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A Comparison of a Mixed-Cell Electrical Conductivity Model to the Volume-Averaging Approximation

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14. ABSTRACT

In this note, a model for mixed-cell electrical conductivity, previously developed by the author, is examined and compared to a simpler model based on volume averaging. Understanding is gained by reformulating the underlying assumptions of the author's model so as to achieve a result that mimics the volume-averaging approach. Then, those revised underlying assumptions are examined for their fidelity to the physical and morphological processes that govern electrical flow in a heterogeneous body. In so doing, an understanding is reached as to why volume averaging does not provide the most favorable match to expected physical behavior of a heterogeneous electrical conductor.

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1. Introduction

The default treatment of mixed-cell properties, in the absence of a more compelling model, is often taken via "volume averaging", in which the averaged (or effective) quantity $\bar{\kappa}$, is obtained by weighing the species-component property values, κ_j, by their respective volume fractions, v_j, for each of the n species found in the cell:

$$\bar{\kappa} = \sum_{j=1}^{n} v_j \kappa_j \quad . \tag{1}$$

With such an approach, the value of $\bar{\kappa}$, for a two-species mixture, for example, will vary linearly between κ_2 and κ_1, as v_1 changes from 0 to 1, respectively.

The model set forth in ARL-TR-8979[1] provides an alternative approach to estimating the electrical conductivity of a mixed cell. One of the hallmarks of the model is that it employs a statistical function $F(\hat{f})$, which provides the likelihood of establishing point-to-point cross-cell connectivity as a function of the volume fraction of conducting material in the domain.[2]

This F function is used to estimate the fraction of viable conducting pathways through the cell that are associated with each combination of material species present. While, on one hand, there is a preference for pathways that possess a higher conductivity (relative to other pathways), the number of pathways available for a given species combination is limited, on the other hand, by the combined volume fraction of those species composing the pathway, through the application of the F function.

2. Origins of the Functions $F(\hat{f})$ and $F(f)$

The function $F(\hat{f})$ provides the likelihood F that point-to-point cross-cell connectivity can be established, given $\hat{f}$ volume fraction of conducting material in the cell. The derivation[2] of the F function was made by metaphorically representing the heterogeneous computational domain as an equivalent square network, comprising randomly distributed conducting and insulating linkages. The F function, for a mixed cell that is idealized as a square 4×4 network of randomly distributed conductors and insulators, is shown in Fig. 1b. In the original treatment, various sizes of square network were considered (2×2, 3×3, 4×4, and a clipped 5×5), of which the 4×4 shown in Fig. 1a is merely a representative example.

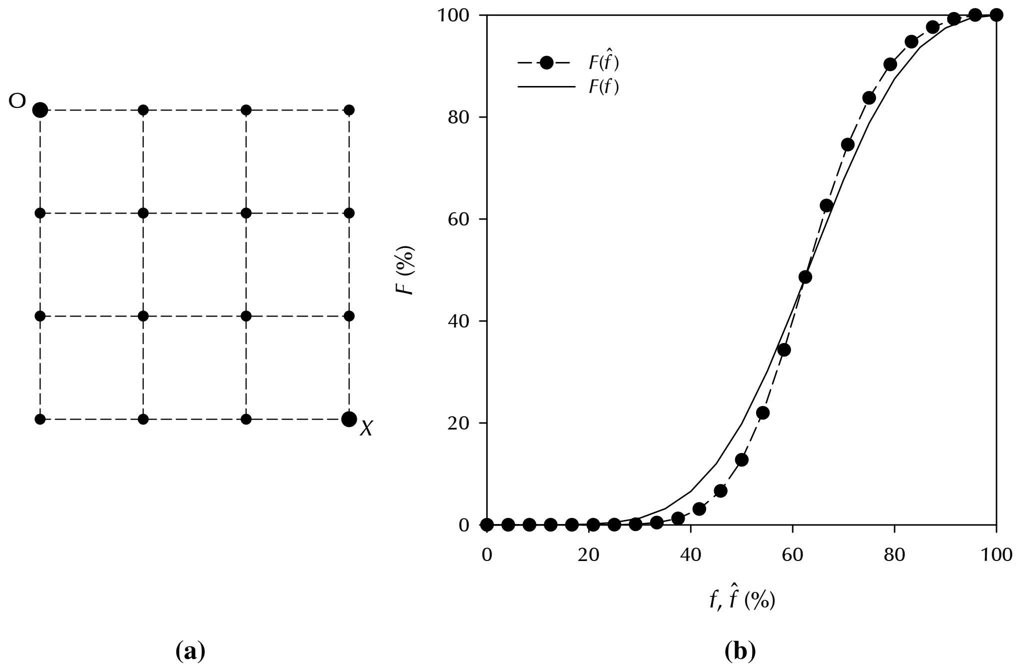

Fig. 1 For a) the given 4×4 network, b) the likelihood of *O*-to-*X* network connectivity *F*, expressed as a function of either the local conduction probability *f* or the global conducting fraction $\hat{f}$ of the network links

Each $m \times m$ network representation has its own unique $F(\hat{f})$ function. However, they all share an *S*-shape similar to that seen in Fig. 1b. This *S*-shape represents threshold behavior, in which the likelihood of connectivity remains very small until the volume fraction of conducting material reaches a threshold. At the threshold, the likelihood of connectivity changes rapidly. Beyond the threshold, the likelihood of connectivity is very high, rapidly approaching a certainty of connection (*i.e.*, $F \rightarrow 1$).

The function $F(f)$, also derived in ARL-TR-8899 and shown in Fig. 1b, is closely related to $F(\hat{f})$. Whereas $\hat{f}$ represents the proportion of total linkages in the network that are conducting (and is, therefore, not a continuous domain for a finite network), the term f instead represents a probability that any given linkage in the network is conducting. As the number of linkages in the network grows without bound, the two functions $F(\hat{f})$ and $F(f)$ become indistinguishable. However, for small finite networks, the $F(\hat{f})$ function becomes sparsely populated and is less closely aligned with $F(f)$, as seen, for example, in the 2×2 network[2] of Fig. 2. Technically, the $F(\hat{f})$ function is only defined at the solid dots of Fig. 2b—the dashed lines are merely linear interpolations between the defined domain points of $\hat{f}$ (with only four linkages in the 2×2 network, the fraction $\hat{f}$ of conducting linkages can only be the five discrete values of 0/4, 1/4, 2/4, 3/4, or 4/4).

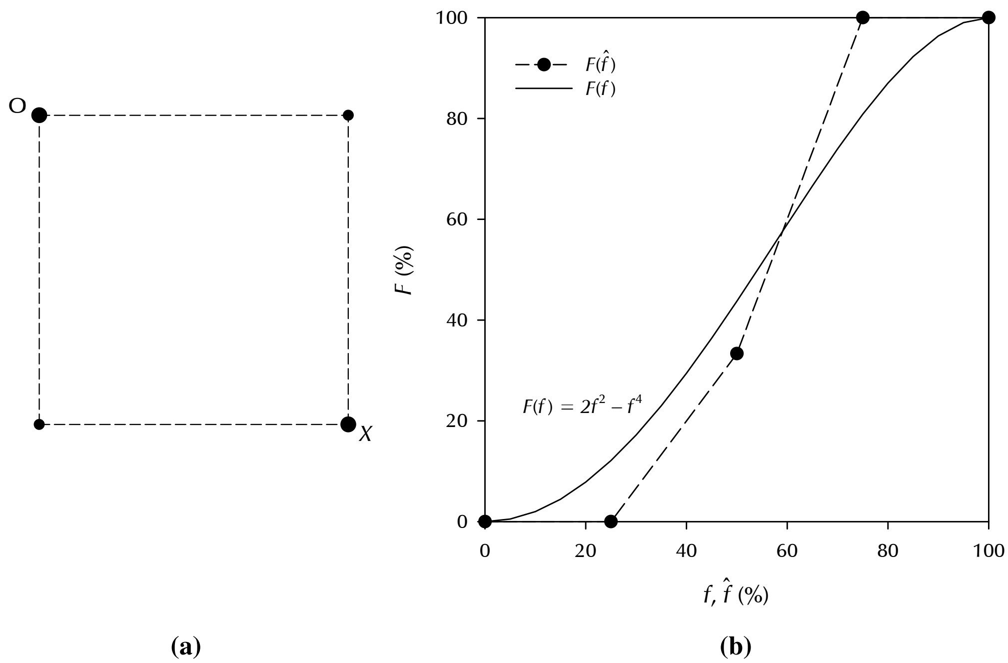

Fig. 2 For a) the 2×2 square network shown, b) the probability of network connectivity, F, with either f or $\hat{f}$ as the independent variable

3. The Question of Volume Averaging

The curious question, which is the subject of this note, arises as to whether the proposed electrical conductivity model of ARL-TR-8979 can, with the appropriate set of assumptions and/or constraints, reduce to a volume-averaged equivalent model, comparable to Eq. 1? The answer to this question is "yes", provided that two assumptions associated with that model[1] are suitably revised. The first required assumption concerns the type of network being used to approximate the morphological connectivity of the mixed cell. The second constraint necessary to achieve the volume-averaging result concerns restricting the variety of material pathways that can carry current in the mixed cell.

3.1 Mixed-Cell Network Morphology

The first step in getting the model of ARL-TR-8979[1] to mimic the response of volume averaging is to choose a different network to metaphorically represent the connectivity in a mixed cell. The $m \times m$ network topographies that were examined in ARL-TR-8899[2] serve the useful purpose of creating a wide number of possible circuits that traverse from points O to X, located on opposite sides of the network. For example, the 4×4 network of Fig. 1a has 184 distinct pathways for moving current from point O to X, should the paths prove conductive. Such a possibility confirms our innate understanding of how current may travel across a heterogeneous solid—a variety of pathways exist, but some of them may be preferred over others based on their relative conductivities.

To take the first step in recovering a model behavior equivalent to volumetric averaging, we need to simplify the network that is taken as the metaphorical equivalent of our mixed cell. In particular, we must adopt the simplest of all networks, the 2×1 network, as depicted in Fig. 3, consisting of a single linkage between points O and X and providing just a single pathway.

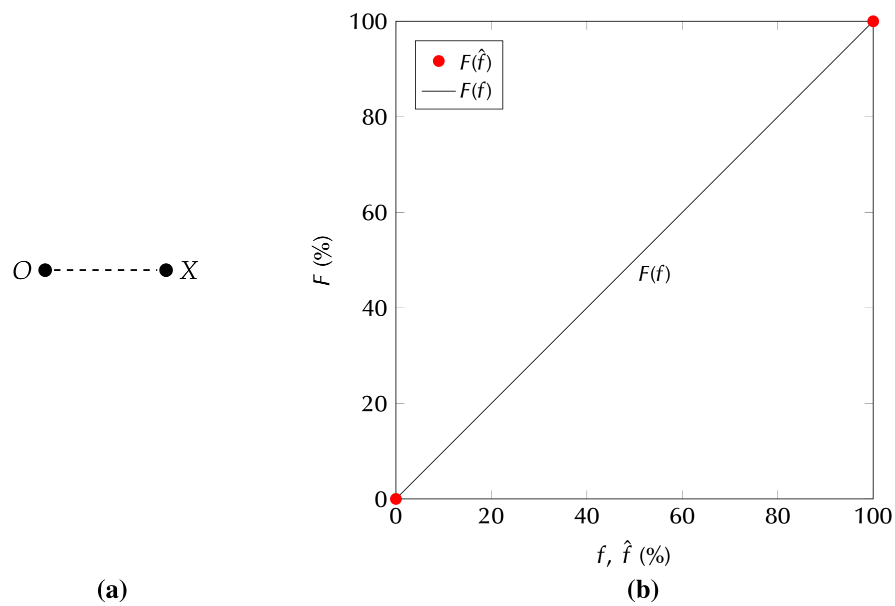

Fig. 3 For a) the 2×1 network that constitutes a revised assumption to the model of ARL-TR-8979, b) the probability of network connectivity, F, as a function of either f or $\hat{f}$

Here, the $F(\hat{f})$ function consists of two points, $(0,0)$ and $(1,1)$. This condition merely recognizes the fact that, with a single linkage in the network, the fraction of conducting linkages, $\hat{f}$, will either be exactly 0 or 1 and that the connectivity of the network, F, hinges completely on the state of that single link. Therefore, it makes sense to turn instead to $F(f)$ as the probabilistic descriptor required by the model. The straight line depicted in Fig. 3b merely reflects the fact that, if the likelihood of the single linkage being conductive is given by f, then the probability of establishing connectivity across the 2×1 network is, likewise,

$$F(f) = f \qquad \text{(revised assumption/constraint).} \tag{2}$$

With this replacement to the F function, the result may be calculated employing the method described in ARL-TR-8979.[1] The resulting mixed-cell electrical conductivity, both with the originally adopted F function and with the simplified replacement, is shown in Fig. 4. The result in Fig. 4b, while much closer to a fully linear result associated with volume averaging, still possesses a small amount of nonlinearity.

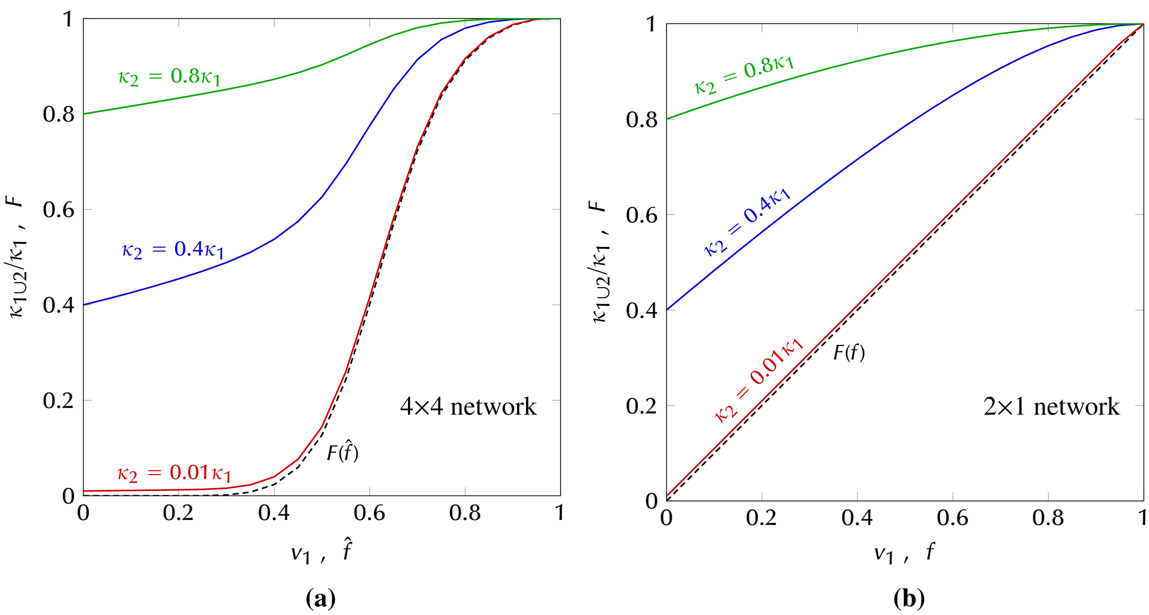

Fig. 4 Electrical conductivity of a two-species mixed cell, under the assumption of a) a 4×4 or b) 2×1 network to model the connectivity of a mixed cell, resulting in different representations for the *F* function

3.2 Electrical Pathway Constraint

In the model proposed in ARL-TR-8979[1] (and, thus, in the results of Fig. 4), there is a hierarchy of conductive preference that favors electrical pathways of greater conductivity. In the implementation adopted, if the material species are numbered in order of decreasing conductivity, the pathway hierarchy is constrained to 1, $1\cap2$, $\ldots$, $1\cap\cdots\cap n$, for a mixed cell of n species. This ordering means that pathways that traverse solely through the most conductive species $\{1\}$ are preferred, but beyond that, all pathways are compound, traversing through a multiplicity of species, preferentially given by the sets $\{1, 2\}$, $\{1, 2, 3\}$, $\ldots$, $\{1, 2, \cdots, n\}$. The rationale for this hierarchy is described in ARL-TR-8979.

To achieve linearized behavior of electrical conductivity κ, which seems almost but not quite achieved in Fig. 4b, the model to describe the conductivity of compound pathways must be revised, by way of assumption. In particular, we must assume that a given piece of matter cannot be part of two different pathways. Therefore, because material species 1 composed the preferred pathways in the mixed-cell "network", pathways encompassing the $1 \cap 2$ set must employ the lower-conductivity species 2 exclusively, such that

$$\kappa_{1\cap\cdots\cap j} = \kappa_j \qquad \text{(revised assumption/constraint).} \tag{3}$$

Pathways that traverse two or more species are unilaterally precluded under this assumption, even though there is little physical rationale for it. It does, however, serve to simplify the resulting equations. This assumption replaces Eq. 4 of ARL-TR-8979.

4. Results

We can now turn to the question of how these two revisions will affect the calculation of electrical conductivity (for reference to what follows, please see Eqs. 4–7 in ARL-TR-8979). Under the assumption of Section 3.1 of this report, which leads to Eq. 2 in the form of $F(v) = v$, the model of ARL-TR-8979 (Eq. 6) simplifies as follows:

$$F_{1\cup\cdots\cup j} = F\Big(\textstyle\sum_{i=1}^{j} v_i\Big) = \sum_{i=1}^{j} v_i \quad . \tag{4}$$

This simplification, by way of Eq. 5 of ARL-TR-8979, leads directly to the result:

$$F_{1\cap\cdots\cap j} = F_{1\cup\cdots\cup j} - F_{1\cup\cdots\cup j-1} = v_j \quad . \tag{5}$$

Take the assumption from Section 3.2, in the form of Eq. 3, along with the result of Eq. 5, and insert them into Eq. 7 of ARL-TR-8979 to obtain the model expression for κ:

$$\kappa = \kappa_{1\cup\cdots\cup n} = \sum_{j=1}^{n} F_{1\cap\cdots\cap j}\,\kappa_{1\cap\cdots\cap j} = \sum_{j=1}^{n} v_j \kappa_j \quad . \tag{6}$$

A comparison of Eq. 6 to the volume-averaged result of Eq. 1 reveals a match! Graphically, Eq. 6 presents as shown in Fig. 5.

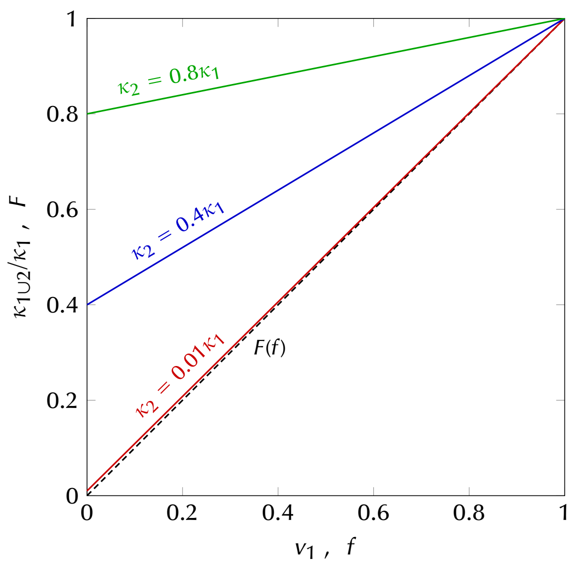

Fig. 5 Electrical conductivity of a two-species mixed cell, incorporating the assumptions embodied in Eqs. 2 and 3 to the model of ARL-TR-8979, captures the behavior of volume averaging

Equation 6, by adopting the two assumptions embodied in Eqs. 2 and 3, captures the behavior of the volume-averaged formulation. In no way is it being recommended to employ the model in such a volume-averaged fashion. The model was indeed developed as an *alternative* to the volume-averaged approach. Nonetheless, the purpose in showing the connection lies in providing a fuller context and understanding of how the model of ARL-TR-8979 operates vis-à-vis the volume-averaged approach.

The result allows one to better critique the deficiency of the volume-averaged approach, by understanding what underlying assumptions are necessary to bring it about. First, by forcing the use of a single-element network to serve as the metaphorical equivalent of the mixed cell, one loses the essential threshold behavior known to exist in distributed (heterogeneous) networks, as represented in Fig. 1b.

Secondly, the pathway restrictions that lead to Eq. 3 represent an unrealistically simplistic notion that electrical pathways through a mixed cell cannot be compounded from two or more species, as would otherwise be found *in situ*. This latter restriction forcibly requires the abandonment of the underlying principle that the current prefers a pathway of lesser resistance and instead treats each of the species in the mixed cell as isolated therein.

5. Conclusion

In this report, the mixed-cell electrical conductivity model introduced in ARL-TR-8979[1] was reimagined, subject to a new set of constraints, in an effort to reproduce a model equivalent to the technique known as volume averaging. The purpose of this exercise is not to put forward the volume-averaging approach, but rather to understand the technical specificities that separate the model of ARL-TR-8979 from that of volume averaging.

This goal was successfully achieved through the adoption of two assumptive changes in the underlying model. First, the network used to metaphorically represent the mixed cell had to be ultimately simplified to a single linkage. In so doing, the tendency toward threshold behavior is removed from the problem, such that the probability of network connectivity becomes directly proportional to the likelihood that any single network linkage is conductive. Secondly, the materials of the mixed cell, which are free to act in concert when placed *in situ*, must instead be assumed to be internally isolated from each other so that electrical pathways across the cell comprise a single material species only.*

With these two assumptive changes in place, the model of ARL-TR-8979 takes on a behavior that has been shown to be mathematically equivalent to the approach known as "volume averaging". It is clear, however, that these two assumptions run counter to our understanding of current flow through a heterogeneous medium.

First, we understand that, in order to disturb the conductivity of a conductor, it is not enough to introduce a minute quantity of low/nonconducting species into the domain—enough pathways can establish themselves around the inclusions so as to retain near-optimal conductivity. Rather, the introduction of low/nonconducting species must be of a magnitude beyond a threshold in order to substantially disrupt the likelihood of establishing high-conductivity pathways. Second, we also understand that, in reality, conductive pathways can establish themselves, which transit

*As pointed out by Berning,[3] these two assumptive changes, taken together, are akin to thinking of the mixed cell as a set of wires, conducting in parallel, one wire for each material species in the mixed cell. All wires are of the same length, and the cross section of each wire is in proportion to the volume fraction of the material species composing it. In such a configuration, each current pathway traverses a single material species and the contribution toward the conductivity for each material species is in proportion to its volume fraction.

multiple, disparate species—there is no scientific justification for requiring that a pathway be confined to a single material species.

These two arguments alone testify against the adoption of a mixed-cell conductivity model based on the principles of volume averaging. Therefore, they serve to reinforce the notion that an alternative approach, perhaps like that introduced in ARL-TR-8979, are better suited to the modeling of mixed-cell conductivity in the context of numerical methods employing magnetohydrodynamic physics.

6. References

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