically address the structure of litter layers in diffusion-reaction models (Li et al., 2000).

The structure of a litter layer is a typical example of an aggregated "soil" structure. Oxygen diffusion in aggregated soils is characterized by a clear distinction between diffusion in the pore phase and in the soil matrix (Rappoldt, 1990). This clear distinction is illustrated in the litter layer by steep oxygen concentration gradients within litter particles and constant atmospheric oxygen concentrations in interparticle pores at average water contents (chapter 2). Steep oxygen concentration gradients within litter are due to the low diffusion coefficient of the organic matter and oxygen consumption within the particles (chapter 3). In interparticle pores, the oxygen diffusion rate is sufficiently high to maintain oxygen concentrations near atmospheric levels at all times when the water content is below ca. 0.6 m$^{-3}$ m$^{-3}$ (chapter 2).

Rappoldt (1990) and Rappoldt and Verhagen (1999) demonstrated that the structure of aggregated soils can be represented by equivalent systems of cylinders with different radii or sheets with different thicknesses. The structure of aggregated soils is characterized by the generalized surface-area-to-volume-ratio, which largely determines diffusion-reaction processes (Rappoldt, 1990). This geometrical property
can be measured in a thin section as a distribution of distances from random points in the soil matrix to the nearest interparticle pores. An equivalent cylinder or sheet system that represents soil structure has the same generalized surface-area-to-volume-ratio as the soil structure.

In this study, we aim to test the applicability of the method as developed by Rappoldt and Verhagen (1999) for litter layers. Applicability of this method for litter layers would be advantageous in large-scale model applications as it is simple and fastworking. Testing the method involves the application of an oxygen diffusion-reaction model both to the equivalent cylinder or sheet system as well as to the organic matter fabric digitized from a thin section. Since the method involves the derivation of a simple equivalent of soil structure, we specifically focus on the error which is hereby introduced. Furthermore, we address effects of using a 2D image instead of a 3D structure. Finally, we discuss effects of sample variability and of the feasibility of distinguishing between organic matter, and inter- and intraparticle pores in a thin section.

4.2 Materials and methods

The method is tested by applying an oxygen diffusion-reaction model both to the equivalent cylinder or sheet system as well as to the digitized organic matter fabric of a thin section. Subsequently, deviations in model results are compared for the cylinder system and the organic matter fabric. For application of the diffusion-reaction model on the organic matter fabric in the litter layer, thin sections of the litter layer were converted to gridmaps in PCRaster GIS, with a distinction between organic matter and pores. These maps were used in a PCRaster diffusion-reaction model, which has also been used in chapter 3. For application of the diffusion-reaction model to the equivalent cylinder system, this system is derived from the distribution of distances from a point in the organic matter to the nearest pore, as measured in the gridmaps. Details of the procedures used are explained below.

From thin section to grid map

A glass column of 6 cm height and a diameter of 10 cm was filled with homogenized Douglas fir organic matter sampled from the F2-layer (highly fragmented needles, see chapter 2 and 3). From these glass columns one vertically (Figure 4.1) and one horizontally cutted thin section were produced. Segments of these thin sections (ca. 2 cm²) were scanned at 1200 dpi, grey scale and converted to the format of the PCRASTER GIS package (PCRaster, 1998). These scanned images were classified to maps with a distinction between organic matter and pores, using a threshold grey value (Figure 4.1). The threshold value was determined as the highest grey value (256 corresponds to white) in cells which clearly corresponded to organic matter tissues in the thin section, as observed by eye. The uncertainty in this method is not
quantified but is expected to be minor due to the excellent colour contrast between organic matter and pore both in the thin section and in the scanned GIS maps.

![Thin section and binary image](image)

**Figure 4.1**: Fig. 4.1a (left): Thin section segment (size 1.7x1.2 cm). Fig. 4.1b (right): Classified map with organic matter and pores, black is organic matter, white is pore.

**Equivalent model system of cylinders or sheets**

Equivalent systems of cylinders or sheets (plate-like structures) that represent the organic matter fabric of a litter sample are derived from the generalized perimeter-length-to-area ratio of a 2D cross section (Rappoldt and Verhagen, 1999). The generalized perimeter-length-to-area-ratio corresponds with the generalized surface-area-to-volume ratio of a 3D structure. By using cross sectional data for the calculations, the organic matter fabric is assumed to be isotropic. In the following section we explain the method in general terms, for equations and exact calculations we refer to Rappoldt (1990) and Rappoldt and Verhagen (1999).

The generalized perimeter-length-to-area ratio is defined by a distance probability density function (pdf), which is the probability density of the distance from a point in organic matter to the nearest pore in the cross section (Rappoldt and Verhagen, 1999). This pdf was automatically measured in a cross section as a frequency distribution of distances from each point in organic matter to the nearest interparticle pore (PCRaster, 1998). An equivalent cylinder system must have the same generalized perimeter-length-to-area ratio and therefore the same pdf as the real organic matter fabric. This equivalent system consists of cylinders with different radii and infinite lengths; the relative abundance of cylinders with radius Ri in the equivalent system set is expressed as the value of a weight function w(R). A weight
\( w \) is the fraction of the total cylinder volume occupied by cylinders with radius \( R_i \). So \( w \) is the probability that a randomly chosen point lies in a cylinder with radius \( R_i \). A set of discrete weights \( w_i \) is found from the requirement that the probabilities \( p_j \) belonging to a chosen number of distance intervals are preserved by the equivalent system (Rappoldt and Verhagen, 1999). Apart from an equivalent cylinder system, an equivalent system of sheets was also calculated. Sheets are plate-like structures with a thickness \( R \) and an infinite width.

In the above description, the measured 2D distances used for the derivation of a cylinder system are assumed to be true 3D distances. However, measured 2D distances in a cross section differ from the true 3D distances from organic matter to the nearest pore, which often lie outside the cross-sectional plane. The distances measured in the cross section therefore are larger than the true ones unless all interparticle pores are perpendicular to the cross section. The use of the measured 2D distance distribution for the calculation of an equivalent set of cylinders therefore leads to a bias in the contribution of various cylinder radii. This problem was solved by cross sectioning a system of cylinders as well (Rappoldt and Verhagen, 1999). The distance distribution of the cross-sectioned cylinder system should then be equal to the measured distance distribution of the real cross section. The cross-sectioned cylinder system is made isotropic by assigning a random orientation to the cylinders. Rappoldt and Verhagen (1999) describe how the weights of an equivalent cylinder system are calculated from the cross-sectional probability density function. This method for the correction of 2D distances to true 3D distances has only been implemented for equivalent cylinder systems and not for sheet systems.

**Application of a diffusion-oxygen consumption model**

We applied an oxygen diffusion-consumption model both to the equivalent cylinder (eq 4.1) or sheet systems (eq. 4.2) as to the gridmap with the digitized organic matter fabric (eq. 4.3). The gridmap with the digitized organic matter fabric has also been used in chapter 2 and 3. Diffusion was modeled with Fick's 2nd law (Crank, 1975).

\[
S \frac{\partial C}{\partial t} = \frac{D}{r} \frac{\partial (r \frac{\partial C}{\partial r})}{\partial r} - Q
\]

[eq. 4.1]

\[
S \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - Q
\]

[eq. 4.2]

\[
S \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} + D \frac{\partial^2 C}{\partial y^2} - Q
\]

[eq. 4.3]
in which:
\[ D = \text{diffusion coefficient (m}^2 \text{s}^{-1}) \]
\[ C = \text{concentration (mol m}^{-3}) \]
\[ S = \text{organic matter porosity (interparticle pores: 0.8 m}^3 \text{m}^{-3}) \]
\[ r = \text{distance from the center (coordinate) (m)} \]
\[ x = \text{distance (m)} \]
\[ Q = \text{oxygen uptake (mol m}^{-3} \text{s}^{-1}) \]
\[ t = \text{time (s)} \]

Oxygen consumption was assumed to be a zero-order reaction, with a constant oxygen consumption rate \( Q_{\text{ref}} \). The oxygen concentration outside cylinders or organic matter was held constant at an atmospheric level. Equations for the calculation of the anoxic volume of the cylinder system are presented in Rappoldt et al. (1990).

For the application of the diffusion-reaction model on the grid map oxygen diffusion transport was calculated between each individual cell and its four neighbouring cells in vertical and horizontal direction. For the calculations we used an explicit finite difference approximation as adapted from Wang and Anderson (1982):

\[
C_{ij}^{n+1} = C_{ij}^{n} + \left[ \left( \frac{C_{i+1,j}^{n} + C_{i-1,j}^{n} - 2C_{ij}^{n}}{A_{x}^2} \right) + \left( \frac{C_{i,j+1}^{n} + C_{i,j-1}^{n} - 2C_{ij}^{n}}{A_{y}^2} \right) \right] \times \left( \frac{D \Delta t}{S} \right) - \frac{Q_{ij}^{n}\Delta t}{S} \]

[eq. 4.4]

with:
\[ C_{ij}^{n} = \text{concentration in cell}_{ij} \text{ (mol m}^{-3}) \text{ at timestep n} \]
\[ C_{i+1,j}^{n}, C_{i-1,j}^{n}, C_{i,j+1}^{n}, C_{i,j-1}^{n} = \text{concentration in upper, lower, left or right neighbouring cell} \]
\[ D = \text{diffusion coefficient (m}^2 \text{s}^{-1}) \]
\[ S = \text{local organic matter porosity (0.8 m}^3 \text{m}^{-3}) \]
\[ A_{x} = A_{y} = \text{cell length (21.2} \times 10^{-6} \text{ m following from the scanning resolution of 1200 dpi)} \]
\[ Q_{ij}^{n} = \text{oxygen uptake in cell } i,j \text{ (mol m}^{-3} \text{s}^{-1}), \text{ at timestep n} \]
\[ \Delta t = \text{timestep (s)} \]

In cells where oxygen supply was lower than the constant oxygen uptake \( Q_{\text{ref}} \) of the zero-order reaction, oxygen uptake (\( Q \)) was set equal to this oxygen supply. The anoxic fraction of the cross-section is defined as:
\[ 1 - \frac{Q}{Q_{\text{ref}}} \]

\( Q \) and \( Q_{\text{ref}} \) refer to bulk oxygen consumption rates, calculated by a summation of all individual cell values of \( Q \) and \( Q_{\text{ref}} \). This procedure is considered to be more accurate than calculating the anoxic fraction of organic matter by summing the
number of cells with an oxygen concentration of zero. In such cells, there may still be an incoming oxygen flux, which is completely consumed. The model was run until equilibrium. Table 4.1 shows the model runs that were performed.

**Testing the method**

For the comparison of the equivalent cylinder system and the digitized organic matter fabrick we evaluated the relation between the anoxic fraction and the process length \( d \), defined as:

\[
d = \sqrt{D^*C/Q}
\]

with:

\( \frac{d}{\text{(m)}} \)
\( D = \text{diffusion coefficient (m}^2\text{s}^{-1}) \)
\( C = \text{external oxygen concentration (mol m}^{-3}) \)
\( Q = \text{oxygen uptake (mol m}^{-3}\text{s}^{-1}) \)

The process length \( d \) may be seen as the length scale at which oxygen concentration gradients occur, and also transitions from oxic to anoxic conditions.

**Table 4.1**: Used values in model runs of diffusion coefficient, external oxygen concentration in interparticle pores and oxygen consumption rates in organic matter. Values of \( d \), calculated with eq. 4.5 are also presented.

<table>
<thead>
<tr>
<th>Run</th>
<th>Diffusion coefficient (m(^2) s(^{-1}))</th>
<th>External oxygen concentration (mol m(^{-3}))</th>
<th>Oxygen uptake (mol m(^{-3}) s(^{-1}))</th>
<th>( d ) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.89E-12</td>
<td>9.375</td>
<td>0.0004</td>
<td>0.210479</td>
</tr>
<tr>
<td>2</td>
<td>2.43E-13</td>
<td>9.375</td>
<td>0.0001</td>
<td>0.150953</td>
</tr>
<tr>
<td>3</td>
<td>2.43E-13</td>
<td>9.375</td>
<td>0.0004</td>
<td>0.075477</td>
</tr>
<tr>
<td>4</td>
<td>1.89E-13</td>
<td>9.375</td>
<td>0.0004</td>
<td>0.066559</td>
</tr>
<tr>
<td>5</td>
<td>2.43E-14</td>
<td>9.375</td>
<td>0.0001</td>
<td>0.047736</td>
</tr>
<tr>
<td>6</td>
<td>2.43E-14</td>
<td>9.375</td>
<td>0.0004</td>
<td>0.023868</td>
</tr>
<tr>
<td>7</td>
<td>2.43E-14</td>
<td>9.375</td>
<td>0.0012</td>
<td>0.013780</td>
</tr>
</tbody>
</table>

**Evaluation of the aspect of shape**

The process length \( d \) is useful for the comparison of model results for the equivalent cylinder set and the original organic matter fabric as it is independent of geometrical quantities like aggregate radius. The anoxic fraction of organic matter depends on the process length \( d \) and on the shape of organic matter fabrics. A deviation in the relation of \( d \) and anoxic fraction for the cylinder set and the digitized organic matter fabric is therefore attributed to shape. This deviation also represents the error that is introduced by the simplification of shape in the derivation of equivalent cylinder systems.

To evaluate the aspect of shape, detailed equivalent cylinder systems were calculated with a frequency distribution of distances with a large number of distance
intervals (21). To evaluate whether cylinder systems of a limited number of cylinders are also satisfactory, a system was calculated with a frequency distribution of distances with only seven distance intervals with increasing class width. The frequency distribution was calculated from 2D cross-sectional distances, and does not take account of a bias in distances in respect to the true 3D distances.

**Cross sectional distances and true 3D distances**
The error introduced by calculating distances from a 2D cross section, was quantified by calculating the relation between the anoxic volume and the process length (d) for two cylinder systems. One is calculated with the assumption that the measured 2D distances are true 3D distances (denoted as 2D cylinder system). The other is calculated by setting the measured 2D distances equal to the 2D distances of the cross-sectioned isotropic cylinder system to be derived (denoted as 3D cylinder system).

**Evaluation of sample variability**
The aspect of sample variability was evaluated by differences in relations between anoxic volume and d for equivalent cylinder systems calculated for different segments. Seven segments were used, for the vertical as well as for the horizontal cross section (Figure 4.2). The segments are regularly distributed over the thin section and all segments are of the size of the segment for which the calculations were performed (Figure 4.1).

![Figure 4.2: Schematic representation of the distribution of segments in the horizontal and vertical thin section. Thin sections are produced from a glass column of 6 cm height and 10 cm diameter. * segment used for comparison of model results for equivalent cylinder systems and organic matter fabric.](image)

**Distinction between inter- and intraparticle pores**
The effect of small pores was studied by calculating cylinder systems for different organic matter fabrics in which pores of different sizes were filtered. The effects of filtered pores were calculated on the relation between anoxic volume and the process length d. The nature of pores, i.e. whether they can be counted as intraparticle pores or interparticle pores, was studied with microscopy.
4.3 Results and discussion

Figure 4.3 shows the distance probabilities that were measured from the organic matter cross section. The distance probabilities were smoothed with a spline function, as the unsmoothed data produced instabilities in further numerical calculations. The distance probabilities in Figure 4.3 are calculated with a uniform class width; the probabilities are highest for the intervals of small distances (0.02-0.06 mm), distances larger than 0.3-0.4 mm are rare. From this distance pdf we calculated equivalent systems of cylinders and sheets. Figures 4.4 and 4.5 give the weights and radii of respectively cylinders and sheets of the equivalent systems.

![Graph showing distance probability density function p(x) of the organic matter. Open symbols are calculated distance probabilities. The smoothed line is produced with a spline function (5 knots). The distance probability at a distance of 0.47 mm was excluded from the function as it produced instabilities in the numerical calculations for the derivation of cylinder and sheet systems.](image)

Figure 4.3: Distance probability density function p(x) of the organic matter. Open symbols are calculated distance probabilities. The smoothed line is produced with a spline function (5 knots). The distance probability at a distance of 0.47 mm was excluded from the function as it produced instabilities in the numerical calculations for the derivation of cylinder and sheet systems.

Equivalent systems of cylinders and sheets were also calculated with distance probabilities calculated with only seven distance interval (increasing class width). Table 4.2 gives the weights and radii of these systems. Small negative values occur for some of the cylinder weights in Figure 4.4 and Table 4.2. Negative values result from a concave geometry of part of the organic matter surrounding pores (Rappoldt and Verhagen, 1999).
Figure 4.4: Weights (or volume fractions) belonging to a model soil consisting of cylinders with different radii. The derivation is performed for uniform and increasing distance intervals, and by assuming the distances in Figure 4.3 to be true three dimensional distances.

Figure 4.5: Weights (or volume fractions) belonging to a model soil consisting of sheets with different thicknesses. The derivation is performed for uniform and increasing distance intervals, and by assuming the distances in Figure 4.3 to be true three dimensional distances.
Aspect of shape

Figure 4.6 shows the relation between anoxic fraction and process length (d) for the 2D cylinders and sheet systems, as well as for the the original organic matter. The deviations in anoxic fractions between cylinder or sheet system and the original organic matter fabric are attributable to a simplification of shape. The anoxic fractions calculated with the digitized organic matter fabric lie in between those represented by the sheet and cylinder model system. The maximum absolute deviation in the anoxic fraction was 0.039 for the sheets system and 0.031 for the cylinder system at different values of d. A realistic process length for the field situation is about 0.08 mm as the corresponding anoxic fraction is 0.1, which agrees with estimates based on measured oxygen profiles (chapter 2). Deviations at this realistic value of d were 0.022 for the sheet system and 0.029 for the cylinder system.

![Graph showing anoxic fraction as a function of process length for cylinders, sheets and the gridmap (left axis). Curves are fitted with a cubic spline function. Deviations in anoxic fractions between digitized organic matter fabric and sheets or cylinders are indicated (right axis). Cylinder and sheet systems are derived from the measured 2D distances.](image)

In Figure 4.6 the relations between anoxic fraction and d are also given for the cylinder and sheets system calculated with only seven distance classes. For the cylinder system the curve did hardly alter from the one calculated with 21 distance intervals (Figure 4.3). Figure 4.7 gives the equilibrium oxygen concentrations in the
digitized organic matter fabric calculated with a realistic process length of 0.08 mm. Regions with zero oxygen concentrations are found in the centers of the largest organic particles.

**Aspect of 2D versus 3D distances**

Anoxic fractions presented in Figure 4.6 are overestimated as the 2D “organic matter-to-pore-distances” measured in the cross section are larger than the true 3D distances. To estimate the error which is hereby introduced we calculated the true 3D distance distribution and corresponding cylinder system, starting from an isotropic organic matter fabric (see method). The difference between calculated anoxic fractions for 2D and 3D model system was 0.086 at the most, and 0.038 at a realistic process length of 0.08 mm (Figure 4.8). Consequently, the error due to the use of cross sectional distances instead of three dimensional ones is about 1.5 times as large as the deviation introduced by simplification of shape.

**Table 4.2:*** Radii and weights of the cylinders and thicknesses and weights of the sheets in cylinder and sheet system derived from measured 2D distances in the organic matter cross section.

<table>
<thead>
<tr>
<th>Radius/ Thickness</th>
<th>0.0212</th>
<th>0.0636</th>
<th>0.1272</th>
<th>0.212</th>
<th>0.318</th>
<th>0.4452</th>
<th>0.5936</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinders Weight</td>
<td>-</td>
<td>0.084</td>
<td>0.3671</td>
<td>0.4633</td>
<td>0.0992</td>
<td>0.0207</td>
<td>0.0003</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.0347</td>
</tr>
<tr>
<td>Sheets Weight</td>
<td>0.0303</td>
<td>0.2858</td>
<td>0.3986</td>
<td>0.2293</td>
<td>0.0409</td>
<td>0.006</td>
<td>0.001</td>
</tr>
</tbody>
</table>

**Aspect of sample variability**

The described deviations in the relation between anoxic volume and d, due to shape or 2D distances were compared with the deviation due to sample variability. Figure 4.9 gives the mean anoxic fraction and standard deviation of seven segments of the horizontal and vertical thin section, in dependence of process length. In addition, relations are drawn between anoxic fraction and process length for seven different segments of the horizontal cross section. The maximum standard deviation from the mean anoxic fraction is 0.05 for the vertical and 0.035 for the horizontal thin section. The standard deviation from the mean anoxic fraction is 0.025 for the vertical and 0.022 for the horizontal thin section at a realistic process length of 0.08 mm (Figure 4.9). These standard deviations are of the same order as deviations due to simplification of shape and slightly lower than the deviation due to the use of 2D cross sectional distances. Since the cross section used in this study was produced from homogenized material sampled from one ectorganic horizon, it is expected that deviations due to sample variability will be larger for samples of intact litter layers. The average anoxic fractions of the horizontal and vertical thin section hardly differ, which indicates that the organic matter fabric is isotropic.
Figure 4.7: Example map with equilibrium oxygen concentrations in organic matter and pores. Process length $d = 0.08$ mm. Oxygen concentration decreases from black (100% saturation) to light grey (0-10% saturation). White denotes interparticle pore space.
Figure 4.8: Anoxic fraction as a function of process length (d) for 2D and 3D cylinder systems. The difference between 2D and 3D fitted curves is indicated (open squares, right axis)

**Aspect of inter- and intraparticle pore distinction**

The calculations described above are based on the classified organic matter fabric of the cross section. In the classification no distinction was made between intra- or interparticle pores. Consequently, any intraparticle pore present had a saturated oxygen concentration at all times, which may not be realistic. To study the effect of small pores on the overall calculated anoxic fraction, we produced a series of organic matter classifications in which pores sized from 1 to 5 cells were removed (0.2 to 0.9 % pore space removed respectively). In addition an organic matter classification was made in which small pores were removed with a width of 2 cells and an undefined length (9.8 % pore space removed). With the distance distributions of resulting organic matter fabrics, equivalent cylinder systems were derived and the relation between anoxic fraction and process length was calculated (Figure 4.10). The removal of pores of one cell size had a large effect: the increase in anoxic fraction in respect to the unfiltered map was 0.089 at a process length of 0.08 mm (Figure 4.10). However, increasing the size of pores to be removed did hardly enlarge the effect further (0-10%).
Figure 4.9: Average and standard deviation of the anoxic fraction, in dependence of the process length (d) for 2D cylinder systems derived for seven different segments of a vertical and horizontal thin section of homogenized Douglas fir litter. The relation between anoxic fraction and d is also shown for the seven different segments of the horizontal thin section. Lines: grey: different segments; black: averages for the vertical (dotted) and horizontal (solid) thin section. Symbols: standard deviation of vertical (•) and horizontal (■) thin section.

The question here is whether pores with the size of 1 cell (21.2 * 21.2 μm) can be counted as intraparticle or interparticle pores. A direct way to make out the nature of one cell pores is to study them in detail in the thin section. Important in this respect is the observation whether those pores are (1) part of an intact cell structure, (2) formed by decomposition due to tunneling of mesofauna or whether they are indeed (3) interparticle pores. Interparticle pores or pores due to tunneling are connected to interparticle pore space and as such can be counted as part of it. Pores of intact cell structures or due to local microbial decomposition are more likely to behave as pores not being part of interparticle pore space.

Figure 4.11 shows a detail of the cross section with pores of one cell size, together with the corresponding part of the binary organic matter fabric. It can be seen that one cell pores, which seemed intraparticle pores in the binary structure, actually are interparticle pores. Intraparticle pores were not classified as pores in the binary organic matter fabric. Therefore, for this thin section the classification of all pore space as interparticle pores is realistic. Furthermore, the applied resolution is appropriate. This realistic distinction between organic matter and pores as used in the unfiltered map, is also in agreement with particle sizes calculated from measured
oxygen profiles (chapter 2). Intra-aggregate pores of intact cell structures (ca. 8 μm) were probably too small to appear in the classified organic matter map.

**Comparison of different effects, and discussion of the method applicability**

The effect of filtering small interparticle pores was by far the largest of all effects. It resulted in a considerable overestimation of the anoxic fraction amounting to nearly 100%. Therefore, filtering of small pores should not be applied in this case. For applications in further studies it is essential to ensure a realistic distinction between organic matter and pores and also between inter- and intraparticle pores.

![Graph](image)

**Figure 4.10:** Anoxic fraction as a function of process length (d) for the unfiltered gridmap and the filtered maps. Results of filtered maps with one cell pores removed were the same as of maps with five cell pores removed. Pores of one cell layer width were removed by first adding a layer of one cell width from the organic matter surface into pore space and then adding a layer back again from the pore space surface to the organic matter.

The absolute error introduced by simplification of shape was 0.022-0.029, which amounted to about 25% of the anoxic fraction. An error of this order is acceptable, since the uncertainties in factors determining the anoxic fraction in a litter layer are expected to be still larger. The anoxic fraction in a litter layer depends on the diffusion coefficient, the oxygen consumption rate and the particle size distribution. Diffusion coefficients are expected to vary within a litter sample as well as between litter samples of different tree species, since diffusion coefficients also showed a large variety in wax layers of living foliar tissues (Schönherr and Riederer, 1989; Schreiber et al., 1996). Variability in particle size distributions of litter layers occur due to differences in the stage of litter fragmentation, and the total thickness of litter.
layers or total litter mass. These properties are known to vary considerably within several meters (Smit, 1999). Differences in particle size distributions and total litter thickness can be covered by applying the method on a representative set of thin sections.

It can be concluded from the above that the method of deriving an equivalent cylinder or sheet system from organic matter fabrics observed in thin sections, is suitable for application in litter layers. Cylinders are preferred to sheets, as the equivalent cylinder system gave satisfactory results with only seven cylinder radii. Furthermore, with cylinders a correction can be made for the use of 2D cross-sectional distances instead of the true 3D distances. In practice however, cross-sectional distances may be used without a correction as the effects of simplification of shape and the use of cross-sectional distances partly compensate each other. With the derived equivalent cylinder system, the calculated anoxic fraction is underestimated, while with the use of cross-sectional distances, the anoxic fraction is overestimated.

**Figure 4.11:** Details of the cross section (right) and corresponding classified map (left) of needle tissue and excrements with small pores. Scale: 1 cell in the left classified map is 21.2 μm * 21.2 μm.

### 4.4 Conclusions

Anoxic fractions calculated with the complex geometry of organic matter observed in the cross section and with the equivalent cylinders or sheets compared well: the digitized organic matter fabric gave results that were in between those of the cylinders and sheets. It appeared to be crucial that a clear distinction between inter- and intraparticle pores can be made. Microscopical observations were conclusive on the nature of observed pores. With the classification of organic matter and pores, the
resolution of the image is relevant: pores in intact organic matter tissues should not appear as individual pores.

An equivalent cylinder system with only seven cylinder radii was sufficient for the representation of the organic matter structure. The derived cylinder system can be easily built in in diffusion-reaction models and offers an excellent opportunity to represent litter layer structures in models simulating anoxic fractions and accompanying production of greenhouse gases in forest soils at different spatial scales (Li et al., 2000).