Explaining the dielectric properties of firn as a density-and-conductivity mixed permittivity (DECOMP)

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The relative dielectric permittivity (RP) of mixtures can be calculated to good approximation by composing its constituents' cubic roots of RP by volume fraction (VF). This is even true for RP's complex continuation, which also treats the conductivity of the material. Firn is a mixture of ice and air. The DECOMP formula links the RP of the ice and its VF, with the RP of the firn. The inversion of the formula is, for most practical applications, possible; the density of firn as well as the ice's RP can then be determined with high spatial resolution from dielectric profiling measurements (DEP) alone. If the ice phase's density and the real component of RP are a constant material property the inversion is feasible. This paper gives an example for numerical inversion of complex-valued dielectric mixing formulae for some known material properties, which is applicable to other composites as well.

1. Introduction

Different aspects of polar firn's dielectric properties have been widely discussed in the literature, but an overall discussion of firn's permittivity in all its complexity is still missing. Ice-core physics and geochemistry focus on the DC and AC conductivity of firn [*Wolff*, 2000; *Wolff et al.*, 1997]. For radio echo sounding (RES) applications the firn density is frequently discussed in relation to the propagation velocity of electromagnetic waves in firn [*Bogorodskiĭ et al.*, 1985; *Hempel et al.*, 2000]. Recent forward modeling of radar traces has shown that high-frequency density variations with depth can explain some of the observed RES reflections in polar firn [*Arcone et al.*, 2005] and that separation of density and conductivity related signals is important for correct interpretations [*Eisen et al.*, 2003]. When linking RES and Dielectric Profiling (DEP) of ice cores [*Moore et al.*, 1990], the problem becomes one of predicting the dielectric properties in the 10–1000 MHz RES frequency range based on the DEP measurements made at frequencies below 1 MHz. The AC permittivity of a homogenous material, such as solid ice, is fully determined by the frequency and two frequency-independent material properties: permittivity and conductivity [*Petrenko and Whitworth*, 1999; *Hobbs*, 1974]. Frequency dependence is, understandably, more complicated for mixtures.

The theory expounded below arose when *Wilhelms* [1996] and *Wilhelms et al.* [1998] interpreted the permittivity of DEP measurements, while other observers focused on the conductivity measurement only [*Moore*, 1989; *Wolff*, 2000]. Early attempts to measure the firn's permittivity by DEP [*Moore*, 1988] were not aggressively pursued. In the publications cited above, the author compared ice-core DEP and gamma-attenuation profiling (GAP) in 5 mm-depth resolution. He verified the applicability of *Looyenga*'s [1965] mixing formula for firn in a complex-valued continuation, as suggested by *Paren and Glen* [1978]. As a conclusion, the author determined the density of polar firn from DEP measurements within a precision of 10% over the whole depth range. However, the question remained how to properly relate the conductivity to the density. The theory of density-conductivity mixed permittivity (DECOMP) as a description of ice's dielectric properties, based solely on the density and the conductivity and accurate to within about 1% will now be outlined[1]. *Shabtaie and Bentley* [1995] discuss suitable mixing models[1] and the Looyenga mixing model (LMM) is their choice model, because of its mathematical symmetry in its two constituents. The now following discussion will thus be based on the LMM.

2. The DECOMP mixing model

Landau and Lifschitz [1982, §9] quote that the cubic root of a mixture's permittivity is the sum of the cubic roots of its constituents' permittivity, weighted by the respective volume fraction. This deduction is valid to second-order terms for isotropic particles, if the deviation of the constituents' permittivity is small compared to the mean permittivity. This is in principle the same assumption as for the mean-field-approximation quoted by *Shabtaie and Bentley* [1995] for derivation of the LMM. The mathematical relation for polar firn's relative permittivity (RP) $\hat{\varepsilon}_F$ as a mixture of ice $\hat{\varepsilon}_I$ and air $\hat{\varepsilon}_A$, with volume fractions (VF) for ice ν_I and air $\nu_A = 1 - \nu_I$ thus is $\sqrt[3]{\hat{\varepsilon}_F} = \nu_I \sqrt[3]{\hat{\varepsilon}_I} + \nu_A \sqrt[3]{\hat{\varepsilon}_A} = \nu_I \sqrt[3]{\hat{\varepsilon}_I} + (1-\nu_I) \sqrt[3]{\hat{\varepsilon}_A} = \sqrt[3]{\hat{\varepsilon}_A} + \nu_I (\sqrt[3]{\hat{\varepsilon}_I} - \sqrt[3]{\hat{\varepsilon}_A})$. *Landau and Lifschitz*' [1982] deduction never made the assumption of real-valued RP, the dielectric behavior of ice can be treated by assuming a complex-valued RP of ice[1] $\hat{\varepsilon}_I = \varepsilon_I' - \varepsilon_I''\mathrm{i}$. The real component (RC) of pure ice's RP is the relative dielectric constant ε_I', while the imaginary component (IC) $-\varepsilon_I'' = -\sigma_I/(\omega\varepsilon_0)$ depends on the pure ice's conductivity σ_I, the angular excitation frequency ω and the permittivity of the vacuum ε_0. The RP of air under normal atmospheric conditions is 1.000576 [*Gerthsen et al.*, 1989], so the assumption of $\hat{\varepsilon}_A = 1$ is valid with less than 0.6‰ relative error. Insertion into the relation above yields an expression for the firn's dielectric properties $\sqrt[3]{\hat{\varepsilon}_F} = 1 + \nu_I (\sqrt[3]{\hat{\varepsilon}_I} - 1) = 1 + \nu_I (\sqrt[3]{\varepsilon_I' - \varepsilon_I''\mathrm{i}} - 1)$, which is solely in terms of the ice's volume fraction and dielectric properties. For the computation of firn's density $\rho_F = \nu_I \rho_I + \nu_A \rho_A$, the air content's contribution $\nu_A \rho_A$ is practically negligible, as $|\rho_F/\rho_I - \nu_I| \leq \nu_A (\rho_A/\rho_I) \leq 1 \times 1.9‰$. The latter figure is estimated from the laws of thermodynamics with the density of polar air[1] $\rho_A \leq 0.0016$ gcm^{-3}. Calculated from the unit cell parameters [*Petrenko and Whitworth*, 1999, and references therein] pure ice's density varies from $0.918 \ldots 0.925$ gcm^{-3} in the $-8 \ldots -60$°C temperature range. This is consistent with a variation of density by about 3‰ in the range of $-60 \ldots 0$°C as reported by *Dantl* [1969]. Compared to the variation with temperature the error limit of $\rho_A/\rho_I = 1.9‰$ is small and

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the volume fraction $\nu_I = \rho_F/\rho_I$ can be calculated without practical loss in precision. For this paper, pure ice's density will be assumed to be $\rho_I = (0.9197 \pm 0.003)$ gcm^{-3}. This is consistent with the density of pure polar ice 0.917 gcm^{-3} reported by *Paterson* [1994, Table 2.1]. In previous applications approximation formulae have been used for the dielectric properties of firn [*Glen and Paren*, 1975; *Miners et al.*, 1997], but these formulae deviate from the precise formula by about 3% [*Bogorodskiĭ et al.*, 1985, Section 3.6.]. All considerations in this paper refer to the DECOMP formula as derived in this section $\sqrt[3]{\hat{\varepsilon}_F} = 1 + \nu_I(\sqrt[3]{\varepsilon_I' - \varepsilon_I''\mathrm{i}} - 1) = 1 + (\rho_F/\rho_I)(\sqrt[3]{\varepsilon_I' - \varepsilon_I''\mathrm{i}} - 1)$.

3. The properties of the pure ice constituent according to DECOMP

DEP and GAP measurements of twenty Antarctic firn and ice cores [*Oerter et al.*, 2000] were used to study the behavior of the DECOMP formula (grey data points in Figure 1). To ensure minimal offsets in the depth scale the measurements wer performed on one combined-measurement bench [*Wilhelms*, 2000]. From the DEP ($\hat{\varepsilon}_F$) and GAP (ρ_F) data as well as the density of pure ice from the literature ρ_I one calculates the permittivity of pure ice with the DECOMP formula[1] $\hat{\varepsilon}_I = \varepsilon_I' - \varepsilon_I''\mathrm{i} = ((\sqrt[3]{\hat{\varepsilon}_F} - 1)/\nu_I + 1)^3$. The DEP scanner is 1 cm wide and in the worst case the measurement is slightly influenced by the ice up to about 2 cm to each side of the scan [*Wilhelms*, 2000, Section 2.3.6.3.], while the GAP scan is confined to a section of ice less than 5 mm wide. To suppress noise from datasets with differing resolution, the DEP and GAP datasets were smoothed by averaging the data and their respective variances and co-variances over 5 cm-long sections (black data points in Figure 1). The RC of pure ice's RP ε_I' scatters around the averaged constant value of 3.110 with a standard deviation 0.053. Considering the 12251 data points of the main population the standard error of the mean would be $0.053/\sqrt{12251} = 0.00048$. Realistically, this is of course an underestimate, but the errors are assumed to be controlled systematically. For purely systematic errors, the error of the mean is the root-mean-square (rms) of the basic population error, and equals 0.056. The actual scatter of pure ice's RP around the average is about[1] 0.035. This finding is consistent with the literature. *Gough* [1973] finds a doping independent RC of ice's RP. *Matsuoka et al.* [1997] find a doping independent RC of RP within 1% error, for marine salt (NaCl), sulfuric acid (H_2SO_4) and nitric acid (HNO_3) in concentrations of up to 10 μg/g. Even for coastal sites, these concentrations are never exceeded. According to *Petrenko and Whitworth* [1999, Section 5.3.1] the RC of RP

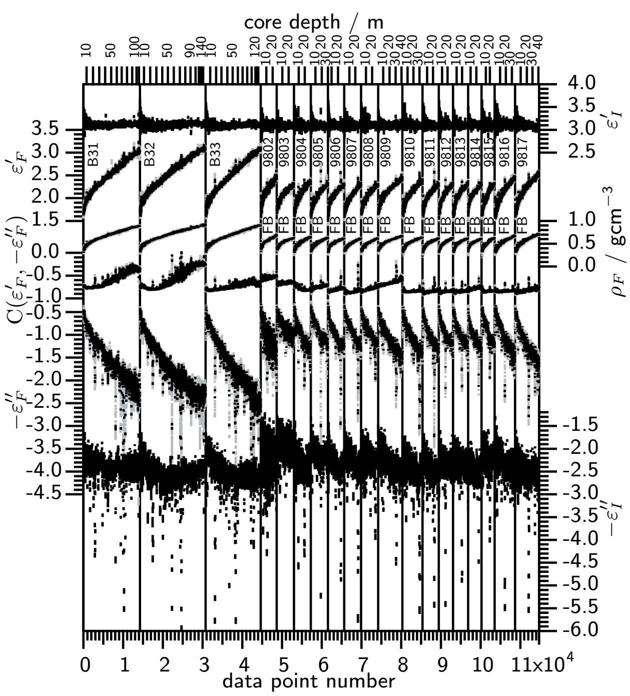

Figure 1. Starting from the RC of RP (ε_F'), GAP density (ρ_F), correlation coefficient of RC and IC of RP (C(ε_F', $-\varepsilon_F''$)) as well as the IC of RP ($-\varepsilon_F''$) (measured with DEP at 250 kHz), the properties of the ice phase RC of RP (ε_I') and IC of RP ($-\varepsilon_I''$) have been calculated with the DECOMP formula. The full DEP data set consists of 114720 measurements with error bars is represented by the grey shaded area. To reduce noise the DEP data have been binned into 5 cm averages before the ice phase's properties were calculated with the DECOMP formula. The binned data set with 12251 entries is plotted with error-bars in solid black on top of the hi-resolution data. The ice phase's RP RC is the topmost and IC is the lowermost curve.

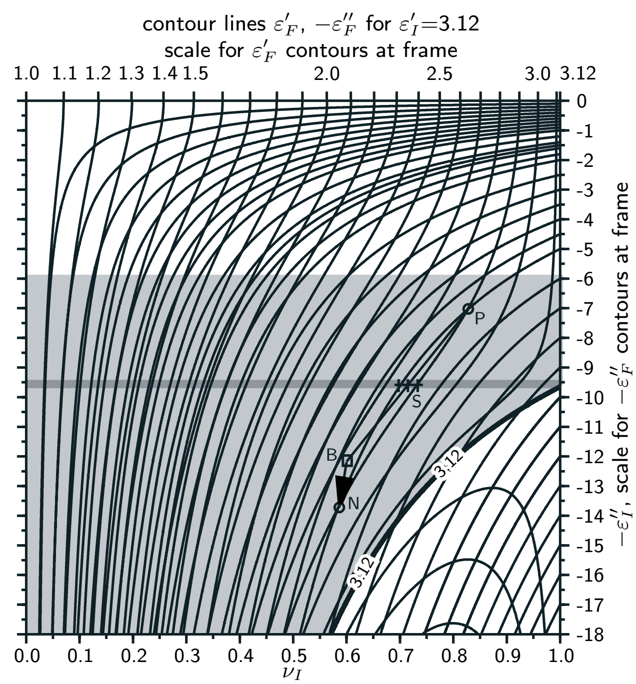

Figure 2. Non-injective properties of the DECOMP map. The ordinate of the $\varepsilon_F' = 3.12$ contour line's intersection with the $\nu_I = 1$ line forming a saddle point (SP) is emphasized in grey. For the counter lines' elevation, refer to the scales on the frame. Note that ε_F' and ε_F'' contour lines intersect twice: the light-grey shading marks the area where two pre-images $\hat{\varepsilon}_I$ exist for an image $\hat{\varepsilon}_F$ inside the plot boundaries. The two appertaining pre-images have been found by mirroring any original pre-image P at the middle of the respective contours' intersections with the SP line (S), and then iterating this starting point B with the Newton algorithm. The fixed point N of the Newton algorithm is the corresponding pre-image to P.

varies only by 1.25% over the 1 MHz–39 GHz range. The RC of RP reported here, which was measured at 250 kHz, is therefore consistent with values reported in the literature; for example, *Auty and Cole* [1952] found a value of 3.1 for a carefully prepared laboratory grown sample, and *Fitzgerald and Paren* [1975] report 3.13±0.02 for a Greenlandic sample. Two-way travel times of radar waves in grounded Greenlandic and Antarctic ice sheets, which exceed 1 km thickness, imply a RC of ice's RP in the range of $3.08\ldots3.11$ [*Bogorodskiĭ et al.*, 1985, Table IX]. *Petrenko and Whitworth* [1999, cover] quote 3.16 for ice at $-20°$C. For purposes of further discussion, we shall assume $\varepsilon'_I = 3.12 \pm 0.04$. This assumption covers the range reported in the literature referenced above, and coincides very well with the determination of ice's RC of RP to 3.110 ± 0.035, as discussed above.

Pure ice's RP IC $-\varepsilon''_I$ is not constant, but varies with the impurity content originating from, for example, the bio-geochemical cycle or volcanic eruptions as well as the influence of ambient temperature during measurement. This is consistent with the accepted opinion in the literature, that the conductivity of polar ice is dependent on its impurity content [e.g. *Wolff*, 2000].

4. Inversion of dielectric data in terms of density and conductivity

The DECOMP formula links the set of pure ice's properties ε'_I, ε''_I and ρ_I to the properties of firn ε'_F, ε''_F and ρ_F. With DEP both components of firn's RP $\hat{\varepsilon}_F$ are measured, where ε'_I and ρ_I are pure ice's material constants. One wonders: is it possible to determine the density of firn and the conductivity of ice solely from DEP measurements with the help of the DECOMP formula? Figure 2 illustrates that the DECOMP map is, in principle, non-injective[1]. In the light-grey shaded area, two existing pre-images $\hat{\varepsilon}_I$ for any given $\hat{\varepsilon}_F$ contour line-intersection can be found, such that more assumptions are required for an unambiguous inversion. In contrast, this means that for any pre-image with IC of RP $\varepsilon''_I \leq 6$ there is no corresponding pre-image in the region $\varepsilon''_I \leq 18$. As no data points were omitted beyond the axis' range in Figure 1, an unambiguous inversion practical with the DECOMP formula as it already exists. If the density of firn is tightly constrained, the DECOMP formula unambiguously determines the firn's density and the pure ice's conductivity from the DEP measurements alone. Firn's density can easily be constrained using the results of empirical densification models, or directly from "bulk" density measurements obtained when logging the core. The inversion of the DECOMP formula with a Newton algorithm will now be described.

Inverting the DECOMP formula $\sqrt[3]{\hat{\varepsilon}_F} = \nu_I(\sqrt[3]{\varepsilon'_I - \varepsilon''_I \mathrm{i}} - 1) + 1$ is equivalent to finding a root $g({}_*\nu_I, {}_*\varepsilon''_I) = 0$ for the function $g(\nu_I, \varepsilon''_I) \equiv \nu_I(\sqrt[3]{\varepsilon'_I - \varepsilon''_I \mathrm{i}} - 1) - \sqrt[3]{\hat{\varepsilon}_F} + 1$. The root for the complex-valued function, g, is found by solving the two real-valued equations for RC and IC simultaneously. A common scheme is to define an iterative Newton mapping that converges to a fix-point[1] $({}_*\nu_I, {}_*\varepsilon''_I)$.

5. Discussion and geophysical applications

For ice core analysis the improvements made possible by application of the DECOMP formula, as presented here, are twofold. Firstly, the inversion of DEP data with the DECOMP formula provides a high-resolution densimeter. The Newton mapping failed to converge in only about 1‰ (121 out of the 114720 sample data points) with improvements possible using better initial guesses for the volume-fraction's starting value. Better guesses could result from either by measuring the density on the core pieces volumetrically, or by first-pass processing of a smoothed data set. Stubborn points should be assessed on a case-by-case. Fitting a proportional line[1] to the 114599 points yields a slope of 0.99406 ± 0.00009. To test the hypothesis, "GAP and DECOMP derive the same density within the most overestimated errors", one must minimize the risk of wrongly rejecting the (null-) hypothesis of "statistically different densities are determined by the two methods". The difference of the GAP- and the DECOMP-determined densities, compared to the random scatter of the difference, is measured by $\chi^2 = \sum_{i=1}^{114599}[(\rho_F - \nu_I\,\rho_I)^2/((\Delta\rho_F)^2 + (\Delta(\nu_I\,\rho_I))^2)]_i = 95643.2$. Thus one would accept the (null-) hypothesis if $\chi^2 \geq \chi^2_c = 97660$, which reduces the risk of rejecting a true hypotheses for 114599 degrees of freedom to a mere $1 : 10^{300}$. As the calculated $\chi^2 < \chi^2_c$, the (null-) hypothesis is rejected confidently at a very high significance level. This supports the hypothesis that GAP and DECOMP provide entirely comparable density measurements, even with the most-overestimated errors. The average standard errors of GAP density (0.01 gcm^{-3}) and DECOMP density (0.015 gcm^{-3}) are also quite comparable, so that DEP measurements can replace the much more complicated GAP measurements. From a practical standpoint, density profiles now be measured rapidly and conveniently in the field using a standard profiling method instead of using radioactive sources or X-ray tubes.

Secondly, elevated conductivity incorporated into the ice from (for example) volcanic eruptions might not be identifiable at all in the firn's IC of RP, but is clearly identifiable in the ice phase's IC of RP. Figure 3 illustrates the mixing effect of density and permittivity. The work by *Eisen et al.* (in preparation) uses the DECOMP formula to disentangle the dielectric properties of firn, rescale the pure ice's IC of RP for the frequency shift from the below 1 MHz DEP frequency to the electromagnetic reflection frequency in the range of 60 MHz, and finally mix the frequency-shifted properties of the firn.

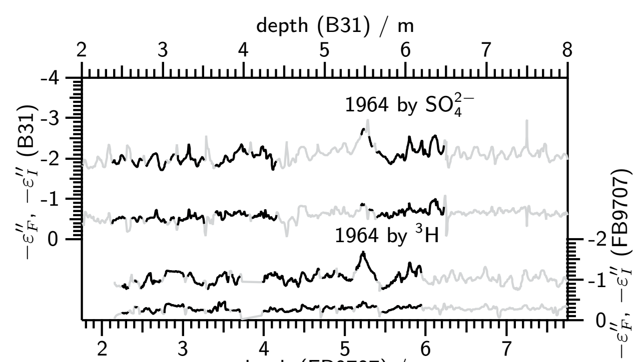

Figure 3. Example for peak identification in the firn. The cores B31 and FB9707 were drilled at the same location DML07 [*Oerter et al.*, 2000] one year apart. Between 5 m and 5.5 m, there is a corresponding maximum of $-\varepsilon''_I$ in both cores that cannot be identified in the $-\varepsilon''_F$ records. The higher conductivity is caused by impurities introduced by a volcanic eruption of Agung, that were deposited in 1964. In FB9707 the peak has been dated by ^{3}H content of the core [*Oerter et al.*, 1999] and in the B31 core, sulfate was measured directly [*Traufetter et al.*, 2004]. In the grey shaded sections the core surface might have been slightly damaged, but with no impact on the measurement. The differing signal level is due to processing at different temperatures.

Few assumptions were made to develop the DECOMP model. Any binary composite with known properties of one phase and known RC of RP can be analyzed with the DECOMP model. Furthermore, this application of DECOMP demonstrates the advancements possible by fitting individual material and composition properties to the dielectric properties of the mixture. Other sets of parameters are likely to work as well. In conclusion the DECOMP application outlined here is a good example of how the interpretation of electrical profiling with dielectric mixing models can improve the understanding of geophysical and geochemical parameters, that are much harder to access otherwise.

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Notes

1. Supporting material is available via Web browser or via Anonymous FTP from "ftp://ftp.agu.org/apend/" (Username = "anonymous", Password = "guest"). Subdirectories in the ftp site are arranged by journal and paper number. Information on searching and submitting electronic supplements is found at http://www.agu.org/pubs/esupp_about.html.

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