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# Radiative transfer equation inversion: Theory and shape factor models for retrieval of oceanic inherent optical properties

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[1] It is shown that the in-water, shape factor formulation of the radiative transfer equation (RTE) (1) yields exact in-air expressions for the remote sensing reflectance $R_{\mathrm{rs}}$ and the equivalent remotely sensed reflectance $RSR_a$ and (2) can be configured for inherent optical property (IOP) retrievals using standard linear matrix inversion methods. Inversion of the shape factor RTE is exact in the sense that no approximations are made to the RTE. Thus errors in retrieved IOPs are produced only by uncertainties in (1) the models for the shape factors and related quantities and (2) the IOP models required for inversion. Hydrolight radiative transfer calculations are used to derive analytical models for the necessary backscattering shape factor, radiance shape factor, fractional forward scattering coefficient, ratio of air-to-water mean cosines, and diffuse attenuation coefficient for in-water upwelling radiance. These models predict the various shape factors with accuracies ranging typically from 2 to 20%. Using the modeled shape factors the in-air remotely sensed reflectance $RSR_a$ can be predicted to within 20% of the correct (Hydrolight-computed) values 96% of the time (or ±0.0005 sr$^{-1}$ 86% of the time) for the synthetic data used to determine the shape factor models. Inversion of this shape factor RTE using field data is a comprehensive study to be published in a later paper. *INDEX TERMS:* 4552 Oceanography: Physical: Ocean optics; 4847 Oceanography: Biological and Chemical: Optics; 4275 Oceanography: General: Remote sensing and electromagnetic processes (0689); 4842 Oceanography: Biological and Chemical: Modeling; *KEYWORDS:* remote sensing, optical oceanography, inverse modeling, radiative transfer theory

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## 1. Introduction

[2] Semianalytic radiance models [*Gordon et al.*, 1988; *Morel and Gentili*, 1996] can be readily inverted by linear matrix methods [*Hoge et al.*, 1999a, 1999b, 2001] to provide oceanic inherent optical properties (IOPs). Such inversions are well conditioned [*Hoge and Lyon*, 1996] and promise a powerful method of simultaneously retrieving constituent absorption and backscattering coefficients in the upper surface layer of the world's oceans using satellite data [*Hoge et al.*, 2001; *Hoge and Lyon*, 2002]. However, semianalytic radiance models (1) do not provide an exact framework to account for all possible environmental and viewing conditions [*Weidemann et al.*, 1995] and (2) contain fixed constants that both obscure insight into the physical radiative transfer processes and limit their flexibility.


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[3] The radiative transfer equation (RTE) can provide exact inverse solutions, but the RTE is not easily inverted for many remote sensing situations [*Zaneveld*, 1995]. Therefore a specific form of the RTE inversion is investigated, namely a modified version of the shape factor formulation of *Zaneveld* [1995]. Some of the motivation for the work herein comes from the distinct need for highly accurate methods to retrieve the absorption coefficients of the chlorophyll accessory pigment phycoerythrin [*Hoge et al.*, 1999b]. To this end the absorption coefficients of chlorophyll and chromophoric dissolved organic matter (CDOM) must be accurately retrieved; otherwise, weaker absorbing constituents (such as phycoerythrin) will be obscured.

[4] In this paper (1) the shape factor form of the RTE is shown to be readily configured into linear form for simultaneous retrieval of oceanic IOPs using standard matrix methods; (2) the RTE inversion is derived for the principal

"big three" IOPs, namely the phytoplankton absorption coefficient, the CDOM + detritus absorption coefficient, and the total constituent backscattering coefficient; (3) shape factor and related models required for the inversion are developed for backscattering and radiance shape factors, the diffuse attenuation coefficient for upwelling radiance, the ratio of average cosines of the air and water downwelling irradiances, and the fractional forward scattering coefficient; and (4) propagation of errors into the IOP state vector resulting from errors in the data-model matrix and hydrospheric vector as well as shape factor and related models are assessed.

[5] Our ultimate objective is to determine if the shape factor RTE matrix inversion methodology will result in accurate algorithms for application to satellite ocean color data. This paper presents the underlying shape factor RTE theory and develops the needed models for the shape factors and related quantities, while future work will describe comprehensive studies of the shape factor RTE inversion of synthetic and real data.

## 6. Discussion

[33] To facilitate a brief comparison of the shape factor models, propagation of errors into the retrieved IOPs, and discussion of future inversion research, all the models are reassembled below.

$$\hat{f}_b = \alpha_1 + \alpha_4 \frac{b}{b_b}\left[1 + \frac{\alpha_2}{\alpha_4}\cos(\alpha_3\,\xi)\right]. \quad (30)$$

$$\hat{B}_f = b_f\left(1 - \hat{f}_L\right) \quad where \quad \hat{f}_L = \alpha_5 + \alpha_6\left(\frac{\lambda}{550}\right)\sin(\alpha_7\theta_s). \quad (31)$$

$$\hat{k} = \alpha_8\, a + \alpha_9\, b_b + \alpha_{10}\sin(\theta_s). \quad (32)$$

$$\hat{R}_\mu = \alpha_{11}\frac{\cos\theta_s}{\cos\left[\sin^{-1}\left(\frac{\sin\theta_s}{n}\right)\right]} = \alpha_{11}\Theta(\theta_s). \quad (33)$$

Although they were derived from a physical basis, it was seen that the models could take various forms. At this early stage of development the above models probably represent the starting point of their eventual evolution.

[34] The highly important $\hat{f}_b$ model contains (1) two IOPs: $b_b$ and $b_f$ (but in a ratio combination $b/b_b = [(b_b + b_f)/b_b] = [1 + b_f/b_b]$), (2) the most model coefficients (four), and (3) the Sun sensor included angle $\xi$ (but not the solar zenith angle $\theta_s$ as do all the other models). In contrast, the $B_f$ model contains (1) the solar zenith angle and one IOP ($b_f$) and (2) the sole wavelength dependence found within the models. The $\hat{k}$ model contains only one IOP, $b_b$, and the solar zenith angle, $\theta_s$. The $\hat{R}_\mu$ model contains no IOPs; only the solar zenith angle $\theta_s$. (Inversion of the shape factor RTE also requires models for those IOPs that are to be retrieved. For example, the phytoplankton absorption coefficient $a_{ph}$, the CDOM/detritus absorption coefficient $a_d$ and total constituent backscattering $b_{bt}$ as given in equation (17). These IOP models [*Hoge and Lyon*, 1996] are considered more mature than the shape factor models. Uncertainty propagated into retrieved IOPs by the IOP models used within a semianalytic radiance model inversion has been studied [*Hoge and Lyon*, 1996].)

[35] Thus, to initiate an iterative inversion, starting values are required for both $b_b$ and $b_f$. Physics demands that $b_b \geq b_{bw}$, where $b_{bw}$ is the backscattering coefficient for water. One possible method for selecting the starting value for $b_b$ is to retrieve it by first executing a semianalytic model inversion [*Hoge and Lyon*, 1996; *Hoge et al.*, 1999a, 1999b, 2001]. Then it can continually be updated after each shape factor RTE inversion in equation (17) since $b_b = b_{bw} + b_{bt}$. Similarly, physics dictates and limits the range of $b_f$ for the first iteration of the shape factor RTE inversion: $b_f \geq b_{fw}$ where $b_{fw}$ is the forward scattering coefficient for water. Although $b_f = b_{fw}$ can perhaps be used as the starting value for the first iteration, future research efforts must develop methods for better (1) selection of starting values and (2) updating of the value during subsequent iterations. Like $b_b$, the $b_f$ can, in principle, be retrieved using equation (17). This too, however, presents some concerns: (1) few if any models exist for $b_f$ to allow its retrieval by equations (17) and (2) a concurrent retrieval of $b_f$ potentially weakens the retrieval of the desired $a_{ph}$, $a_d$, and $b_{bt}$. Detailed error propagation analyses of the shape factor RTE inversion are outside the scope of this present paper, but a brief discussion of the relative influence of the shape factor models on the desired IOP state vector, $\boldsymbol{p} = [a_{ph}(\lambda_g), a_d(\lambda_d)\, b_{bt}(\lambda_b)]^T$, is provided in the following section.

### 6.1. Uncertainties in the IOP State Vector *p*

#### 6.1.1. Sensitivity of *p* to Perturbations in the Data-Model Matrix *D*

[36] As already noted, the inversion of the shape factor form of the RTE is exact from the standpoint of radiative transfer theory, and uncertainties in the retrieved IOPs within the IOP state vector $\boldsymbol{p}$ are due only to the accuracy of the (1) shape factor models and their related quantities and (2) IOP models. Perturbations within $\boldsymbol{D}$ arise, for example, from the water-leaving radiances, scalar irradiances, IOP models, and backscattering shape factor contained within it. Similarly, uncertainties in $\mathbf{h}$ arise from the radiances, irradiances, hydrospheric constants (or IOP constants $a_w$ and $b_{bw}$) for sea water, as well as $f_b$, $dL_u(\lambda_i)/dz$, $b_f(\lambda_i)$, $f_L(\lambda_i)$, and $\cos\theta$. Relative to $\boldsymbol{h}$, the data-model matrix, $\boldsymbol{D}$, plays the major role in the propagation of errors into $\boldsymbol{p}$ since $\|\boldsymbol{p} - \boldsymbol{p}'\|/\|\boldsymbol{p}\| \leq \kappa(\boldsymbol{D})\,(\|\Delta_{\boldsymbol{D}}\|/\|\boldsymbol{D}\| + \|\delta_{\boldsymbol{h}}\|/\|\boldsymbol{h}\|)$, where $\|\boldsymbol{D}\|$ is the determinate of $\boldsymbol{D}$ and $\kappa(\boldsymbol{D}) = \|\boldsymbol{D}\|\,\|\boldsymbol{D}^{-1}\|$ [*Ortega*, 1990; *Hoge and Lyon*, 1996]. The latter expression is the condition number of $\boldsymbol{D}$, and $\Delta_{\boldsymbol{D}}$ and $\delta_{\boldsymbol{h}}$ represent uncertainty or perturbation of $\boldsymbol{D}$ and $\boldsymbol{h}$, respectively. Here $\boldsymbol{p}'$ is the perturbed solution of $\boldsymbol{p}$. The first expression simply states that to first order the relative error in $\boldsymbol{p}$ can be $\kappa(\boldsymbol{D})$ times the relative error in $\boldsymbol{D}$ and $\boldsymbol{h}$. Thus the propagation into $\boldsymbol{p}$ of the relative errors of both $\boldsymbol{D}$ and $\boldsymbol{h}$ is governed by the condition number of $\boldsymbol{D}$. For any norm, $1 \leq \kappa(\boldsymbol{D}) \leq \infty$. For the limiting cases: $\kappa(\boldsymbol{D}) = 1$, $\boldsymbol{D}$ is said to be perfectly conditioned, while for $\kappa(\boldsymbol{D}) = \infty$, $\boldsymbol{D}$ is singular. For intermediate values of $\kappa(\boldsymbol{D})$ the interpretation of the condition number is very subjective and must be evaluated separately. For large $\kappa(\boldsymbol{D})$ the $\boldsymbol{D}$ matrix is said to be ill conditioned and large errors may be found in $\boldsymbol{p}$. For small $\kappa(\boldsymbol{D})$ the $\boldsymbol{D}$ matrix is said to be well-conditioned and smaller errors may be found in $\boldsymbol{p}$. Of the shape factor components only $f_b$ occurs in $\boldsymbol{D}$ (via $V$) and therefore provides the strongest influence on the IOP retrieval errors.