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Convergence of the Bouguer–Beer law for radiation extinction in particulate media

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ABSTRACT

Radiation transport in particulate media is a common physical phenomenon in natural and industrial processes. Developing predictive models of these processes requires a detailed model of the interaction between the radiation and the particles. Resolving the interaction between the radiation and the individual particles in a very large system is impractical, whereas continuum-based representations of the particle field lend themselves to efficient numerical techniques based on the solution of the radiative transfer equation. We investigate radiation transport through discrete and continuum-based representations of a particle field. Exact solutions for radiation extinction are developed using a Monte Carlo model in different particle distributions. The particle distributions are then projected onto a concentration field with varying grid sizes, and the Bouguer–Beer law is applied by marching across the grid. We show that the continuum-based solution approaches the Monte Carlo solution under grid refinement, but quickly diverges as the grid size approaches the particle diameter. This divergence is attributed to the homogenization error of an individual particle across a whole grid cell. We remark that the concentration energy spectrum of a point-particle field does not approach zero, and thus the concentration variance must also diverge under infinite grid refinement, meaning that no grid-converged solution of the radiation transport is possible.

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1. Introduction

Radiation heat transfer can become the dominant mode of energy transport in high-temperature systems. In such cases it is important to resolve the processes of absorption, emission, and scattering within a participating medium in order to make accurate predictions of the heat transfer. These predictions may be complicated by the fact that the participating media may be stochastically distributed [1–6] or evolving in time due to external forcing as in a turbulent flow [7,8].

Predictions of radiation transport are further complicated when the participating medium is not continuous, as in the case of a cloud of small particles. Continuum radiative transfer models based on Mie theory rely on an upscaling of the particle–radiation interaction under the assumption that the particles are non-interacting, have a large wavelength-to-clearance ratio, and are randomly distributed in space [9]. Many of these restrictions are violated in natural processes in which particles are clustered together, causing dependent scattering or non-exponential radiation attenuation. In recent years there have been a number of studies of particle-resolved radiation transport [2,10,11]. In particular, the study of radiation transport through stochastic particle distributions has shown that in the presence of spatial correlations, the rate of radiation attenuation may be reduced or enhanced depending on whether the particle positions are positively or negatively correlated [12].

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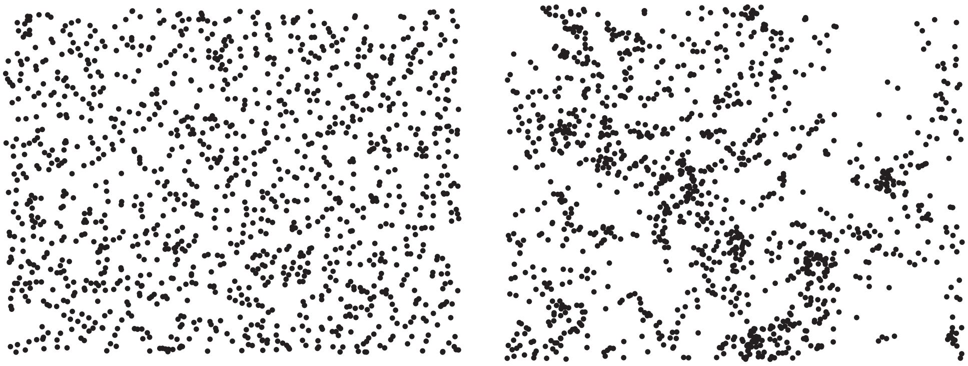

Fig. 1. A visual comparison of Poisson-distributed particles (left) and turbulence-clustered particles (right).

A ubiquitous example of non-uniform particle clustering is in turbulent particle-laden flows. In these cases, the particles are carried by the surrounding fluid, which undergoes frequent velocity fluctuations. Due to the particle inertia, the particle velocities can lag the local fluid velocity, leading to a segregation of particles out of regions of high fluid vorticity and into regions of high shear [13–15]. The resulting particle spatial distributions deviate significantly from Poisson distributions, as may be seen in Fig. 1. This phenomenon is commonly referred to as preferential concentration and has been shown to be an important process in droplet growth in clouds [16] and fuel–air mixing in spray combustion processes [17]. The controlling parameter for the relative magnitude of preferential concentration is the Stokes number St, which compares the aerodynamic response time of a particle $\tau_p = \rho_p d_p^2/18\mu$ to a characteristic flow time scale τ_f. When the flow time scale is chosen to be the Kolmogorov time scale based on the small eddy turnover time τ_η, the Stokes number that maximizes preferential concentration is $St \approx 1$ [18,19]. Recent work has also investigated the dynamics of heated particles in a turbulent flow, showing that clustering effects can affect the temperature statistics and the particle settling rates [20–22]. Thus radiation transmission through a turbulent cloud with particles with Stokes numbers close to 1 is likely to show larger fluctuations than through a cloud with a uniform particle distribution, especially if heat transfer effects are taken into account.

It is common to use an Eulerian methodology [23], Euler–Lagrange methodology [24] or a particle-resolved simulation [25] to treat the interaction of particles with a surrounding fluid to simulate the effects of particle clustering. In these cases, the particles are treated as discrete entities and the interaction between a given particle and the surrounding fluid can be treated either exactly or with the use of a model based on drag laws. The particle-resolved simulation approach is the most accurate as it has the closest representation of the true physics, though the Eulerian and Euler–Lagrange methods (both based on continuum treatments of the particle–fluid forcing) can yield close agreement. The interaction of radiation with discrete particles is a much more complex problem, the solution of which would require either particle-resolved ray-tracing or a detailed electromagnetic scattering computation [26,27]. The level of computational effort required to perform such calculations may be infeasible in general, especially in a multi-physics context in which radiation transport may be just one part of a larger simulation. Thus the use of continuum models for radiation are a more appealing alternative since they would permit the use of more efficient transport calculations such as the discrete ordinates method [28].

In order to perform predictive computations of radiation transport in particle-laden turbulent flows with a continuum model for the particle–radiation interaction, we must first validate the continuum model and prove that it is an effective representation of the underlying transport through a discrete particulate medium. In this work we compare the solutions of radiation transport in particulate media for continuum representations on a grid against the exact solutions in discrete representations. The error in the continuum representation is measured as a function of the ratio of particle diameter to grid size, and the convergence behavior is demonstrated for various grid and particle sizes. For the purposes of simplicity, we limit ourselves to the case of cold, purely absorbing media, for which the radiation transport in uniformly distributed particulate media is described by the Bouguer–Beer (BB) law.

2. Background

2.1. Bouguer–Beer law

The attenuation of radiation in a particulate medium can be derived in a probabilistic framework. When particles are randomly distributed in space, the probability of finding a given number of particles N in a volume V is given by the Poisson distribution:

$$P_N = \frac{\lambda^N \exp(-\lambda)}{N!} \tag{1}$$

where P_N is the probability, and $\lambda = nV$ is the expectation of the number of particles in the volume. If we were to trace a ray from a random initial location through a randomly-distributed particle-laden medium, the probability of the ray being transmitted through the volume is equal to the probability that no particles lay in the volume

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