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SOME CLASSICAL MIXING FORMULAS IN THE TIME DOMAIN

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Abstract: This paper discusses a time domain approach to the effective-medium modeling of dielectrically heterogeneous materials. Special emphasis is put on the dispersive behavior of the mixture. Specifically, the Debye model is treated. In terms of the geometry of the mixture, the present analysis is carried out for inclusions of ellipsoidal or spherical form.

MIXTURE FORMULAS IN THE TIME DOMAIN

The classical mixing theories use a static or quasistatic treatment of the inclusions embedded in a host medium and the polarizabilities of the inclusions. In the time domain, the evaluation of the effective permittivity operator requires evaluation of inverse Fourier transforms or calculation of convolutions and operator inverses.

In the present paper we consider linear, isotropic, temporally dispersive dielectric materials. In a time domain setting, the constitutive relations have the general form, see [2]:

$$\begin{cases} \boldsymbol{D}(\boldsymbol{r},t) = \varepsilon_0 \left[\epsilon \boldsymbol{E}\right](\boldsymbol{r},t) = \varepsilon_0 \left\{\varepsilon_\infty(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r},t) + (\chi * \boldsymbol{E})(\boldsymbol{r},t)\right\} \\ \boldsymbol{B}(\boldsymbol{r},t) = \mu_0 \boldsymbol{H}(\boldsymbol{r},t) \end{cases}$$

where the vacuum permittivity is ε_0 and the vacuum permeability μ_0, and the operation denoted by $*$ stands for the temporal convolution. The function $\varepsilon_\infty(\boldsymbol{r}) \geq 1$ describes the instantaneous (optical) response of the material. The dispersive part is described by the susceptibility kernel $\chi(\boldsymbol{r},t)$ as a function of time. Due to causality, the susceptibility kernel χ vanishes for $t < 0$, but it can have a discontinuity in the origin, *i.e.*, it can happen that $\chi(t = 0^+) \neq 0$. Although this option of discontinuity across the origin is sometimes doubted in the literature (see, for example [1, p. 310], [4]), it does not violate causality. In fact, the Debye model, which models the dispersive behavior of polar liquids in the microwave regime excellently, is an example of a case where $\chi(t = 0^+) \neq 0$.

NON-DISPERSIVE BACKGROUND—DEBYE MODEL FOR ELLIPSOIDAL INCLUSIONS

Consider a mixture of dispersive ellipsoidal inclusions in a dispersionless background. The ellipsoidal inclusions are located in random positions with their axes aligned in the host medium. The time domain Maxwell Garnett formula, written for a non-dispersive background medium, ε_b, and dispersive inclusions with optical response ε_∞ and susceptibility kernel $\chi(t)$ implies that the effective permittivity dyadic of the mixture is

$$\boldsymbol{\epsilon}_{\text{eff}} = \epsilon^x_{\text{eff}}\hat{\boldsymbol{x}}\hat{\boldsymbol{x}} + \epsilon^y_{\text{eff}}\hat{\boldsymbol{y}}\hat{\boldsymbol{y}} + \epsilon^z_{\text{eff}}\hat{\boldsymbol{z}}\hat{\boldsymbol{z}}, \qquad i = x, y, z$$

where the effective permittivity in the ith direction is

$$\epsilon^i_{\text{eff}} = \varepsilon^i_{\infty,\text{eff}} + \chi^i_{\text{eff}}* = \varepsilon_b + \varepsilon_b f\left(\varepsilon_\infty - \varepsilon_b + \chi*\right)\left[\varepsilon_b + N_i\left(1-f\right)\left(\varepsilon_\infty - \varepsilon_b + \chi*\right)\right]^{-1}$$

This expression is well defined unless $\varepsilon_b + N_i\left(1-f\right)\left(\varepsilon_\infty - \varepsilon_b\right) = 0$. The permittivity operators (functions) contain the depolarization factors N_i of the ellipsoids [3]. Specifically, for a Debye-mixture, $\chi(t) = \beta\exp[-t/\tau]$, $t > 0$, the optical response and the susceptibility functions are

$$\begin{cases} \varepsilon^i_{\infty,\text{eff}} = \varepsilon_b + \varepsilon_b f \dfrac{\varepsilon_\infty - \varepsilon_b}{\varepsilon_b + N_i\left(1-f\right)\left(\varepsilon_\infty - \varepsilon_b\right)} \\ \chi^i_{\text{eff}}(t) = \dfrac{f\varepsilon_b^2\beta H(t)}{\left[\varepsilon_b + N_i\left(1-f\right)\left(\varepsilon_\infty - \varepsilon_b\right)\right]^2}\exp\left[-\left(\dfrac{1}{\tau} + \dfrac{N_i\left(1-f\right)\beta}{\varepsilon_b + N_i\left(1-f\right)\left(\varepsilon_\infty - \varepsilon_b\right)}\right)t\right] \end{cases}$$

A MIXTURE OF TWO DISPERSIVE MATERIALS

If the background medium and the inclusions are both dispersive, the time domain Maxwell Garnett formula can still be written in the standard form. For spherical inclusions we have

$$\epsilon_{\text{eff}} = \varepsilon_{\infty,\text{eff}} + \chi_{\text{eff}}(t) *$$

where the optical response of the mixture is

$$\varepsilon_{\infty,\text{eff}} = \varepsilon_{\infty,\text{b}} + 3\varepsilon_{\infty,\text{b}} f \frac{\varepsilon_{\infty,\text{i}} - \varepsilon_{\infty,\text{b}}}{\varepsilon_{\infty,\text{i}} + 2\varepsilon_{\infty,\text{b}} - f(\varepsilon_{\infty,\text{i}} - \varepsilon_{\infty,\text{b}})}$$

We now focus on the special case of spherical Debye inclusions in a Debye background material, which susceptibility kernels we denote by

$$\begin{cases} \chi_b(t) = \dfrac{\varepsilon_{s,b} - \varepsilon_{\infty,b}}{\tau_b} \exp\left(-\dfrac{t}{\tau_b}\right) H(t) \equiv \alpha_b \exp(-t\beta_b) H(t) \\ \chi_i(t) = \dfrac{\varepsilon_{s,i} - \varepsilon_{\infty,i}}{\tau_i} \exp\left(-\dfrac{t}{\tau_i}\right) H(t) \equiv \alpha_i \exp(-t\beta_i) H(t) \end{cases}$$

In the case $\tau_b \neq \tau_i$, we get the following explicit expression for the effective susceptibility kernel:

$$\chi_{\text{eff}}(t) = c_1 \chi_b(t) + c_2 \chi_i(t) + c_3 \chi_+(t) + c_4 \chi_-(t) + c_5 \chi_b(t) \frac{t}{\tau_b}$$

where the coefficients are

$$\begin{cases} c_1 = 1 + a_1 \left(1 - \dfrac{\alpha_+}{\beta_+ - \beta_b} - \dfrac{\alpha_-}{\beta_- - \beta_b}\right) + a_3 \left(\dfrac{\alpha_+ \beta_b}{(\beta_+ - \beta_b)^2} + \dfrac{\alpha_- \beta_b}{(\beta_- - \beta_b)^2}\right) \\ c_2 = a_2 \left(1 - \dfrac{\alpha_+}{\beta_+ - \beta_i} - \dfrac{\alpha_-}{\beta_- - \beta_i}\right) \\ c_3 = -\varepsilon_{\infty,\text{eff}} + \varepsilon_{\infty,b} - a_1 \dfrac{\alpha_b}{\beta_b - \beta_+} - a_2 \dfrac{\alpha_i}{\beta_i - \beta_+} - a_3 \dfrac{\alpha_b \beta_b}{(\beta_+ - \beta_b)^2} \\ c_4 = -\varepsilon_{\infty,\text{eff}} + \varepsilon_{\infty,b} - a_1 \dfrac{\alpha_b}{\beta_b - \beta_-} - a_2 \dfrac{\alpha_i}{\beta_i - \beta_-} - a_3 \dfrac{\alpha_b \beta_b}{(\beta_- - \beta_b)^2} \\ c_5 = a_3 \left(1 - \dfrac{\alpha_+}{\beta_+ - \beta_b} - \dfrac{\alpha_-}{\beta_- - \beta_b}\right) \end{cases}$$

where

$$\begin{cases} a_1 = \dfrac{\varepsilon_{\infty,\text{eff}} - \varepsilon_{\infty,b}}{\varepsilon_{\infty,b}} - \dfrac{\varepsilon_{\infty,\text{eff}} - \varepsilon_{\infty,b}}{\varepsilon_{\infty,i} - \varepsilon_{\infty,b}} \left(1 + \dfrac{\varepsilon_{s,i} - \varepsilon_{\infty,i}}{\varepsilon_{\infty,b}} \dfrac{\tau_b}{\tau_i - \tau_b}\right) \\ a_2 = \dfrac{\varepsilon_{\infty,\text{eff}} - \varepsilon_{\infty,b}}{\varepsilon_{\infty,i} - \varepsilon_{\infty,b}} \left(1 + \dfrac{\varepsilon_{s,b} - \varepsilon_{\infty,b}}{\varepsilon_{\infty,b}} \dfrac{\tau_i}{\tau_i - \tau_b}\right) \\ a_3 = -\dfrac{(\varepsilon_{\infty,\text{eff}} - \varepsilon_{\infty,b})(\varepsilon_{s,b} - \varepsilon_{\infty,b})}{\varepsilon_{\infty,b}(\varepsilon_{\infty,i} - \varepsilon_{\infty,b})} \\ 2\beta_\pm = f_i \alpha_i + \beta_i + f_b \alpha_b + \beta_b \pm \sqrt{(f_i \alpha_i - \beta_i + f_b \alpha_b + \beta_b)^2 + 4 f_i \alpha_i (\beta_i - \beta_b)} \\ \alpha_\pm = \dfrac{\beta_i - \beta_b}{\frac{(\beta_\mp - \beta_b)}{(\beta_\pm - \beta_b)} - \frac{(\beta_\mp - \beta_i)}{(\beta_\pm - \beta_i)}} \end{cases}$$

and

$$\chi_\pm(t) = \alpha_\pm \exp(-\beta_\pm t) H(t)$$

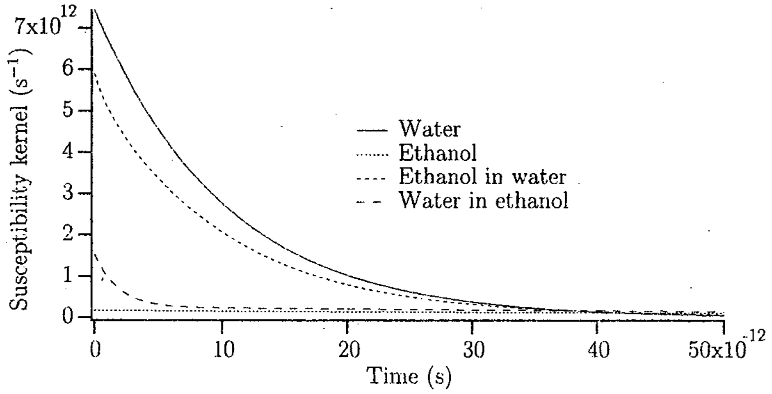

Figure 1: The susceptibility kernels for water, ethanol, ethanol–in–water mixture (20% ethanol), and water–in–ethanol mixture (80% ethanol).

Consequently, $\chi_{\text{eff}}(t)$ is a linear combination of four Debye kernels and one modified Debye kernel. We also have that

$$\min(\beta_i, \beta_b) < \beta_- < \max(\beta_i, \beta_b) < \beta_+, \qquad \alpha_\pm > 0$$

This implies that the relaxation time $\tau_+ = 1/\beta_+$ is less than both the relaxation times τ_i and τ_b, whereas $\tau_- = 1/\beta_-$ assumes a value between τ_i and τ_b.

Numerical results for a Debye–in–Debye medium (ethanol and water, 20-80% and 80-20%) are displayed in Figure 1. The figure shows that although the mixture curves resemble in form the Debye-kernels of water and ethanol, they are not exactly exponentially decaying. Another interesting detail of Figure 1 is the fact that the water–in–ethanol mixture has a slightly stronger memory for times after 40 ps compared to both water and ethanol, although the difference is very small.

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