**A Homogenization Approach to Multi-Scale Radiative Transfer in Nano-Structures**

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**ABSTRACT**

We propose a homogenization approach for modelling thermal radiative transfer in nano-structured materials to obtain an effective radiative transport equation (RTE). The approach is based on the concept of moment-linking—the macroscopic moments of an effective RTE are matched to the moments of the underlying electrodynamic solution. Here we present the approach and discuss anticipated results and future directions.

**1. Introduction**

Radiative transfer in complex hetero-structured media has garnered much attention in the recent decade [1]. When the heterogeneous features of such media are sufficiently large, the radiative transfer equation (RTE) can be applied at discrete levels, which drastically simplifies the analysis. Recent developments provide a strong theoretical foundation for the use of the single and multiple RTE continuum approaches in macro-structured media consisting of multiple components with arbitrary-shaped discrete-level geometry and arbitrary radiative properties of the constituents [2]. Studies on predicting thermal characteristics, in particular radiative properties, of nano- and micro-structured media are nearly absent in the literature and pose serious challenges to model. Of particular interest here are the high-temperature processes considered in the emerging field of solar thermochemistry [3] where multi-scale materials have already appeared in experimental investigations [4].

The connection between the electrodynamic description of light and the ray description that underlies the RTE in discrete and continuous random media has been explored by numerous authors and was shown to be valid in limiting cases [5,6]. In this work, we propose a method for the multi-scale simulation of porous media exhibiting wavelength-scale features where the RTE may not be strictly valid, but the energy transfer within the media can still be represented by it.

**2. Proposed methodology**

We consider the limiting case of the RTE written in terms of a phase-space energy densityfor a cold scattering medium [5],



Here, *σ* is the scattering coefficient,*k* is the wave-vector,  is the *i*th component of the phase velocity vector, and Φ is the scattering phase function. The permeability and permittivity of the local medium is given by *ε* and *μ*. Space and time are denoted *x* and *t*. Note that the phase-space energy density has the units of J m-3µm3, i.e. energy density per wave-vector, and the scattering phase function is properly normalized and should ensure that scattering only takes place within a certain wavenumber band. For the reader more comfortable with an RTE written in terms of a specific intensitywe point out that for a medium with a dilute collection of independent scatterers we have where is the speed of light in the background medium. We would like to connect this equation to the fields obtainable by a solution to Maxwell’s equations but we do not propose to do so by directly deriving the RTE from them. Instead, we express the coefficients defining the medium—namely  andin terms of quantities that can be readily calculated using both the RTE and Maxwell’s equations, the macroscopic moments.

The moments of the RTE are calculated by



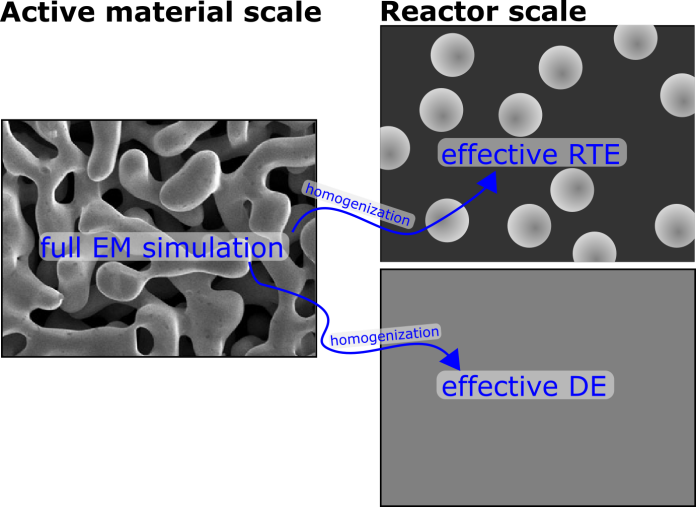
where and are positive integers. If we assume the RTE to exist in a region of infinite extent and impose the energy density goes to zero at infinite, we can obtain a set of ordinary differential equations in time for the moments by multiplying Eq. (1) by and integrating over all wave-vectors and space:



Defining the moments for the electrodynamic problem requires a more sophisticated approach because ???please add a very short explanation?. First, we need to take a physical model that exists in configuration space only (Maxwell’s equations), and project it in a meaningful way into the phase space. Ryzhik et al. [5], among others, utilizes the Wigner function for this purpose,

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The vectoris defined by and the star denotes the complex conjugate. This quantity has been shown to be analogous to the phase-space energy density in that its zeroth and first moments in wave-vector correspond to the internal energy and the energy flux, respectively. It satisfies a RTE under limiting circumstances; see [7]. The Wigner function is not positive definite, so its interpretation as a phase space energy density is limited to the high-frequency case. Regardless, the proper moments can be obtained by



**Figure 1. A concept diagram for the moment linking homogenization process in the context of a thermochemical reactor with a nano-structured active material. An effective diffusion equation was not discussed here but will be considered by an analogous approach to the RTE case considered here.**



where tr represents the trace operation.

We are now ready to state the approximation underlying the proposed homogenization process. We impose that the ODEs given by (3) fit the time dependent moments calculated by a solution to Maxwell’s equations for the geometry under study. In other words, we impose that



This imposition has been shown to give excellent agreement when approximating radiative transfer by a diffusion equation [7]. Figure 1 is a representation of the proposed scale-linking process. For the case of a medium that strictly satisfies the RTE—that is, dilute independent scatterers—the transport coefficients obtained from the electrodynamic solution should exactly correspond to the proper transport coefficients. When the medium does not satisfy the conditions for a RTE to be valid, we expect the fitting process proposed here to give *effective* transport coefficients. All electrodynamic information that is lost in the RTE description, namely interference effects, will be coarsely contained within them and the *effective* RTE solved on the large scale.

**3. Future work**

With the conceptual connection between scales in place, the future work will focus on the validation of the propose theory. The ?add the precise name? moments will be computed by solving Maxwell’s equations on the exact geometry of infinite extent. First, scattering of a plane, monochromatic wave by a single non-absorbing sphere will be considered because the availability of an exact solutionin that case. Next, the problem involving an independently scattering medium as considered by Mishchenko et. al [6] will be considered because the RTE has been rigorously derived in this limit using the Wigner function used [5]. In order to extend the approach to cases of porous materials we propose to solve Maxwell’s equations on a large sample of the proposed geometry using computational electrodynamics. The FDTD method is the promising solution method because open source, scalable codes implementing it are readily available to solve the problem presented.

Some foreseen challenges are discussed here to conclude the present study. The scattering phase function is a continuous function of the incoming and outgoing wave-vectors. Thus, it is impossible to be represented exactly by a finite number of moments. Consequently, an approximate expression in terms of determinable expansion coefficients must be decided upon. The approach to excite a representative element of a porous system is still an outstanding problem. While an individual scatterer can be excited by a plane, monochromatic wave, the analogous case for a porous element has not been identified yet.

**References**

[1] L.A. Dombrovsky and D. Baillis. *Thermal Radiation in Disperse Systems: An Engineering Approach*. Begell House, New York and Redding (CT), 2010.

[2] W. Lipiński, D. Keene, S. Haussener, and J. Petrasch. Continuum radiative heat transfer modeling in media consisting of optically distinct components in the limit of geometrical optics. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 111:2474–2480, 2010.

[3] R. Bader and W. Lipiński. Solar thermochemical processes. In *The World Scientific Handbook of Solar Energy* (ed. Crawley, G. M.) (World Scientific, 2016).

[4] P. Furler et al. Thermochemical CO2 splitting via redox cycling of ceria reticulated foam structures with dual-scale porosities. *Physical Chemistry Chemical Physics*, 16(22):10503–10511, 2014.

[5] L. Ryzhik, G. Papanicolaou, and J.B. Keller. Transport equations for elastic and other waves in random media. *Wave Motion*, 24(4):327–370, 1996.

[6] M.I. Mishchenko, J.M. Dlugach, M.A. Yurkin, L. Bi, B. Cairns, L. Liu, R. Lee Panetta, L.D. Travis, P. Yang, and N.T. Zakharova. First-principles modeling of electromagnetic scattering by discrete and discretely heterogeneous random media. *Physics Reports*, 632:1–75, 2016.

[7] K. Razi Naqvi and S. Waldenstrøm. Brownian Motion Description of Heat Conduction by Phonons. *Physical Review Lett*ers, 95(6):065901, 2005.