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ANNUAL LETTER REPORT

Ocean Optical Modeling: Light Field Structure, Internal Radiant Emission, and Vertical Inhomogeneities

ONR *Grant Number:* N00014-89-J-3137/P00002

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both supercomputer facilities utilize the Unicos 6.0 operating system. Thus the executable code developed at the NCSC can run directly on the POPS system without any recompiling.

NOARL Optics Workshop - Intercomparison of Optical Models

In March of 1991, NOARL (now NRL) sponsored a workshop on modeling in oceanographic optics. Many issues were raised about code efficiency, assumptions about the nature of suspended particles for absorption and volume scattering functions, skylight, wavy interfaces, etc.

Improvements in the NOARL optical model were presented which have seen extensive use in the subsequent modeling efforts. These improvements are detailed in the other research sections of this report. We agreed to do an intercomparison of all the models represented at the workshop. This will be done with each investigator simulating the output from a series of canonical models running the same internal variables and conditions.

Two-Flow model: Progress toward solving it and related equations

This model is a popular approximation to the full radiative transfer equation. The major uses for it are to derive algorithms for quantifying remote sensing observations and using them to predict chlorophyll concentration, primary productivity, etc. It is simple and most of its terms can be measured directly. However, the fundamental difficulty faced by all of the simplifications of the radiative transfer equation proposed so far is the presence of multiple scattering. I have incorporated multiple scattering variables into the NOARL model to allow assessment of this factor for any model or simulation.

For any depth increment of a simulation involving photon penetration, it is possible in the NOARL model to take the photon flux through that increment and determine if the photons are not scattered, single scattered, second order scattered, or third order and higher scattered. The primary contributions of these classes of photons respectively are to either downwelling or upwelling flux, to the backscattered fraction of the penetrating photons, or as photons penetrating in the same general direction as they started (downwelling or upwelling) but with an increased mean photon path due to the altered trajectories. This generates possibilities of interactions within the hydrosol that can't be predicted with single-scattering approximations where the mean photon path remains constant. In essence, this effort allows the incorporation of the volume scattering function in our modeling and approximations that was not attempted before. The usual assumption has been that variations in the volume scattering function for different classes of particles were not significant. The results that follow definitely demonstrate that this is not the case.

The unmodified Two-Flow model is an attempt to determine the amount of radiant energy absorbed and the amount of radiant energy scattered from either the downwelling or upwelling photon streams into the opposite or backward flowing stream of photons. This is done with a pair of differential equations describing the downwelling and upwelling photon flows and with simple terms for absorption and backscattering. One simplifying assumption is that the backscattering components of the photon streams are entirely uniform. However, the fully integrated radiative transfer equation requires a term for the backscattered flux that allows for the interaction of the volume scattering function and the radiance distribution, i.e. the backscattered fluxes are not uniform and isotropic. This interaction term measures the increase in backscattered flux beyond the amount predicted from knowledge of the simple backscattering coefficient. The shape factors (r_d and r_u) measure this augmenting of the backscattered flux and they must be equal to each other and to 1.0 in order for the simple coupled differential equations of the Two-Flow model to be solvable. We have tested these assumptions of the unmodified Two-Flow model with realistic optical parameters for the absorption and scattering of typical algal cells and for the volume scattering functions of bacteria, organic detritus, and quartz-like suspended mineral matter.

A major result of the NOARL Monte Carlo simulations is that the shape factors are neither equal to each other nor equal to 1.0. With this result the unmodified Two-Flow model is rendered unsolvable. The downwelling shape factor r_d varies from about 1.3 at zero depth to 1.5 after penetration of a few optical depths. This result holds for chlorophyll concentrations of 0.05 mg/m^3 to 20.0 mg/m^3 and Air Mass 1. For an Air Mass 2 the r_d coefficient increased to 1.5 even at the surface at chlorophyll concentrations of 0.05 mg/m^3 to 1.0 mg/m^3. Also the r_d coefficient increased to 1.9 at the surface and decreased to 1.75 at greater optical depths for chlorophyll concentrations of 5.0 mg/m^3 to 20.0 mg/m^3.

In addition, the r_u coefficients show a much greater variability, increasing with chlorophyll concentration in addition to increasing with an increase in Air Mass. The r_u values for chlorophyll concentrations of 0.05 mg/m^3 to 1.0 mg/m^3 are from 3.0 to 4.5 for Air Masses 1 and 2. For chlorophyll concentrations of 5.0 mg/m^3 to 20.0 mg/m^3 the r_u values range from 5.5 to 8.0 for Air Mass 1 and from 6.0 to 8.9 for Air Mass 2. The effect of increasing to Air Mass 2 is equivalent to increasing the chlorophyll concentration by factors of 1.5 to 2.0. A major contribution to this increase in the r_u coefficient compared to r_d is the presence of bacteria. When the bacterial contribution to the scattering is replaced by organic detritus, the r_u coefficient drops to about 2.2 at chlorophyll concentrations of 0.05 mg/m^3 to 1.0 mg/m^3 while it drops to about 4.0 at chlorophyll concentrations of 5.0 mg/m^3 to 20.0 mg/m^3.

Furthermore, the ratio of these two coefficients (r_u/r_d) is not constant but a non-linear function of chlorophyll concentration. The r_u/r_d ratio is nearly constant at 2.4 for chlorophyll concentrations between 0.05 and 0.5 mg/m^3. The bacterial concentration is nearly constant at these chlorophyll levels. With increase in chlorophyll concentration the ratio increases nonlinearly to about 5.5 at a chlorophyll concentration of 20.0 mg/m^3. The inability of various irradiance inversion algorithms for remote sensing etc. to make predictions for both low chlorophyll waters and high chlorophyll waters may be explained by these results. Although the two shape factors increase in value with an Air Mass of 2 compared to an Air Mass of 1, the r_u/r_d ratio remains primarily a function of chlorophyll concentration.

Thus the r_d and r_u coefficients vary differently because of the differing shapes of the radiance distributions involved and the different manners in which the volume scattering function contributes to the backscattered photon stream. A major contributor to this variation appears to be bacteria. However, the variation in the r_d coefficient is much less than that of the r_u coefficient. So far r_d appears to be a well-behaved function, approaching a limit that we can predict based on knowledge of the Air Mass. If our simulations give us a robust estimate of the r_d coefficient, then the equations of the Two-Flow model will contain 3 unknowns, the absorption coefficient, the backscattering coefficient, and the r_u coefficient. We can extend the Two-Flow model with an equation for calculating the absorption that I have developed earlier, the Three-Parameter model. Once this extension is made to produce a 3 differential equation system (The Net Flow/Two Flow model), we will have only two unknowns in the system.We are developing this system as method of determining the backscatter coefficient by inverting remotely sensed reflectance information and knowledge of the in-water irradiance field.

In addition to the above investigations, we are also looking into the possibility of improving remote sensing algorithms for quantifying satellite observations, and estimating the backscattering coefficient, with Zaneveld's (1982) model. The Zaneveld equation contains another shape factor, f_b, which is assumed to be 1.0. The NOARL model contains detailed volume scattering functions for most of the known suspended materials of the marine hydrosol. Zaneveld (1982) tested this assumption about f_b with a limited array of radiance distributions and volume scattering functions. Using Zaneveld's approximate equations, we have demonstrated that the estimated backscattering coefficient is consistently too high (Weidemann and Stavn, 1991). The results of the NOARL simulations indicate that the value of f_b is closer to 0.8. If this is the case, which we actively investigating now, then we can propose more efficient approximations to Zaneveld's equation. It does appear to be robust and will probably be quite useful when the radiance-irradiance information it requires is available. The Zaneveld equation requires more information than does the Net Flow-Two Flow model. We are investigating the possible trade-offs between the two approaches.

<u>Water Raman scattering</u>

The water Raman scattering function in the NOARL model has been improved and updated for optimum simulation of the effects of water Raman scattering in the oligotrophic ocean and possible interactions of this process with dissolved and suspended organic matter. Water Raman emission studies are conducted over a 10 nm waveband to simulate the results available with current optical technology. The bandwidth of water Raman emission from one line source can be 30 - 50 nm however. Thus, the NOARL optical model incorporates three different source bandwidths with appropriate corrections of the water Raman scattering cross section to allow for emission in a specific 10 nm bandwidth. This allows us to account for dissolved or suspended materials (chlorophyll, pheopigments, xanthophylls, gelbstoff, etc.) that may have one or several narrow absorption peaks. If a narrow absorption peak of other materials occurs in only one of the water Raman source bandwidths, then the effects on water Raman emission will be highly specific for the material in question. The highly specific effects of a material competing with the water molecule for photons would be impossible to predict otherwise. This will also allow the prediction of possible "windows" of water Raman emission in waters with perhaps a heavy load of materials that do not absorb in the regions of the potential water Raman source wavelengths.

In addition, the magnitude and shape of the water Raman scattering function is affected by the variable depolarization across the emission bandwidth and this factor has been incorporated into the NOARL optical model. The depolarization ratio differs for mid-band, lower-band, or upper-band Raman emissions. A high depolarization ratio means a larger water Raman scattering cross section: energy is contributed from both 90 degrees and 0 degrees relative to the propagation of the original beam, thus we have a relatively larger contribution to the total Raman emission. In addition to the quantitative variation in the Raman emission coefficient, the shape of the volume scattering function will vary from spherical to the classic "dumbbell shape" of the Rayleigh scattering function.

A general survey of water Raman emission phenomena from the UV region to the red region of light has been completed. At depths of 80 - 100 m in the oligotrophic open ocean, about 50% of the photons in the light field are transpectrally scattered from the water molecule (Stavn and Weidemann, 1992). These are photons of wavelength longer than about 510 nm. The photons of the red region are mostly of water Raman origin at any appreciable depth. The contribution of chlorophyll fluorescence at 683 nm is well known but the augmentation of the light field at other wavelengths has not been generally recognized. The major effect of water Raman scattering at wavelengths shorter than 510 nm is to contribute to the upwelling irradiance, the Raman contribution being from about 5% to 10%. Preliminary results on the skylight contribution indicate that skylight may suppress the production of water Raman emission. There are indications that longer wavelength skylight may promote water Raman emission. These effects will vary with Air Mass (greater water Raman emission at Air Mass 2) and they are now under active investigation.

Projected Activities

I am at present being considered for the position of Adjunct Associate Professor at UNC-Chapel Hill. John Bane of the Institute of Marine Sciences at Chapel Hill has presented me with this opportunity. The advantage here is the opportunity to sponsor a graduate student at the Ph.D. level. We are also planning possible joint research efforts and some participation in advanced oceanography courses at the Institute of Marine Sciences.

The potential of simulation on the Cray Y-MP is just beginning to open up. The scientific support staff of the NCSC projects the possibility of running the NOARL model at perhaps 100 - 150 MFLOPS per CPU second, roughly an increase in order of magnitude of efficiency over what the code is capable of now. The exciting possibility that is now being proposed is the vectorization of the Monte Carlo code. To my knowledge, this has not been done before for ocean optical models. The optimum vectorization may increase efficiency beyond even what they are projecting now. I am in the process of receiving initial training in this area at the NCSC. Still another exciting possibility is putting the Monte Carlo output (detailed radiance distributions for example) into a visualization paradigm. The NCSC has been designated a national center for work in visualization and the possible modes of analysis of the simulation output will be multiplied.

The area of photon emission due to fluorescence is really beginning to open up. The possible and demonstrated sources of fluorescence are gelbstoff, chlorophyll, xanthophylls, carotenes, etc. The sources can be both cellular and dissolved organic matter. I have received invitations from Charles and Clarice Yentsch and David Phinney of the Bigelow laboratories, West Boothbay Harbor, Maine, to share ideas and research experiences to best attack this growing area.

We are continuing to investigate remote sensing applications with the goal of determining the best method of estimating the backscattering coefficient: Zaneveld (1982) with more information needed or the Net Flow/Two Flow model using an estimate of the r_d value that approaches a maximum of 1.5 - 2.0 depending on the Air Mass.

A longer term interest is to investigate the role of multiple scattering itself; it is especially of importance in the heating of the surface layers by coccolithophore blooms in the Gulf of Maine. We have here confirmation of the the optical energy trapping, likely due to multiple scattering, at the water/air interface that I had predicted previously on theoretical and empirical grounds.

With the information described above well in hand in the next couple of years, we will then be ready to attack the more complex problem of the optical properties of coastal waters.

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