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Title: Infrared Backscattering

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Recent Work:

All particles in the atmosphere are not spherical. Moreover, the scattering properties of randomly oriented nonspherical particles are not equivalent to those of spherical particles no matter how the term "equivalent" is defined. This is especially true for scattering in the backward direction and at the infrared wavelengths at which some atmospheric particles have strong absorption bands. Thus calculations based on Mie theory of infrared backscattering by dry or insoluble atmospheric particles are suspect.

To support this assertion, I note that peaks in laboratory-measured infrared backscattering spectra show appreciable shifts compared with those calculated using Mie theory. One example is ammonium sulfate. We have had some success in modeling backscattering spectra of ammonium sulfate particles using a simple statistical theory called the CDE (continuous distribution of ellipsoids) theory. In this theory, the scattering properties of an ensemble are calculated. Each member of the ensemble, an arbitrary ellipsoid, does not necessarily correspond to each particle in a suspension of naturally occurring nonspherical particles. Nevertheless, the properties of the two ensembles are similar. Spectra calculated with the CDE theory are in better agreement with measurements than those calculated using Mie theory.

In the original version of the CDE theory, all ellipsoidal shapes had equal probability. Recently, Tim Nevitt applied a modified version of this theory to measured spectra of scattering by kaolin particles. The particles were platelike, so the probability distribution of ellipsoidal shapes was chosen to reflect this. As with ammonium sulfate, the wavelength of measured peak backscattering is shifted longward of that predicted by Mie theory. Even the original CDE theory, in which no information about the shape distribution is used, predicts more accurately the position of peak backscattering. When the shape distribution is accounted for, agreement between theory and experiment is even better.

The CDE theory is only a first tentative step. It is limited to particles small compared with the wavelength of the incident light. Although this condition is satisfied, at CO_2-laser wavelengths, for some particles in the atmosphere, it is not satisfied for all such particles. Thus a better theory is needed.

There are two aspects of the problem of calculating infrared backscattering by irregular particles: (1) Constructing a theory capable of accurately calculating backscattering by an arbitrary particle (or at least some range of nonspherical particles); (2) Deciding what is meant by "irregular" and how to treat irregularity statistically.

For about the past two years, my colleague Shermila Singham and I have been tackling the first of these two problems using a method originally developed by Purcell and Pennypacker. We call this method the coupled-dipole method, although it recently has acquired other names. In this method, a particle is approximated by a cubic array of point dipoles, the polarizabilties of which are determined by the refractive index of the particle of interest. Each dipole is excited not only by the incident field but by the fields of all the other dipoles. If the array contains N dipoles, 3N linear equations for the cartesian field components at each lattice site must be solved, from which the scattered field is readily obtained. If N is less than about 300, the 3Nx3N coefficient matrix of the 3N linear equations can be inverted using standard techiques. When N is greater than about 300, however, the matrix inversion approach fails because of insufficient computer storage. In an attempt to overcome this limitation, we reformulated the coupled-dipole method in such a way that the field at every dipole site is a series, each term of which can be interpreted as arising from multiple (coherent) scattering of different orders. This enables us to calculate scattering for N greater than 300, but eventually the scattering-order series diverges. At what point it diverges depends on the particle refractive index and shape; N = 5000 is a good approximate upper limit. Thus we have run into the same problems that plagued Purcell and Pennypacker and others who have adopted their method.

This summer, Shermila and I reformulated the coupled-dipole method in such a way that we obtain a series that must converge. Unfortunately, this method is impracticable given the speed of the present generation of computers. It works, but at the expense of a staggering amount of computer time.

Recently, several papers on the coupled-dipole method (which they call the digitized Green's function method) were published by George Goedecke and Sean O'Brien of New Mexico State University. Once the mathematical decorations are expunged from their work, what remains is no more than the coupled-dipole method. Moreover, they compute fields by matrix inversion, thus are limited to arrays of at most a few hundred dipoles.

Recently, other papers, either in press or to be submitted, have been sent to us by their authors. Bruce Draine, at Princeton, has applied the coupled-dipole method (which he calls the discrete dipole approximation) to the calculation of scattering and absorption by interstellar grains. Draine was able to treat particles of fairly high refractive index with size parameter up to about five. Yet to do so he had to restrict himself to particles with a high degree of symmetry. Draine is now collaborating with Graeme Stephens and Piotr Flatau at Colorado State University.

Although it is frustrating for us to have reached a size-parameter barrier, it is comforting to know that no one else has been able to surmount it. To date, no one who has worked on the coupled-dipole method has been able to overcome its limitations. To surmount the size-parameter barrier will require either radically new approximations based on physical reasoning or an increase in computer speed of at least a factor of ten, preferably much more. Computers are likely to become faster, but this will not occur overnight.

Fortunately, as a practical matter, the size-parameter limitations of the coupled-dipole method are of no serious consequence to calculating infrared backscattering by irregular atmospheric particles. At a wavelength of 10 μm, for example, the size parameter is less than 2 for particles with characteristic linear dimension less than about 2 μm. We can treat such particles using the coupled-dipole method.

Plans for Further Work:

I have been hampered in the past by the lack of a capable graduate student. The original proposal was written by Tim Nevitt, then a graduate student working on a doctoral degree in meteorology at Penn State. Our intention was that his doctoral research would be supported by the NASA grant. Unfortunately, by the time we received it--two years after submssion--Tim had left Penn State to take a position at 3M. This left me without a graduate student. After a year of floundering by myself, I went on sabbatical leave for a year. During the past year I have been working with Shermila Singham on the coupled-dipole method. Tim Nevitt has continued to work on the problem of infrared backscattering, but he cannot devote much time to it since he has a full-time, demanding job.

Recently, my situation has improved. Tracy Moore has left the Air Force to work with me. He has a degree in physics so we speak the same language. He did a second BS degree, in meteorolgy, at Penn State while an Air Force officer. He was the best student in all of my classes. When he left, he told me that he was going to return, and he has made good on his word. Despite the fact that he now has three children, he resigned his commission in the Air Force to take up voluntarily the exiguous life of a graduate student. Thus he is highly motivated and I expect great things of him. When I return to Penn State in

August, I am going to put him to work at using the coupled-dipole method for calculating infrared backscattering by irregular particles. Penn State now has a Supercomputer link, which we hope to make use of.

Publications:

Singham, S. B. and C. F. Bohren, 1988: Light scattering by an arbitrary particle: The scattering-order formulation of the coupled dipole method. J. Opt. Soc. Am. A (in press).

Bohren, C. F. and S. B. Singham, 1988: Backscattering by nonspherical particles: A review of methods; suggested new approaches. J. Geophys. Res. (submitted).

Nevitt, T. J., 1988: Backscattering by irregularly shaped particles: A comparision between theory and experiment. J. Geophys. Res. (submitted).

Singham, S. B. and C. F. Bohren, 1988: A hybrid method in light scattering by an arbitrary particle. Appl. Opt. (submitted).

NASA/MSFC GLOBAL SCALE ATMOSPHERIC PROCESSES RESEARCH PROGRAM

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APPROVAL

NASA/MSFC FY88 GLOBAL SCALE ATMOSPHERIC PROCESSES RESEARCH PROGRAM REVIEW

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The information in this report has been reviewed for technical content. Review of any information concerning Department of Defense or nuclear energy activities or programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

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