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Project Summary

Effects of Suspended Sediments on Penetration of Solar Radiation into Natural Waters

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Aquatic photochemical and photobiological processes that affect chemical fate depend on both the amount and the spectral composition of solar radiation penetrating to depths in natural waters. In turn, the depth of penetration, as a function of wavelength, depends on the dissolved and suspended material in these waters. As a consequence, the rates of photochemical transformation, as well as the impact on photobiological processes, depend on the optical properties of these water bodies as determined by their dissolved and suspended material. In particular, because photochemical processes are frequently governed by radiation in the ultraviolet region of the spectrum, the optical properties of natural waters in this spectral region are especially important.

In this study, several theoretical models were developed and some unique experimental data were collected for characterizing the optical properties of various natural waters. Particular emphasis was placed on optical properties in the ultraviolet region of the spectrum. Optical properties were modeled in terms of their dissolved materials and suspended sediments so that the solar radiant energy penetrating to depths in these waters can be calculated from available or easily collected experimental data. The theoretical models, with input of these data, can then be used to calculate the rates of photochemical and photobiological processes in various aquatic environments.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

A variety of chemical pollutants are known to be widespread contaminants of natural waters. Concern over the environmental impact and persistence of these pollutants has prompted studies of processes that transport and transform these chemicals in rivers and lakes. Many of these chemicals have been shown to undergo photochemical transformation, particularly as a function of the amount of ultraviolet (UV) and near-UV radiation.

Photochemical and photobiological processes that take place in water bodies depend on both the intensity and the spectral composition of solar radiation penetrating to depth. The depth of radiant energy penetration depends on the attenuation characteristics of the water, which, in turn, is a function of the dissolved and suspended material in the water. Consequently, the rates of photoprocesses in natural waters depend on the materials in these waters and how these materials influence the optical properties of the water.

The range of optical properties for different bodies of water is so large, as is the variability within a body of water with time, that it is currently impractical to make meaningful *in-situ* optical measurements for a representative sample of natural waters. A practical alternative to measuring the optical properties for a wide range of waters directly is to theoretically model the optical properties and to base the inputs of the model on more easily or routinely obtained experimental data.

Several models have been developed and tested for the purpose of calculating key optical properties based on a knowledge of the dissolved and suspended material in the water. In addition, we have obtained unique laboratory experimental data, with emphasis on the UV spectral region, for selected dissolved and suspended material We have used the more complete of our models to simulate realistic field data, which are then used for sensitivity analyses and the further development of simple practical models.

These results show how to characterize various natural waters theoretically, in terms of their constituents and consequent optical properties, so that the spectral radiant energy versus depth can be estimated. Thus, the models solve numerous practical environmental problems associated with the optical properties of natural waters. In particular, the results of this research provide a basis for both the theoretical and experimental study of photoprocesses in natural waters.

The figure shown herein summarizes the relationship between the experimental and theoretical work carried out in this project. Field data are represented by triangles. These data serve as both inputs to and checks of the classification schemes and predictive models. Predictive models are portrayed as boxes; parameters calculated by means of these models are represented by circles. In the figure, the lower dashed area refers to the Baker-Smith component model of the diffuse attenuation coefficient for irradiance The upper dashed box outlines our Monte Carlo modeling and the various inputs to and calculated outputs from this model The left hand side of the figure shows important constituents of the water (chlorophyll, dissolved organic material, suspended particulate material), which are relatively easily measureable in the field and serve as inputs to the models The right hand side of the figure shows the calculated outputs from the models (spectral radiance, irradiance and the diffuse attenuation coefficient), which are the optical properties necessary to model in water photoprocesses.

Experimental results (input data)

Inherent optical properties of a medium are independent of the geometrical configuration of light-field within the water. Included within the set of inherent optical properties are the absorption coefficient, a, and the volume scattering function, $\beta(\theta)$. The absorption coefficient is a measure of the radiant energy lost in passing through the medium, and the volume scattering function is a measure of the scattering characteristics of the medium. It can be shown theoretically that the set (a, $\beta(\theta)$) of inherent optical properties of a medium are a sufficient and complete set for the description of the optical properties of a medium under any circumstance. Figure 1 indicates how these optical properties serve as inputs to the models for selected constituents of natural waters.

The optical properties of water as a function of wavelength are dependent on both the inherent properties of water itself and the dissolved and suspended material in the water. The optical properties of pure water serve as a natural limit and a baseline for natural waters. We have collected and summarized the most recent and most reliable data for the optical properties of pure water, in the spectral region from 200-800 nm, and these serve as basic input data (the triangle "water") to the models.

Important constituents that are frequently found in natural waters and significantly influence their optical properties include chlorophyll (due to phytoplankton), dissolved organic material, and suspended particulates. The respective triangles and subsequent boxes shown in the figure represent the experimentally determined and/or indi-

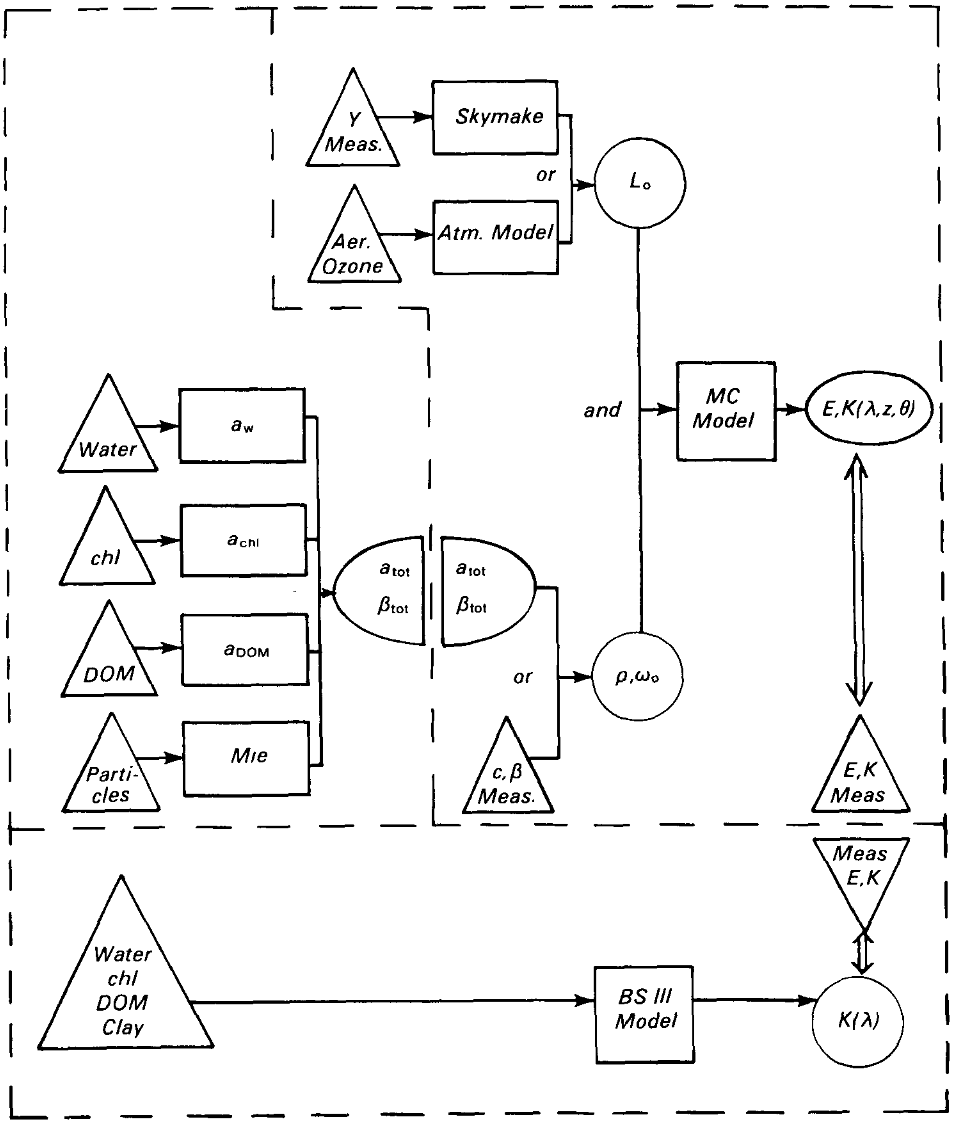

Figure 1. Relationships between experimental field data and computer models.

vidual component model input of these parameters to the larger Monte Carlo model (box labeled "MC model").

As an example, consider the path (in the figure) from the triangle "particles" to the box "Mie" to the circle "a, β." Suspended particulate material is relatively easily and routinely measured for various natural waters. Thus, information on the amount and size distributions of particulate material for various waters is relatively common. Mie scattering theory represents an analytic solution of the scattering of light by small spherical particles From particle size distributions as input, the Mie theory can be used to calculate the absorbing and scattering properties of the water containing these particles. This information in turn can be used as the required input to the Monte Carlo model

Complete modeling of radiation penetrating to depth in natural waters requires as input the solar spectral irradiance, which is incident upon the water surface having passed through the atmosphere. Atmospheric data inputs include the ratio of sky to total irradiance (triangle "Y meas "), as input to the model "skymake," or alternatively, data on the atmospheric aerosol and ozone concentration, as input to an atmospheric model that emphasizes the UV region of the spectrum

Our project used existing data sources and in addition obtained unique optical data, which emphasized the UV region of the spectrum, for selected representative water types. Known amounts of dissolved organic material (DOM) and terrigenous material (clay) were added to a tank of filtered water, and the optical properties were continually monitored These data were then used to describe and model the influence of each substance individually on the attenuation of radiant energy in water These data are represented by the triangle so labeled and are input to the Baker-Smith III component model.

Theoretical results (models)

Modeling will continue to play an important role in the understanding and prediction of spectral radiation behavior under water, because field data are difficult and relatively expensive to obtain Also, once a working model exists, it can be used to extend and extrapolate the necessarily limited field data Use of the models also permits one to investigate problems where it is particularly difficult to obtain field data (e.g., low sun angles or great depths), to study unsampled water types by simulation, to simulate large variations in b/c or $\beta(\theta)$, and to do general sensitivity studies. Such modeling helps verify our understanding of submicroscopic processes and provides an important theoretical link between the constituents of an optical medium and their resultant optical properties.

Our investigation of computational methods is outlined in the figure where predictive models are represented by boxes. For solution to the radiative transfer equation, most of our work has focused on Dave's code for an iterative solution and a Monte Carlo code adapted from Kirk for a more generally useful solution. Both of these codes were extensively modified to suit our purposes: the Dave code because it did not directly apply to aquatic media and the Kirk code because it was comparatively inefficient. We also used a code that provided the solutions to the Mie equations to deduce the inherent optical properties for water from the particle size distribution of suspended particles. The results of the Mie solutions can then be used in either the Dave or Monte Carlo models.

As anticipated in Figure 1, the required data inputs to the Monte Carlo model are optical properties of water for which we had extensive data bases or for which we developed appropriate component models. These component models take as input the relatively routine data in the form of concentrations of the component of interest (e.g., chlorophyll, DOM, particulates) and output the diffuse attenuation for irradiance (for example the lower dashed area in Figure 1). Both the Monte Carlo model that we developed and our component models have been compared against experimental data and have been shown to agree extremely well.

Overall results (spectral irradiance and photolysis rates)

In developing models for the aquatic environment, we first considered the input radiance distribution, LO. Both an analytical approach (the atmospheric model of Dave) and an experimental approach ("skymake") were useful depending on the specific problem and input data available. The inherent optical properties of waters, based on representative dissolved and suspended components, also were modeled. These individual component models provide the absorption and volume scattering function (or alternatively the single scattering albedo and phase function for scattering) as input to the Monte Carlo model.

The Monte Carlo model can then be used to calculate the underwater spectral irradiance, $E(\lambda, z)$, and the spectral diffuse attenuation coefficient, $K(\lambda, z, \theta)$. Alternatively, if the concentrations of key components are known, the multicomponent model shown at the bottom of the Figure can be used to calculate E and K.

Once the underwater spectral irradiance can be calculated, it is possible to calculate the rates of underwater photoprocesses in general and chemical photolysis rates in particular. Equally important, the rates of these photoprocesses can be calculated as a function of all the input variables, for example, as a function of atmospheric properties, sun angle, and various water properties. Thus these photoprocesses can be characterized in terms of various environmental parameters.

Conclusions and Recommendations

The experimental and theoretical study of environmental processes in important practical situations can be complex and expensive. This research demonstrated the cost effectiveness of an integrated theoretical and experimental program where limited, but specifically chosen, data were used to test and refine models. These models, in turn, were used to simulate realistic field data for sensitivity analyses and the further development of simple practical models.

Our investigations have obtained valuable new data and created theoretical models that provide solutions to diverse environmental problems dealing with natural waters. This work also suggests new directions for further productive research. Specific recommendations include: (1) more complete experimental work in controlled environments (e.g., tank experiments) with emphasis on determining the optical effects when these are mixed, (2) work to increase the speed and efficiency of the Monte Carlo model and the use of this model for continued sensitivity analysis directed toward specific practical problems, (3) the development and application of other solutions of the radiative transfer equation that can be expected to provide increased insight into the fundamental processes underlying various significant environmental problems, and (4) the use of Mie scattering theory to compute the inherent optical properties of various natural sediments and the subsequent use of these in our biooptical component model to compute the apparent optical properties for waters of interest.

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The complete report, entitled "Effects of Suspended Sediments on Penetration of Solar Radiation into Natural Waters," (Order No. PB 83-238 188; Cost: $10.00, subject to change) will be available only from:

National Technical Information Service
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