A partial susceptibility approach to analysing the magnetic properties of environmental materials: a case study

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SUMMARY
An approach to expressing the magnetic properties of environmental materials in terms of the contributions of the magnetic susceptibilities of specific magnetic components is reported. The approach links the partial susceptibilities of discrete particles, domains or mineral fractions with the concentration-dependent parameters by means of multiple linear regression methods. The case study, using the Liverpool street dust data set, demonstrates that the technique is able to model the contributions of the main magnetic components satisfactorily. Several factors may have a significant impact on the regression results. These include the validity of the linear proportional relationships between partial susceptibilities and the relevant concentration-dependent parameters, the adequacy of the variable selection procedure and the regression model, and the suitability of certain magnetic parameters.

Key words: concentration-related parameters, magnetic susceptibility, multiple linear regression, partial susceptibilities, street dust.

INTRODUCTION
One of the most urgent needs in environmental magnetism is to present magnetic measurement results in terms of mineral and grain size contributions quantified by both empirical and theoretical models of the relationships between magnetic properties and magnetic components (Oldfield 1991, 1999). There have been several complementary attempts to do this. Hunt (1986) used the statistical procedure of discrimination analysis to establish variations in the magnetic signature between groups of dusts. Thompson (1986) described two approaches to modelling magnetization data: the first modelling the magnetic properties of natural materials in terms of mixtures of possible source materials, and the second modelling the magnetic properties of natural materials in terms of mixtures of magnetite and haematite crystals of varying concentrations and grain sizes. Another attempt is represented by the development of empirically derived mixing models to estimate the contributions of magnetically differentiated types of source material (e.g. Yu & Oldfield 1989; Lees 1997). On the basis of the magnetic properties of some synthetic submicron magnetites, Maher (1988) proposed a method of magnetic granulometry using a sequence of measurements, such as the ratio $\frac{Z_{ARM}}{SIRM}$ and $Z_{FD}$ percentage, which has been further tested by Oldfield (1994) and Dearing et al. (1997). Robertson & France (1994) and Stockhausen (1998) tried to discriminate among magnetic phases using cumulative log Gaussian functions to model IRM acquisition curves. Recently, von Dobeneck (1998) and Frederichs et al. (1999) introduced the concept of partial susceptibilities for quantitative analysis of carriers of magnetic susceptibility in marine sediments.

In this paper, von Dobeneck (1998) and Frederichs et al.’s (1999) proposal is developed. First, the concept of partial susceptibilities and the relevant concentration-dependent parameters are described. Second, the Liverpool street dust data set is used as a case study. Finally, factors that may have a significant impact on the approach are discussed.

METHODS
The observed total magnetic susceptibility of an environmental sample, $Z_{TOTAL}$, is the sum of the partial susceptibilities of discrete particles, domains or mineral fractions. The partial susceptibilities are of ferrimagnets, $Z_{FERRI}$; canted antiferromagnets, $Z_{ANTIFERRO}$; paramagnets, $Z_{PARA}$; and diamagnets, $Z_{DIA}$. The susceptibility of ferrimagnetic components ($Z_{FERRI}$) in a sample can also be considered as the total contribution of superparamagnetic domain (SP), stable single domain (SSD), and multidomain (MD) grains ($Z_{SP}$, $Z_{SSD}$, and $Z_{MD}$). Small MD grains could demonstrate pseudo-single domain behaviour. For magnetite, SP and SSD threshold grain sizes (in diameter) are estimated as 0.025–0.030 and 0.05–0.06 μm (or 0.079–0.084 μm) (Dunlop & Özdemir 1997). Therefore, $Z_{TOTAL}$ can be expressed as

$$Z_{TOTAL} = Z_{SP} + Z_{SSD} + Z_{MD} + Z_{ANTIFERRO} + Z_{PARA} + Z_{DIA}.$$  (1)
$z_{\text{TOTAL}}$ is usually routinely measured by means of low-field AC susceptibility $z_{\text{LF}}$ (low frequency), which represents the total contribution of magnetic materials in a sample, but partial susceptibilities are rarely directly measured except for high-field susceptibility, $z_{\text{HIGH}}$, which detects the total contribution of paramagnetic, diamagnetic, and canted antiferromagnetic components (Richter & van der Pluijm 1994). However, the concentrations of discrete magnetic minerals and their fractions can be estimated by other magnetic-concentration-related parameters. There is evidence that some concentration-dependent parameters can be used as proxies for the related magnetic components in a sample. First, frequency-dependent susceptibility $z_{\text{FD}}$ is related to SP components. When the SP grain concentration, rather than the grain size distribution, dominates both $z_{\text{FD}}$ and $z_{\text{SP}}$ values, a linear relationship between $z_{\text{SP}}$ and $z_{\text{FD}}$ is expected. Measurements of environmental materials show that $z_{\text{FD}}$ values can be considered as a loose indication of the amount of SP material present in a sample (Dearing et al. 1996). Second, SSD grains can be estimated by anhysteretic remanent magnetization (ARM) or susceptibility of ARM ($z_{\text{ARM}}$). SSD can be regarded as independent of grain size. However, $z_{\text{ARM}}$ values are associated with SSD grain sizes (King et al. 1982; Maher 1988). Therefore, when $z_{\text{ARM}}$ is dominated by the SSD grain concentration, rather than the grain size distribution, $z_{\text{ARM}}$ is expected to be related linearly to $z_{\text{SSD}}$. Dearing et al.’s (1997) study on representative Welsh soil samples suggests that where soils have reasonably constant proportions of grains in the SP and SSD size ranges, $z_{\text{ARM}}$ may be used to estimate the concentration of fine ferrimagnetic grains. Third, weak field (e.g. 20 mT) isothermal remanent magnetization (IRM) or low reverse field (e.g. $-20 \text{ mT}$) demagnetization of saturation isothermal remanent magnetization (SIRM) can be used to identify the presence of soft components (mainly MD grains). Thompson’s (1986) calculations suggest that $z_{\text{SIRM}}$ can be regarded as independent of grain size. $z_{\text{ARM}}$ was obtained on 1 cm$^3$ samples using a Molspin pulse magnetizer, and measured on a Molspin spinner magnetometer. Measurements are expressed as susceptibility of ARM ($z_{\text{ARM}} - 10^{-5} \text{ m}^3 \text{ kg}^{-1}$) by dividing the remanence by the steady field. Acquisition of isothermal remanent magnetization in fields of 20 mT (IRM$_{20\text{mT}}$), 1 T (SIRM), $-20 \text{ mT}$ (reverse) (IRM$_{-20\text{mT}}$), and $-300 \text{ mT}$ (reverse) (IRM$_{-300\text{mT}}$) was carried out using a Molspin pulse magnetizer, and measured on a Molspin spinner magnetometer. Measurements are expressed in $10^{-7} \text{ A}^2 \text{ m}^{-2}$ for IRM$_{20\text{mT}}$, SIRM, (SIRM=IRM$_{-20\text{mT}}$), and (SIRM=IRM$_{-300\text{mT}}$) on a mass-specific basis, and as percentages (per cent) for reverse field ratios of SOFT ($-20 \text{ mT}$) and HARD ($-300 \text{ mT}$). High-field susceptibility $z_{\text{HIGH}}$ was obtained on 1 cm$^3$ samples using a Molspin vibrating sample magnetometer in a field of 0.8–1 T. Measurements are expressed as a mass-specific term ($10^{-7} \text{ m}^3 \text{ kg}^{-1}$).

The magnetic measurement data were then analysed. Samples with values more than 1.5 box-lengths away from the box of the box-plot were identified as outliers and excluded before carrying out other statistical analysis. In the linear regression analysis, samples with standardized residual values of more than two standard deviations above or below the regression line were also detected as outliers and eliminated. The magnetic measurement results show that the $z_{\text{HIGH}}/z_{\text{LF}}$ values range from 1.5 to 3.8 per cent (average 2.5 per cent), indicating that the total contribution of paramagnetic, diamagnetic, and canted antiferromagnetic components to the total susceptibility are not significant. SOFT percentage (33.5–42.8 per cent) and HARD percentage (0.1–4.2 per cent) values and $z_{\text{LF}}$ values ($>50 \times 10^{-8} \text{ m}^3 \text{ kg}^{-1}$, with the exception of one sample) also suggest that the dominant magnetic minerals are ferrimagnetic (Oldfield & Richardson 1990; Dearing et al. 1996). By comparing the $z_{\text{SP}}$ percentage (0.9–2.5 per cent) and $z_{\text{ARM}}$ (0.09–0.19 $\times 10^{-3} \text{ m}^3 \text{ A}^{-1}$) data with a semi-quantitative mixing model (Dearing et al. 1997), the proportions of SP, SSD, and MD grains are estimated as $~10$, $~0$, and $~90$ per cent, respectively. Therefore, the dominant magnetic minerals are ferrimagnetic, in which the main components are MD and SP grains.

**MODELLING OF FERRIMAGNETIC SUSCEPTIBILITY $z_{\text{FERRI}}$**

Since the sum of the partial susceptibilities of paramagnetic, diamagnetic, and antiferromagnetic components ($z_{\text{FERRA}} + z_{\text{DIA}} + z_{\text{ANTIFERRO}}$) is estimated by $z_{\text{HIGH}}$, from eq. (1), we have $z_{\text{FERRI}} = z_{\text{TOTAL}} - z_{\text{HIGH}}$, or $z_{\text{FERRI}} = z_{\text{LF}} - z_{\text{HIGH}} - z_{\text{SP}} - z_{\text{SSD}}$, and $z_{\text{SSD}}$ can be determined by means of the multiple linear regression using $z_{\text{HIRM}}$, $z_{\text{ARM}}$, and SOFT [$=(z_{\text{SIRM}} - z_{\text{IRM}}_{-20\text{mT}})/2$ or IRM$_{-20\text{mT}}$]. Therefore, the multiple linear regression equations to calculate...
$Z_{FERRI}$ can be written as

$$Z_{FERRI\text{cal}} = z_1Z_{FED} + z_2Z_{ARM} + z_3SOFT,$$  \hspace{1cm} (2)

$$Z_{FERRI\text{cal}} = z_4Z_{FED} + z_5Z_{ARM} + z_6IRM_{\text{20mT}},$$  \hspace{1cm} (3)

where $z_1$, $z_2$, and $z_3$ are the partial regression coefficients.

Using the simultaneous method, the regression result of eq. (2) is

$$Z_{FERRI\text{cal}} = 17.226Z_{FED} + 7.646Z_{ARM} + 11.800SOFT.$$  \hspace{1cm} (4)

The multiple linear regression correlation coefficient $R^2$ is 0.997, close to unity, and the difference between $Z_{FERRI\text{cal}}$ and $Z_{FERRI\text{cal}}$ is 0.6 per cent on average (Table 1), indicating a high degree of agreement between observations and calculations. A test of the regression results is made by comparison between the partial susceptibility contributions from modelling and another approach. In eq. (4), the calculated $Z_{SP}$, $Z_{SSD}$, and $Z_{MD}$ contribute 30.9, 1.6, and 67.5 per cent to $Z_{FERRI\text{cal}}$ on average. Considering the grain size dependence of magnetic susceptibility, which shows higher values for SP grains than for SSD or MD grains (Maher 1988), the regressed partial susceptibility results are consistent with those of the mixing model (SP, SSD, and MD grain proportions ~10, ~0, and ~90 per cent).

Using the stepwise method, from eq. (2), we obtain

$$Z_{FERRI\text{cal}} = 17.593Z_{FED} + 11.954SOFT.$$  \hspace{1cm} (5)

Fig 1 compares $Z_{FERRI\text{cal}} = (Z_{LF} - Z_{HIGH})$ and $Z_{FERRI\text{cal}}$. As shown in Table 1, eq. (5) also gives a good estimate of $Z_{FERRI\text{cal}}$, and the contributions of SP, SSD, and MD grains. Examination of the partial regression coefficients in eq. (4) shows that $z_1$ and $z_3$ are significant at the 0.01 level, but that $z_2$ is not significant at the 0.05 level, suggesting that $Z_{ARM}$ does not contribute reliably to the regression equation. This is confirmed by the stepwise method resulting in eq. (5), which does not include $Z_{ARM}$. Therefore, eq. (5) is more appropriate for application than eq. (4).

For eq. (3), using the simultaneous method, we get an erroneously negative $z_2$ value, since the relationship between $Z_{MD}$ and $Z_{ARM}$ is positive. Alternatively, using the stepwise

Table 1. The modelling results of the partial susceptibilities of the Liverpool street dust data set.

<table>
<thead>
<tr>
<th>Eq.*</th>
<th>Sample number</th>
<th>Multiple $R^2$</th>
<th>Mean difference (per cent)</th>
<th>SP proportion (per cent)$^d$</th>
<th>SSD proportion (per cent)$^d$</th>
<th>MD proportion (per cent)$^d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4)</td>
<td>79</td>
<td>0.997$^a$</td>
<td>0.6$^a$</td>
<td>30.9$^a$</td>
<td>1.6$^a$</td>
<td>67.5$^a$</td>
</tr>
<tr>
<td>(5)</td>
<td>79</td>
<td>0.997$^a$</td>
<td>0.5$^a$</td>
<td>31.6$^a$</td>
<td>0.0$^a$</td>
<td>68.4$^a$</td>
</tr>
<tr>
<td>(6)</td>
<td>72</td>
<td>0.995$^a$</td>
<td>1.8$^a$</td>
<td>31.1$^a$</td>
<td>0.0$^a$</td>
<td>68.9$^a$</td>
</tr>
<tr>
<td>(9)</td>
<td>79</td>
<td>0.964$^d$</td>
<td>0.5$^d$</td>
<td>30.7$^d$</td>
<td>0.0$^d$</td>
<td>69.3$^d$</td>
</tr>
<tr>
<td>(10)</td>
<td>78</td>
<td>0.964$^d$</td>
<td>-0.9$^d$</td>
<td>30.9$^d$</td>
<td>0.0$^d$</td>
<td>69.1$^d$</td>
</tr>
<tr>
<td>(11)</td>
<td>75</td>
<td>0.940$^d$</td>
<td>0.8$^d$</td>
<td>32.0$^d$</td>
<td>0.0$^d$</td>
<td>68.0$^d$</td>
</tr>
</tbody>
</table>

*Eq. (4): modelling $Z_{FERRI}$ by using SOFT and the simultaneous method; eq. (5): modelling $Z_{FERRI}$ by using SOFT and the stepwise method; eq. (6): modelling $Z_{FERRI}$ by using IRM$_{20mT}$ and the stepwise method; eq. (9): modelling $Z_{TOTAL}$ by using the simultaneous method (only including three independent variables: $Z_{FED}$, $Z_{ARM}$, and SOFT); eq. (10): modelling $Z_{TOTAL}$ by using SOFT and the stepwise method; eq. (11): modelling $Z_{TOTAL}$ by using IRM$_{20mT}$ and the stepwise method (only including the first two independent variables entered).

*After excluding outliers.

$^a$ Between $Z_{FERRI\text{cal}} = (Z_{LF} - Z_{HIGH})$ and $Z_{FERRI\text{cal}}$; difference: $(Z_{FERRI\text{cal}} - Z_{FERRI\text{cal}})/Z_{FERRI\text{cal}}$.

$^b$ Between $Z_{TOTAL\text{obs}} = (Z_{LF} + Z_{HIGH})$ and $Z_{TOTAL\text{cal}}$; difference: $(Z_{TOTAL\text{cal}} - Z_{TOTAL\text{obs}})/Z_{TOTAL\text{obs}}$.

$^d$ SP, SSD, and MD proportions: proportions of ferrimagnetic components.

![Figure 1](https://academic.oup.com/gji/article-abstract/138/3/851/578960/25 December 2018)
method, we obtain
\[ Z_{\text{FERRI(cal)}} = 17.498 Z_{\text{FD}} + 27.723 \text{IRM}_{20\text{mT}}. \]  
(6)

The modelling results of eq. (6) are similar to those of eq. (5) (see Table 1). As discussed above, IRM$_{20\text{mT}}$ can be used for the same purpose as SOFT on the basis that they both represent soft components in a sample. Fig. 2 shows a good linear correlation between SOFT and IRM$_{20\text{mT}}$ in our data set. In practice, reverse field remanence can be precisely remeasured and confirmed much more easily.

**MODELLING OF TOTAL SUSCEPTIBILITY \( Z_{\text{TOTAL}} \)**

Using HIRM as a proxy for the concentration of canted antiferromagnetic components, from eqs (1)–(3), the regression equations for modelling \( Z_{\text{TOTAL}} \) can be expressed as

\[ Z_{\text{TOTAL,cal}} = a_0 + a_1 Z_{\text{FD}} + a_2 Z_{\text{ARM}} + a_3 \text{SOFT} + a_4 \text{HIRM}, \]  
(7)

\[ Z_{\text{TOTAL,cal}} = a_0 + a_1 Z_{\text{FD}} + a_2 Z_{\text{ARM}} + a_3 \text{IRM}_{20\text{mT}} + a_4 \text{HIRM}, \]  
(8)

where \( a_0, a_1, a_2, a_3, \) and \( a_4 \) are the partial regression coefficients.

For eq. (7), using the simultaneous method, we get an erroneously negative \( a_4 \) value, since the relationship between \( Z_{\text{ANTIFERRO}} \) and HIRM is positive. Eliminating the HIRM term, using the simultaneous method, we obtain

\[ Z_{\text{TOTAL,cal}} = 1.256 + 17.560 Z_{\text{FD}} + 0.107 Z_{\text{ARM}} + 12.416 \text{SOFT}. \]  
(9)

\( R^2 \) is 0.964, and the difference between \( Z_{\text{LD}} \) and \( Z_{\text{TOTAL,cal}} \) is 0.5 per cent on average (Table 1), indicating a high degree of agreement between \( Z_{\text{LD}} \) and \( Z_{\text{TOTAL,cal}} \). The estimated \( Z_{\text{SP}}, Z_{\text{SSD}}, \) and \( Z_{\text{MD}} \) contribute 30.7, 0.0, and 69.3 per cent to \( Z_{\text{FERRI(cal)}} \), consistent with the results of the mixing model (SP, SSD, and MD grain proportions \( \sim 10, \sim 0, \) and \( \sim 90 \) per cent), since SP grains show higher magnetic susceptibility values than SSD and MD grains (Maher 1988). \( R^2 \) between \( Z_{\text{FERRI(obs)}} \) and \( Z_{\text{FERRI(cal)}} \) is 0.965, and the difference between \( Z_{\text{FERRI(obs)}} \) and \( Z_{\text{FERRI(cal)}} \) is 2.6 per cent on average. The constant term, which may reflect magnetic measurement uncertainties, contributions of \( Z_{\text{ANTIFERRO}}, Z_{\text{PARA}}, \) and \( Z_{\text{SHA}}, \) and deviations from the linear proportional relationships between \( Z_{\text{SP}} \) and \( Z_{\text{FD}}, Z_{\text{SSD}}, \) and \( Z_{\text{ARM}}, Z_{\text{MD}}, \) and SOFT, is unlikely to represent the contributions of any discrete magnetic components.

Using the stepwise method, the regression result of eq. (7) is

\[ Z_{\text{TOTAL,cal}} = -1.291 + 17.635 Z_{\text{FD}} + 12.388 \text{SOFT}. \]  
(10)

Comparison between \( Z_{\text{TOTAL,obs}} = Z_{\text{FD}} \) and \( Z_{\text{TOTAL,cal}} \) is shown in Fig. 3. The modelling results of eq. (10) are similar to those of eq. (9) (see Table 1). Similar to that between eqs (4) and (5), comparison between eqs (9) and (10) suggests that eq. (10) is more suitable for application than eq. (9), since \( z_2 \) in eq. (9) is not significant at the 0.05 level.

For eq. (8), the simultaneous method is also unsuccessful due to negative \( z_2 \) and \( z_4 \) values. When the stepwise method is applied and three independent variables (\( Z_{\text{FD}}, \text{IRM}_{20\text{mT}}, \) and \( \text{HIRM} \)) are included in the model, the \( z_4 \) value is again negative. However, if the regression model only includes the first two independent variables entered, we have

\[ Z_{\text{TOTAL,cal}} = -25.775 + 20.808 Z_{\text{FD}} + 31.693 \text{IRM}_{20\text{mT}}. \]  
(11)

Table 1 shows that the modelling results of eq. (11) are similar to those of eq. (10), suggesting the success of eq. (11). For eq. (11), the mean difference between \( Z_{\text{FERRI(obs)}} \) and \( Z_{\text{FERRI(cal)}} \) is 17.4 per cent, higher than that of eq. (10) (2.5 per cent), suggesting an overestimation of \( Z_{\text{FERRI(obs)}} \), which results in a higher negative value of the constant term. Therefore, eq. (10) gives a better estimate of \( Z_{\text{FERRI}} \) than eq. (11). Comparison between eqs (10) and (11), the former using SOFT, the latter \( Z_{\text{FERRI}}, \) to estimate the content of MD grains, suggests that the partial susceptibility approach may be sensitive to some magnetic parameters, such as SOFT and \( \text{IRM}_{20\text{mT}} \). The regression process of eq. (8), using the stepwise method, shows that an inadequate model will cause the failure of the partial susceptibility approach.

**DISCUSSION AND CONCLUSIONS**

The partial susceptibility approach assumes linear positive proportional relationships between \( Z_{\text{SP}} \) and \( Z_{\text{FD}}, Z_{\text{SSD}}, \) and \( Z_{\text{ARM}}, Z_{\text{MD}}, \) and SOFT or \( \text{IRM}_{20\text{mT}}, \) and \( Z_{\text{ANTIFERRO}} \) and HIRM. As discussed above, there is evidence to support these assumptions.
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However, in some situations, some assumptions do not hold. Dearing et al. (1997) suggested that a zero \( x_{FD} \) value does not result in zero content of SP grains in the Welsh soil samples, indicating the non-proportional relationship between \( x_{FD} \) and \( x_{MD} \). In the Liverpool street dust data set, the relationship between SOFT and IRM\(_{30mT}\) is not proportional (see Fig. 2), suggesting that the relationship either between \( x_{MD} \) and SOFT or between \( x_{MD} \) and IRM\(_{30mT}\) is not proportional. In addition to the contribution of MD grains, SOFT and IRM\(_{20mT}\) also include the contribution of fine viscous grains, which may not be significant in our samples due to the small concentrations of SP grains. HIRM, defined as \( (\text{SIRM} - \text{IRM}_{-300mT})/2 \), could exclude the contribution of some soft canted antiferromagnetic components. Deviations from the assumptions of linear proportionality will lead to increased uncertainties in the regression results. Contributions of more than one ferromagnetic mineral and effects of grain interactions in the samples may also cause violations of the assumptions of linear proportionality.

The case study results are summarized in Table 1. They demonstrate the success of the partial susceptibility approach in modelling the contributions of the main magnetic components. The case study shows that several factors may have a significant impact on the regression results. First, different variable selection procedures, for example the simultaneous method and the stepwise method, may generate considerably different regression equations. Second, an adequate regression model is important to obtain a reasonable regression result. Finally, the technique may be sensitive to some magnetic parameters, such as SOFT and IRM\(_{30mT}\). It is unlikely that the constant term in the regression equation represents the contributions of any discrete magnetic components. As a consequence, in some circumstances, the regression equations fail to model the contributions of the partial susceptibilities.

Two points are essential in the application of the partial susceptibility technique. First, different regression models and methods (for example the simultaneous method and the stepwise method) should be tested for selecting suitable variables and developing regression equations. Second, the technique is successful only if the modelling results give a reasonable estimate of the contributions of the partial susceptibilities, which can be assessed by comparison with those from other approaches, such as the semi-quantitative mixing model (Dearing et al. 1997).

The advantage of the technique is that complex magnetic data are reduced to magnetic susceptibilities, which can then be compared quantitatively against each other in the percentage or ratio form. In other words, based on routine magnetic measurement data, this technique provides an approach to presenting magnetic mineralogy, grain size, and concentration in terms of partial magnetic susceptibilities.

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