COMPUTATIONAL EVALUATION OF AN APPROXIMATE THEORY FOR THE OPTICAL PROPERTIES OF SOOT

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Introduction. The absorption and scattering (optical) properties of soot are needed both to predict the continuum radiation properties of soot and to interpret nonintrusive optical measurements to find soot concentrations and structure. This is a challenging problem, however, because soot consists of small primary particles that combine into branched aggregates that exhibit neither simple Rayleigh nor Mie scattering behavior [1]. Nevertheless a potentially useful approximate theory for soot optical properties (denoted RDG-FA theory in the following) has been developed recently, based on the Rayleigh-Debye-Gans (RDG) scattering approximation while assuming that soot aggregates are mass-fractal objects [2-7]. In particular, recent measurements of both soot structure and scattering properties for soot aggregates found in flame environments have exhibited good agreement between RDG-FA predictions based on the structure measurements, and the scattering measurements [2,3]. Unfortunately, these soot populations involved relatively large soot aggregates so that it was not possible to adequately test RDG-FA theory in the small-angle (Guinier) regime where use of the RDG scattering approximation is least reliable. Thus, the objective of the present investigation was to undertake theoretical evaluation of RDG-FA theory, emphasizing the Guinier regime. The evaluation was based on computations using the ICP approach of Iskander et al. [8], which provides a more exact treatment of aggregate scattering in the Guinier regime than RDG-FA theory, by including effects of multiple and self-induced scattering. A full description of this study can be found in Farias et al. [9].

Theoretical Methods. Simplified RDG-FA predictions of soot optical properties were based on methods described in [2-7] but attention was focused on the approach of Köylü and Faeth [2] which extends the method of Dobbins and Megaridis [7] to provide an improved treatment of the large-angle (power law) regime.

The soot structure approximations of the RDG-FA and ICP calculations were the same. In addition, each primary particle constituted an ICP computational cell, which is satisfactory for primary particle optical size parameters $x_p \leq 0.4$ within the Guinier regime [9]. Present results were obtained as averages over various orientations of individual aggregates and populations of fractal aggregates of specified size (N primary particles), unless noted otherwise.

Aggregates were numerically simulated by cluster/cluster aggregation, following Jullien and Botet [10]. This involved starting with individual and pairs of primary particles, and attaching them to each other randomly. This procedure was used to form progressively larger aggregates but with the additional restriction that the aggregate fractal dimension, D_f, should be in the range 1.7-1.8 and the fractal prefactor, k_f, should be roughly 8 for $N > 8$ in order to match typical soot aggregate properties [1-3]. Some typical projected images of soot aggregates constructed in this manner are illustrated in Fig. 1 for N = 16, 64 and 256. The appearance of the aggregates varies considerably with direction of projection and from aggregate to aggregate within a population of given size; nevertheless, they are qualitatively similar to past observations and simulations of soot aggregates [1].

Results and Discussion. Discrepancies between RDG-FA and ICP predictions mainly increased with increasing x_p and scattering angle. Evaluation of ICP using Mie scattering predictions for compact spherical aggregates, and reasonably definitive experimental results for fractal aggregates in the power-law regime, however, indicated problems with ICP at large x_p and scattering angles due to truncation errors in the ICP algorithm. Thus, evaluations using ICP at large x_p were limited to the Guinier regime. Within this regime, discrepancies between RDG-FA and ICP were less than 10% for $x_p \leq 0.4$, indicating agreement within computational uncertainties.

Some typical normalized differential scattering patterns found from the RDG-FA and ICP theories are illustrated in Fig. 2, for the worst case condition, $x_p = 0.4$. The results are plotted as $k^2C^a_{vv}(\theta)$, where k = wave number and $C^a_{vv}(\theta)$ = aggregate optical cross section at an angle θ, in order to highlight effects of aggregate size on differential scattering patterns. The Guinier regime involves $\theta < 20°$, $40°$ and $90°$ for N = 256, 64 and 16, respectively; within this range of conditions the agreement between RDG-FA and ICP clearly is excellent. Combined with reasonable performance of RDG-FA predictions during recent experimental evaluations emphasizing the power law regime, these results suggest that RDG-FA theory is a reasonably effective way to treat the optical properties of soot for $x_p \leq 0.4$, which usually is the range of interest.

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Fig. 1 Projected images of simulated soot aggregates.

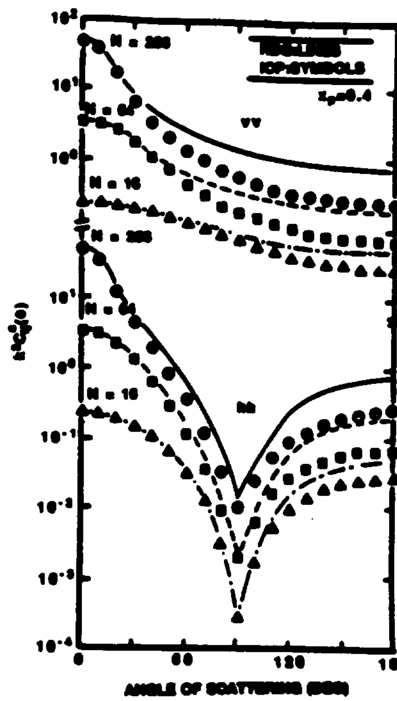

Fig. 2 RDG-FA and ICP predictions of normalized scattering patterns for soot aggregates of various size.