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ON THE NUMERICAL CHARACTERISTICS OF AN INVERSE SOLUTION FOR THREE-TERM RADIATIVE TRANSFER

W. L. DUNN† and J. R. MAIORINO‡

Department of Nuclear Engineering, North Carolina State University, Raleigh, NC 27650, U.S.A.

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Abstract—Certain numerical characteristics of an inverse formulation for three-term scattering radiative transfer are investigated. Specifically, approximate solutions to the direct problem are constructed by the F_N and Monte Carlo methods, allowing approximation of the various surface angular moments and related quantities needed for the inverse calculation. Several numerical schemes are employed in order to demonstrate the computational characteristics for some specific phase functions. The numerical results indicate that the single-scatter albedo can be calculated fairly consistently and accurately, but the higher order coefficients of the scattering law are more difficult to obtain by this method.

1. INTRODUCTION

We are concerned here with the practical application of the inverse formulation given by Siewert[1] for radiative transfer in plane geometry with a three term phase function. We consider first the equation of radiative transfer of the form

$$\left(\mu\frac{\partial}{\partial t}+1\right)I(\tau,\mu)=\omega\int_{-1}^{1}f(\mu|\mu')I(\tau,\mu')\,\mathrm{d}\mu',\ \ \tau\in[L,R] \tag{1}$$

subject to

$$I(L,\mu)=F_1(\mu),\ \mu>0, \tag{2}$$

$$I(R,\mu)=F_2(\mu),\ \mu<0, \tag{3}$$

where $I(\tau,\mu)$ is the radiation intensity, τ is the optical variable, μ is the direction cosine of the propogating radiation with respect to the positive τ direction, ω is the sinlge-scatter albedo, $f(\mu|\mu')$ is a probability density function (pdf) describing the scattering law inside the slab atmosphere contained in $L\leq\tau\leq R$, and F_1 and F_2 are known incident distributions. Next, we consider the specific pdf

$$f(\mu|\mu')=\tfrac{1}{2}[1+b_1\mu\mu'+b_2P_2(\mu)P_2(\mu')], \tag{4}$$

where b_1 and b_2 are constants and $P_2(x)$ is the Legendre Polynomial of Order 2. Similarly, we restrict our analysis to the specific incident distributions given by

$$F_1(\mu)=A_l\mu^{\beta},\ A_l=0\text{ or }1, \tag{5}$$

and

$$F_2(\mu)=A_r\mu^{\beta},\ A_r=0\text{ or }1, \tag{6}$$

where β is a nonnegative integer. Following Siewert,[1] we define the following quantities:

$$\alpha=\omega b_1/3, \tag{7}$$

$$\beta=2\omega b_2/5, \tag{8}$$

$$\gamma=(5-9\alpha)/[10(1-\alpha)], \tag{9}$$

†Present address: Operations Analysis Division, Research Triangle Institute, P.O. Box 12194, Research Triangle Park, NC 27709, U.S.A.

‡Permanent address: Institute de Pesquisas Energeticas e Nucleares, Cidade Universitaria, Sao Paulo, Brazil.

$$S_\nu = \int_0^1 I(R, \mu)\mu^\nu F_2(\mu)\,d\mu - \int_0^1 I(L, -\mu)\mu^\nu F_1(\mu)\,d\mu,\ \nu = 0, 2, 4, \tag{10}$$

$$I_\nu(x) = \int_{-1}^1 I(x, \mu) P_\nu(\mu)\,d\mu,\ \nu = 0, 1, 2, \tag{11}$$

$$K(x) = \int_{-1}^1 I(x, \mu)\mu^2\,d\mu, \tag{12}$$

$$L(x) = \int_{-1}^1 I(x, \mu)\mu^3\,d\mu, \tag{13}$$

$$M(x) = \int_{-1}^1 I(x, \mu)\mu^4\,d\mu, \tag{14}$$

$$N(x) = \int_{-1}^1 I(x, \mu)\mu^5\,d\mu, \tag{15}$$

$$M_2(x) = \tfrac{3}{2}L(x) - \tfrac{1}{2}I_1(x), \tag{16}$$

and

$$U(x) = -\frac{2}{15}\frac{\omega}{1-\omega}\frac{1}{1-\alpha}\, I_1(x)\frac{3}{2}N(x) + \gamma L(x), \tag{17}$$

where $P_\nu(\mu)$ is the Legendre Polynomial of order ν and $x = L$ or R. Siewert[1] has derived the following set of formulas using these quantities which can, in principle, be used to effect the inverse calculations for the quantities ω, b_1 and b_2:

$$4S_0 = g_1(\omega, \alpha, \beta) = \omega[I_0^2(R) - I_0^2(L)] - 3\alpha[I_1^2(R) - I_1^2(L)] + \frac{5}{2}\beta[I_2^2(R) - I_2^2(L)], \tag{18}$$

$$4S_2 = g_2(\omega, \alpha, \beta) = \frac{\omega}{1-\omega}[I_1^2(R) - I_1^2(L)] - 3\frac{\alpha}{1-\alpha}[K^2(R) - K^2(L)] + \frac{5\beta}{2-\beta}[M_2^2(R) - M_2^2(L)], \tag{19}$$

and

$$4S_4 = g_3(\omega, \alpha, \beta) = \frac{1}{3}\frac{1}{1-\alpha}\left(\frac{\omega}{1-\omega}\right)^2[I_1^2(R) - I_1^2(L)] - \left(\frac{1}{1-\alpha}\right)^2\left(\frac{\omega}{1-\omega} + \frac{9}{5}\alpha^2\right)$$
$$[K^2(R) - K^2(L)] + \frac{1}{1-\alpha}\left\{\frac{2\omega}{1-\omega}[I_1(R)L(R) - I_1(L)L(L)] - 6\alpha\right.$$
$$\left.[K(R)M(R) - K(L)M(L)] + 3\alpha[L^2(R) - L^2(L)]\right\} - \frac{5\beta}{2-\beta}$$
$$\left\{2[M_2(R)U(R) - M_2(L)U(L)] + \frac{2}{3}\left(\gamma - \frac{9}{7}\right)\frac{\beta}{2-\beta}[M_2^2(R) - M_2^2(L)]\right.$$
$$\left. + \left[\frac{3}{2}M(R) - \gamma K(R)\right]^2 - \left[\frac{3}{2}M(L) - \gamma K(L)\right]^2\right\}. \tag{20}$$

For a specific inverse formulation to be much practical value, it should converge to a solution reasonably close to the true solution given approximate input. We demonstrate the numerical characteristics of this particular formulation in the following sections.

2. ANALYSIS AND RESULTS

In order to evaluate inverse solutions numerically, a means of generating approximations to the intensity and/or various moments of the intensity is first needed. If it is difficult to measure these experimentally, one can use exact or approximate solutions to the direct problem. For our purposes, the F_N method developed by Siewert[2,3] was selected, in which surface intensities can be approximated by using

$$I(L,-\mu)=\sum_{\alpha=0}^{N} a_\alpha{}^\alpha\mu,\ \mu>0 \tag{21}$$

and

$$I(R,\mu)=\sum_{\alpha=0}^{N} b_\alpha{}^\alpha\mu,\ \mu>0, \tag{22}$$

where N defines the order of the F_N approximation. Here, the a_α and b_α are obtained by the methods described by Siewert, Maiorino, and Ozisik.[3] Once the surface intensities are known, the other surface quantities needed for the inverse computation can be determined from Eqs. (10)–(17).

For simplicity, we consider only the case of unitary isotropic incidence at the left boundary and a free surface condition on the right boundary, corresponding to $A_l = 1$, $A_r = 0$, and $\beta = 0$. Various order F_N results were generated for the case $\omega = 0.9$, $b_1 = b_2 = 1$. The results, shown in Table 1, indicate convergence to about four significant figures by F_9 or F_{10}. As a means of verifying these F_N solutions, a Monte Carlo algorithm was designed. Monte Carlo and F_N calculations were compared for two values of the single scatter albedo, $\omega = 0.8$, and $\omega = 0.99$. The results in Table 2 demonstrate sufficient agreement between the two methods to suggest that these approximate F_{10} solutions are correct to several significant figures.

There are two questions to be addressed concerning the numerical characteristics of this inverse formulation. Firstly, is the solution to Eqs. (18)–(20) with approximate moments (say four significant figures) unique and sufficiently close to the true solution of the equations with correct moments? Secondly, is the system sufficiently well-behaved that a simple numerical search will converge quickly and unambiguously to the solution? In an effort to answer the first question, a simple test (designated as *TI*) was devised which consisted in solving each of Eqs.

Table 1. Surface quantities calculated by the F_N method for a unit slab with $\omega = 0.9$, $b_1 = b_2 = 1$.

	F_6	F_7	F_8	F_9	F_{10}
$I_0(R)$	0.46500	0.46527	0.46535	0.46537	0.46535
$I_0(L)$	1.34693	1.34670	1.34661	1.34657	1.34656
$I_1(R)$	0.27533	0.27534	0.27534	0.27534	0.27534
$I_1(L)$	0.36184	0.36186	0.36186	0.36186	0.36186
$I_2(R)$	0.06294	0.06281	0.06276	0.06276	0.06277
$I_2(L)$	-0.05056	-0.05044	-0.05040	-0.05037	-0.05037
K (R)	0.19696	0.19696	0.19696	0.19696	0.19696
K (L)	0.41527	0.41527	0.41527	0.41527	0.41527
L (R)	0.15342	0.15341	0.15341	0.15341	0.15341
L (L)	0.19268	0.19268	0.19268	0.19268	0.19268
M (R)	0.12563	0.12562	0.12562	0.12562	0.12562
M (L)	0.24381	0.24381	0.24381	0.24381	0.24381
$M_2(R)$	0.09247	0.09245	0.09245	0.09245	0.09245
M2(L)	0.10810	0.10809	0.10809	0.10809	0.10809
N (R)	0.10635	0.10633	0.10634	0.10634	0.10633
N (L)	0.13131	0.13131	0.13131	0.13131	0.13131
S_0	-0.34693	-0.34670	-0.34661	-0.34657	-0.34656
S_2	-0.08194	-0.08194	-0.08194	-0.08194	-0.08194
S_4	-0.04381	-0.04381	-0.04381	-0.04381	-0.04381

Table 2. Comparison of F_N and Monte Carlo surface quantities for $b_1 = b_2 = 1$.

	$\omega = 0.8$		$\omega = 0.99$	
	F_{10}	M.C. (80,000)*	F_{10}	M.C. (100,000)*
$I_0(R)$	0.3951	0.3960	0.5475	0.5479
$I_0(L)$	1.2733	1.2704	1.4311	1.4303
$I_1(R)$	0.2403	0.2407	0.3157	0.3157
$I_1(L)$	0.3928	0.3935	0.3255	0.3257
$I_2(R)$	0.0636	0.0634	0.0609	0.0604
$I_2(L)$	-0.0418	-0.0408	-0.0595	-0.0592
K (R)	0.1741	0.1743	0.2231	0.2229
K (L)	0.3966	0.3963	0.4374	0.4373
L (R)	0.1366	0.1367	0.1726	0.1723
L (L)	0.2049	0.2060	0.1770	0.1771
M (R)	0.1123	0.1124	0.1407	0.1404
M (L)	0.2337	0.2336	0.2558	0.2558
$M_2(R)$	0.0847	0.0847	0.1010	0.1006
M2(L)	0.1124	0.1123	0.1028	0.1028
N (R)	0.0954	0.0955	0.1187	0.1185
N (L)	0.1395	0.1396	0.1216	0.1216
S_0	-0.2733	-0.2704	-0.4311	-0.4303
S_2	-0.0632	-0.0630	-0.1041	-0.1040
S_4	-0.0337	-0.0336	-0.0559	-0.0558

* The quantity in parentheses indicates the number of Monte Carlo histories.

(18)–(20) for each of the parameters in terms of the other two. Equations (18) and (19) are linear in the parameters and the solutions are straightforward; Eq. (20) yields quadratic equations for each of the variables. By substituting approximate moments and the exact values of two of the parameters into these equations, it can be seen how close the third parameter is to its true value. While this is not a direct answer to the first question, it offers substantial insight towards its answer.

Several cases defining different phase functions were considered using test *TI* and other tests to be described subsequently. The cases considered are indicated in Table 3. In applying test *TI*, the solution of each equation for ω was quite good, the solutions for α not so good, and the solutions for β poor, as the selected results in Table 4 indicate. The F_{10} moments were rounded to four significant figures to generate these results. In order to investigate the sensitivity of the solution to the degree of accuracy of the moments, solutions using test *TI*

Table 3. The specific phase function for several cases.

Case	ω	b_1	b_2	α	β	Comments
1	0.800	1.000	1.000	0.267	0.320	
2	0.900	1.000	1.000	0.300	0.360	
3	0.990	1.000	1.000	0.330	0.396	
4	0.992	0.600	0.000	0.198	0.000	linearly anisotropic
5	0.800	0.000	0.500	0.000	0.160	Rayleigh scattering
6	0.800	2.01	1.56	0.536	0.500	8-term scattering*

* $b_3 = 0.674$, $b_4 = 0.222$, $b_5 = 0.0472$, $b_6 = 0.00671$, $b_7 = 0.00068$, $b_8 = 0.00005$.

Table 4. Results of test $T1$ for several cases with F_{10} moments rounded to four significant figures.

Solution from equation	ω	α	β	Case
*	0.800	0.267	0.320	1
18	0.801	0.263	0.123	
19	0.800	0.267	0.553	
20	0.806	0.239	0.325	
*	0.990	0.330	0.396	3
18	0.990	0.322	0.029	
19	0.990	0.327	1.57	
20	0.990	0.326	1.19	
*	0.992	0.198	0.000	4
18	0.992	0.165	-1.97	
19	0.992	0.192	1.71	
20	0.992	0.192	1.43	
*	0.800	0.536	0.500	6
18	0.792	0.566	-0.793	
19	0.800	0.536	0.806	
20	0.801	0.506	0.537	

* These are the exact values for the indicated cases.

were obtained with three-, four-, and six-significant figure input for Case 2. The results are shown in Table 5 and tend to indicate that the solutions to Eq. (20) for α and β are not very close to the true solutions, even for six-significant figure input. Finally, solutions to Case 5 were considered, where both the true value of β and $\beta = 0$ were used in the equations for ω and α, as shown in Table 6, in order to test the sensitivity of the solutions to the value of β used.

The results obtained using test *TI* tend to indicate the following:

(a) The solution of the approximate set of equations for ω is quite near the true solution and fairly insensitive to the value of β (see Table 4).

Table 5. Results of test $T1$ for case 2 as a function of input accuracy*.

Solution from equation	Number of significant figures	ω	α	β
†	--	0.900	0.300	0.360
18	3	0.896	0.339	2.21
18	4	0.900	0.304	0.561
18	6	0.900	0.299	0.334
19	3	0.899	0.304	0.0890
19	4	0.900	0.301	0.551
19	6	0.900	0.300	0.611
20	3	0.901	0.291	-0.0835
20	4	0.901	0.286	0.322
20	6	0.901	0.285	0.364

* F_{10} moments were rounded to the number of significant figures indicated for input.

† These are the actual values for case 2.

Table 6. Dependence of test $T1$ for case 5 on the value of β used.

Solution from equation	ω	α	β	Comments
--	0.800	0.000	0.160	Actual case 5 values
18	0.800	-0.003	-0.008	β = 0.160
18	0.800	0.000	-0.008	β = 0
19	0.800	0.000	0.297	β = 0.160
19	0.801	-0.005	0.297	β = 0
20	0.807	-0.036	0.163	β = 0.160
20	0.801	-0.006	0.163	β = 0

(b) The solution for α obtained from Eq. (19) is generally better than the solutions for α from Eqs. (18) or (20).

(c) The values of β obtained by solving the different equations are rarely reproducible and seldom near the true value; hence, a unique solution of the approximate equations for the triplet (ω, α, β) may not exist and even if it does, it may not be sufficiently near the solution of the exact equation.

These results offer only modest encouragement to attempt a three-term inverse solution numerically. However, in order to demonstrate the types of results that might be obtained we employed several algorithms to effect the inverse calculation. The algorithms $T2$, $T3$, and $T4$ consist of the following: Algorithm $T2$ involves solving Eqs. (18) and (19) for ω and α in terms of β, then solving Eq. (20) for β, given ω and α. An iterative procedure results, requiring only an initial estimate for β. Algorithm $T3$ is a variant of $T2$ which uses the fact that solutions for ω and α are rather insensitive to β. Here, test $T2$ is taken through only one iteration, with the starting point $\beta = 0$. Algorithm $T4$ consists in utilizing a straightforward pattern search to locate the minimum of an objective function obtained as the square of the sum of the squares of certain residuals, i.e.

$$\Omega(\omega, b_1, b_2) = [(\omega - h_1)^2 + (b_1 - h_2)^2 + (b_2 - h_3)^2]^2, \tag{23}$$

where h_1, h_2 and h_3 are solutions of Eqs. (18)–(20) for ω, b_1 and b_2 respectively. The minimum of this objective function is the solution to Eqs. (18)–(20). Fymat and Lenoble[4] discuss a similar approach to another inverse problem.

Results of these three inverse algorithms are presented in Table 7 for Cases 1 and 2. These techniques consistently yield accurate values for ω. We note that algorithm $T2$ yields solutions that are within about 0.1% for ω, 1% for α, and 10% for β, for Cases 1, 2, and 3. Comparison of entries 6 with 7 and 14 with 15 tend to verify that the F_{10} calculations are not good to more than about four- or five-significant figures, since not much improvement in accuracy of the inverse calculation is achieved in going from five-significant figure to unrounded double precision input. We note also that algorithm $T4$ with five-significant figure input computes all parameters, including β to within three digits in the third decimal place, which is generally less than 1% error. Even for only two-significant figure input, algorithm $T4$ yields reasonable results (see entry 12). Also, the $T3$ results show that the calculation for β is extremely sensitive to the values of ω and α, since after one iteration the computed values of β are very poor while the computed values of ω and α are moderately good. Finally, we note that two derivative-based search algorithms were also attempted, but gave no better results.

3. CONCLUSION

This study has shown that the third equation in Siewert's[1] inverse formulation is extremely sensitive to the accuracy of the input moments. This input affects the behaviour of this system of equations for three-term inverse analysis. A one-step inverse algorithm ($T3$) yields values of ω and α that are reasonable but values of β that are small by approximately an order of

Table 7. Inverse calculations using different algorithms and F_{10} input rounded to the number of significant figures shown.

Entry	Algorithm	Number of significant figures	ω	α	β	Case
1	Exact	--	0.800	0.267	0.320	1
2	T2	*	0.801	0.270	0.336	
3	T3	4	0.794	0.238	0.043	
4	T4	5	0.799	0.266	0.320	
5	Exact	--	0.900	0.300	0.360	2
6	T2	*	0.900	0.303	0.380	
7	T2	5	0.900	0.300	0.351	
8	T3	4	0.896	0.269	0.035	
9	T4	5	0.900	0.301	0.362	
10	T4	4	0.900	0.301	0.362	
11	T4	3	0.899	0.299	0.352	
12	T4	2	0.907	0.299	0.366	
13	Exact	--	0.990	0.330	0.396	3
14	T2	*	0.990	0.333	0.422	
15	T2	5	0.990	0.326	0.354	
16	T3	4	0.990	0.330	0.008	
17	T4	5	0.990	0.330	0.393	
18	Exact	--	0.800	0.000	0.160	5
19	T3	4	0.797	0.018	0.024	
20	T4	5	0.800	0.001	0.160	

*Double-precision F_{10} intensities were used.

magnitude (see Table 7). However it is noted that both iterative algorithms attempted, one of them ($T4$) with only two-significant figure input, converged to solutions that were excellent for ω and α and fair for β, for the cases considered.

The inverse computation has the properties that the solutions for ω and α are relatively insensitive to the value of β assumed (see, for instance, Table 6) and that convergence is rather slow, typically requiring between 100 and 200 iterations. Thus, this inverse formulation consistently computes ω and α satisfactorily, even if β is not computed accurately. This results in, for instance, the ability to identify Rayleigh scattering (with $\alpha = 0$) but not linearly anisotropic (with $\beta = 0$), since the inverse computation will yield a near-zero value for α in the Rayleigh scattering case but probably not a near-zero value for β in the linearly anisotropic case (see Tables 4 and 7). Similarly, we note that ω and α are reasonably correct even for phase functions with more than three terms (see Table 4), although again β is not. The ultimate conclusion then, is that this inverse formulation is a useful one provided too great reliance need not be placed on the value of β computed and a slow convergence is not unacceptable.

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