

6.4 NUMERICAL SOLUTION OF SCHWARZCHILD'S EQUATION USING THE "MODTRAN INFRARED LIGHT IN THE ATMOSPHERE" WEBSITE AND A SPREADSHEET

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1. INTRODUCTION

I begin with a personal note: I am retired from an academic career in condensed matter physics, during which time a standard freshman/sophomore physics of the environment course was often included in my teaching assignment. After retirement, I decided to teach myself basic one-dimensional atmospheric physics by studying textbooks on the subject, but I had no available personal contact with anyone expert in the field who could help me in this enterprise. The major impediment to my progress was that no numerical solution to Schwarzschild's equation (SE) was demonstrated in any of the ten textbooks I purchased and studied (Andrews 2010; Archer 2006; Bohren & Clothiaux 2006; Goody & Yung 1989; Houghton 2007; Liou 1980; Petty 2006; Pierrehumbert 2014; Taylor 2014; Wallace & Hobbs 2006).

Such a numerical solution to the SE is demonstrated here and can be carried out using a spreadsheet. The result is obtained using transmittance values from the free online website "Modtran Infrared Light in the Atmosphere" (MILIA n.d.). The two cases studied are:

1. The observer looks down from 70 km to observe outgoing long-wave radiation (OLR) that is transmitted through a path from ground to 70 km through a U.S. standard atmosphere containing only 400 ppm CO₂ as a greenhouse gas (GHG).
2. The observer looks down from 70 km to observe OLR that is transmitted through a path from ground to 70 km through a U.S. standard atmosphere containing only 800 ppm CO₂ as a GHG.

In both cases, the emissivity of the Earth's surface is assumed to be 0.971.

A symbolic solution of the SE for the vertical, outgoing long-wave *intensity* (OLI) for one wavelength, as given by Petty (2006, Eqs. 8.27–8.28), is shown as Equation 1 below. For simplicity in notation, Petty suppresses subscripts that indicate the dependence on frequency.

$$I \uparrow (\infty) = I \uparrow (0) \epsilon t^* + \int_0^\infty B(z) \left[\frac{dt(z,\infty)}{dz} \right] dz \quad (1)$$

The first term to the right of the equal sign corresponds to the radiance leaving the surface multiplied by the emissivity ϵ times the transmittance t^* between the Earth's surface and an infinity point. The infinity point is often, but not necessarily, a point near the top of the atmosphere. The second term, involving an

integral, corresponds to the upward OLI emitted by the atmosphere itself. In this second term, $B(z)$ corresponds to the black body radiance term in units of $W/m^2 \text{ Sr}$ at altitude z whilst the term in square brackets is the derivative of the transmittance between altitude z and the infinity point. Note that the intensity at the Earth's surface, $I(0) \uparrow (z)$, has units of watts per meter squared per steradian, since from Lambert's law, the available emission solid angle totals π steradians available in the upper hemisphere.

The first term to the right of the equality in Equation 1 is easy to calculate. Difficulties can arise in computing the integral term, which corresponds to the atmospheric contribution to the OLI. Other terminology may be used; for instance, in the "underlying program output" for MILIA, the term used for OLI is "integrated radiance."

Points A, B, and C are now discussed, relative to the physics behind Equation 1 above.

1.1 POINT A

Consider a situation for which the infinity point limit Z is 1000 meters and steps of $dz = 1$ meter are used. Since the downward-looking virtual observer has a detector at $Z = 1000$ m, the limiting transmittance as z approaches 1000 m must correspond to zero material between the virtual detector and the point $Z = 1000$ m. *Thus, the limiting value of the transmittance at $z = Z$ must be unity.* This condition must be obeyed for a correct numerical solution.

1.2 POINT B

There is a second interesting feature of Equation 1 that one notices when comparing an atmosphere with 400 ppm CO₂ relative to an atmosphere with 800 ppm CO₂ and assuming the same vertical path and atmospheric location region. Consider the behavior of the first term to the right of the equality in contrast to the integral term. First note that the value of $B(z=0)$ is the same for both compositions. However, t^* is smaller for the 800 ppm than for the 400 ppm composition. It follows that

$$I \uparrow (0) t_{400}^* - I \uparrow (0) t_{800}^* \quad (2)$$

is a *positive* number.

Next, consider the integral term to the right of the equal sign in Equation 1. The net *change* in transmittance $t^*(z, Z)$ is between $z = 0$ and the value *unity* at $z=Z$. Then the absolute value of the change in transmittance $\Delta t_{800}^*(0,z)$ between $z = 0$ and $z= Z$ is $1 - t_{800}^*(0,Z)$. By a similar argument, the corresponding absolute value of the change in transmittance $\Delta t_{400}^*(0,z)$

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between $z = 0$ and $z = Z$ is $1 - t_{400}^*(0,Z)$. Then one has Equation 3:

$$\Delta t_{400}^*(0,Z) - \Delta t_{800}^*(0,Z) = t_{800}^*(0,Z) - t_{400}^*(0,Z), \quad (3)$$

which is a *negative* number, and finally

$$\int_0^Z B(z) \left\{ \frac{[dt(z,Z)_{400}]}{dz} \right\} dz - \int_0^Z B(z) \left\{ \frac{[dt(z,Z)_{800}]}{dz} \right\} dz, \quad (4)$$

which is also a *negative* number.

1.3 POINT C

The solution to SE illustrated in Equation 1 is, strictly speaking, only applicable to monochromatic radiation (Liou 1980). Techniques for overcoming this problem by performing an angular integral of diffuse transmittance over the available π Sr have been developed (Liou 1980). The online program Spectral Calc (n.d.) uses such methods to yield a correct answer for the vertical OLI, in units of watts/meter² Sr, even if a wide range in ω is used. I quote the following personal communication from Tom Marshall (Marshall, Gordley, & Chu 1994):

“Schwarzschild’s equation is applicable only for monochromatic radiation. It does not apply to broad band. The Spectralcalc results are correct, at least to within the accumulated numerical errors (<.1%) and errors in the spectroscopy.”

Here, SpectralCalc is used to obtain values of OLI that are compared to the results obtained using MILIA.

The transmittance values used here extend over a wide band width, and therefore the solution to Equation 1 is, strictly speaking, not valid. However, the errors produced by ignoring the non-monochromatic nature of the radiation can be shown to be on the order of ~ 4 % relative error in the OLI if the method of using MILIA as described here is used. The method described has several advantages: (a) The source of the transmittance values is a free online program accessible by the student. (b) The wavenumber range used is between 2 ω n and 2200 ω n, which is wide enough so that one can use the Stefan–Boltzmann law to estimate $B(z)$ in equation. 1 (c) The approach to the condition for which the transmittance value must approach unity as z approaches 70 km is sufficiently gradual that one may use 1 km step sizes in Equation 1.

I will outline the method of demonstrating a solution to SE by using MILIA in Section II, and the ~4 % error will be tolerated. Section III will discuss the methods of correcting for the effects of the non-monochromatic nature of the radiation by using the “diffusivity factor approximation.” Section IV describes a modification of the diffusivity factor (DF) approximation, and section V is a summary of the manuscript results.

2. NUMERICAL SOLUTION TO THE SE USING OUTPUT FROM “MODTRAN, INFRARED LIGHT IN THE ATMOSPHERE” WITH NO DIFFUSIVITY FACTOR CORRECTIONS.

First, the MILIA (n.d.) program is accessed. Then, the user should set the concentration buttons all equal to zero except for CO₂, which is set for the default concentration of 400 ppm. The “U.S. Standard Atmosphere” location is chosen. The default setting of the virtual observer is 70 km looking *down*. The value of OLR calculated for these settings is 345.4 w/m². To find the output for transmittance, one must click the “Show Raw Model Output” button and scroll down to the last page. Note that the “average transmittance” value is 0.8841 and that an Earth’s surface emissivity of 0.971 is assumed. One also finds that, with the “looking down” setting, the user can only access path settings 70 km to ground, 69 km to ground, and so on, eventually reaching 1 km to ground. These are not the paths needed to calculate the integral term in Equation 1. One must select “looking up,” so that the virtual observer is now looking up from the ground to 70 km. Press “raw model output” and scroll down again. (I note that the “average transmittance” has changed from 0.8841 looking down to 0.8842 looking up. This relative difference between transmittance looking up and down is 0.01%, but theoretically there should be *no* difference in transmittance looking up and looking down. I suspect that this 0.01% difference may be due to round-off error of some sort within the computer program.) Use the “looking up” setting, which means looking up from z to 70 km. Change the values of z and assume that the vertical transmittance value between two points A and B is the same whether the observer looks up from point A to point B or down from point B to point A. Transmittance values can be obtained looking down from 70 km to altitude z for altitudes $z = 1$ km, 2 km, and so on up to $z = 69$ km and finally 70 km. These are the transmittance values needed as input to integrate the integral term for OLI in Equation 1. The temperature values for the U.S. standard atmosphere can be generated using the free online website “digital Dutch” (n.d.). The radiance is given, to a good approximation, by the equation

$$\text{Radiance} = \sigma T^4 / \pi \quad (5)$$

In Equation 5, σ is the Stefan–Boltzmann constant. One can check the accuracy of Equation 5 by using the SpectralCalc Black Body Calculator. That app is now available for use without a subscription. Choosing the frequency range between 2 ω n and 2200 ω n, emissivity 0.971, and temperature 288.15K, the Black Body Calculator yields a radiance of 123.865 W/m² Sr, which is within 0.45% of the result obtained by Equation 5. The spreadsheet used to compute the atmospheric contribution to the OLI can be found in the last comment at <https://www.skepticalscience.com/Science-Climate-Change-online-class-Coursera.html>. As of Jan 6, 2018 this last comment consists of seven columns of numbers. These columns comprise the altitude in km, the transmittance for 400 ppm where CO₂ is the only GHG between the altitude and 70 km, the derivative of the transmittance relative to altitude, temperature in K, radiance computed using the Stefan–Boltzmann law, the product of derivative and radiance, and the trapezoidal rule applied to this product.

The user can copy and paste the table mentioned above into an Excel spreadsheet. The result of this calculation is the atmospheric contribution to the OLI, which is obtained by summing the entries in the “trapezrule” column. The “Product” column is the product of the “derivative” column and the radiance (“Rad”) column. The trapezoidal rule is applied to the “Product” column and the sum of all the trapezoid entries gives the atmospheric contribution to the OLI. This is the last term to the right of the equality in Equation 1, with the ∞ point being 70 km. The value of the atmospheric contribution to the OLI is 7.4 W/m²Sr.

The $I \uparrow (0) \epsilon t^*_{400}$ term is equal to 124.425 W/m² Sr multiplied by 0.971 multiplied by 0.8842, or 106.8 W/m²Sr. The contribution of the atmosphere to OLI is calculated in the spreadsheet to be equal to 7.4 W/m²Sr. The total OLI then becomes 114.2 W/m²Sr. From SpectralCalc, the correct OLI would be equal to 109.4 W/m² Sr, indicating that there is then a relative error in my computed value of 4.3%—on the high side of the correct result. The “trapezoidal rule” is used to find the atmospheric contribution by numerical integration. One expects that the calculated OLI would be on the high side because of the non-monochromatic nature of the infrared. In the next section, the DF correction for this effect is discussed. Before finishing this section, I show below in Fig. 1 a comparative plot of the derivative of the 400 ppm and 800 ppm transmittance versus altitude curves.

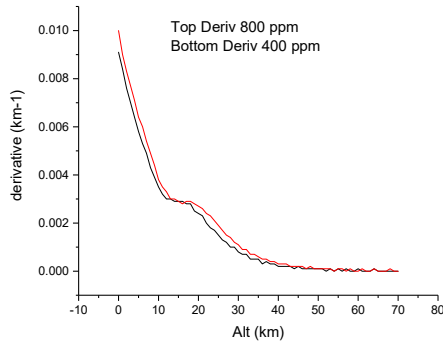


Fig. 1. Comparative plots of the derivatives of the 400 ppm CO₂ versus 800 ppm CO₂ curves versus altitude.

It may be seen in Fig. 1 that both slopes do approach zero as z approaches 70 km, and the transmittance therefore approaches one in this limit. But the initial slope is greater for the 800 ppm curve. Therefore, the relationship expressed in Equation 4 above is satisfied. There is a characteristic “hill” feature in both curves around the altitude at which one passes into the tropopause.

3. THE DIFFUSIVITY FACTOR APPROXIMATION

Let τ represent the optical thickness of a vertical path between two levels in the atmosphere and $\mu_{effective}$

represent the cosine of an effective zenith angle ϑ for a model path that is not vertical. For a judicious choice of ϑ , one can not only replace the monochromatic solution to SE with the solution over a wide band of frequencies; in addition, the terms to the right of OLI can also, to a good approximation, be multiplied by π so as to yield the upward diffusive flux (OLR) in units of watts per square meter (Petty 2006, pp. 213–214; Pierrehumbert, 2014, pp. 190–191). The value of optimum ϑ is usually taken to be about 53 degrees, so the reciprocal of $\cos \vartheta$ is then $1.66 = 5/3$ (Petty 2006, pp. 213–214). However, Pierrehumbert points out that there could be more than one “judicious choice” of ϑ , and he recommends a default angle of 60 degrees “unless there is a compelling reason to adopt another value” (Pierrehumbert 2014, pp. 190–191).

A recent study by Zhao and Shi (2013) is useful in the present context. These authors apply new DF theory directly to the upward and downward radiative intensities in units of w/meter² sr. They point out that the DF has an upper and lower limit where the upper limit is two for small optical depth and the lower limit of the DF is unity for large optical depth. In between these extremes, the DF might have any possible intermediate value. Their Equation 16 allows one to compute the DF as a function of optical depth.

4. MODIFICATION OF THE DF APPROXIMATION FOR THE CASE WHERE CO₂ IS THE ONLY GHG

The user of MILIA cannot change the angle of the IR radiation path, but I wish to discuss the DF both in terms of MILIA, and the DF as discussed in texts. The DF as discussed in textbooks is formulated in terms of varying the path angle from vertical. I developed a simple but accurate approximation, which—instead of changing the path from vertical—produces the same effect on the DF by altering the concentration of CO₂. The approximation is valid only in cases in which CO₂ is the only GHG. The approximation can be applied when using packages such as Modtran6, MILIA, and Spectral Calc—packages that allow one to control atmospheric compositions. The justification for this approximation is outlined in the following paragraph.

If Q_A is defined as the specific concentration of CO₂, ρ_A is defined as the partial pressure of CO₂, and ρ_{tot} is the partial pressure of the total gas, then $Q_A = \rho_A / \rho_{tot}$ (Pierrehumbert 2014, Eq. 4.62). Many expressions in atmospheric textbooks that contain Q_A also contain $\cos \vartheta$, and these quantities appear together in combination as $Q_A / \cos \vartheta$. For example, the mean transmission function between pressures p_1 and p_2 for a single Lorentzian line is derived by Pierrehumbert (2014 Eq. 4.63) and is given below as Equation 6. The definitions of all symbols other than Q_A and $\cos \vartheta$ are not relevant to the argument.

$$\tau(p_1, p_2) = \left(\frac{1}{\Delta}\right) \int_{-\Delta/2}^{\Delta/2} \left[\exp^{-1\left(\frac{1}{g m \cos \vartheta}\right) \int_{p_1}^{p_2} Q_A S(T) \gamma / (v'^2 + \gamma^2) dp} \right] dv' \quad (6)$$

Since the concentration of CO₂ in the atmosphere is constant almost all the way up to 100 km, and CO₂ is a

dilute gas, then Q_A is a constant in Equation 6, as is $(1/\cos \theta)$. The term $Q_A / \cos \theta$ may then be brought out of the integral in the exponent and becomes a multiplying factor. Say that one is using a package such as SpectralCalc and is working with a 400 ppm atmosphere of CO_2 . Consider the DF corresponding to a concentration of 400 ppm and an effective zenith angle of 60 degrees. To an extremely good approximation, to apply the DF correction, all that needs to be done is to (a) change the concentration entered into SpectralCalc from 400 ppm to 800 ppm so that Q_A is changed to Q_B where $Q_B / Q_A = 2$, but (b) leave the path vertical. For MILIA, one is not given the option of changing the output from a vertical path, so the approximation described is necessary.

This assertion may be checked by using SpectralCalc. Consider SpectralCalc results for Case A versus B above. I use 400 ppm CO_2 as the only GHG with the observer looking down towards the Earth. I obtain from SpectralCalc the transmittance between the surface and 10 km and a band from 500 wn to 850 wn . For a vertical path, the transmittance is 0.50225. (a) Now keep the same concentration and band limits but use a nadir angle of 60 degrees. The SpectralCalc transmittance changes to 0.44992. (b) Finally, I set the path to vertical again but set the concentration to 800 ppm. The new SpectralCalc transmittance is 0.45014, so that the percentage relative difference (RD) between transmittance values for Case A versus Case B is given by $\%RD = \{ [(0.45014 - 0.44992)] / 0.45014 \}$ times 100 = 0.042%. From the simple approximation derived above, one may apply the DF corresponding to a zenith angle of 60 degrees by simply multiplying the concentration of CO_2 by two and keeping the path vertical. Then the OLI obtained using an uncorrected concentration of 800 ppm in a vertical path would be the maximum possible correction to the 400 ppm CO_2 vertical path, according to Zhao and Shi.

The uncorrected OLI value is then 113.40 $\text{W/m}^2\text{Sr}$, and the error relative to the SpectralCalc result of 109.4 $\text{W/m}^2\text{Sr}$ is reduced to ~3.6 % by thus obtaining the uncorrected OLI for the 800 ppm concentration. But the corrected value of the OLI is still too large by this same value of 3.6%.

The 60-degree effective zenith angle case would result in the maximum possible DF correction according to the paper by Zhao and Shi (2013), and therefore, on face value, the results here are in contradiction to accepted diffusivity factor theory. An interesting aspect of this discrepancy is that the OLI actually calculated by MILIA using integration over angles is in excellent agreement with SpectralCalc, whereas the results obtained by using the transmittance values obtained by MILIA to numerically compute Equation 1 are off by a few percent.

One possible source of error in my treatment here is that Earth's emissivity of 0.971 is built into the MILIA program. There must be some scattered or reflected IR leaving the Earth if the emissivity is less than one, implying a breakdown of the two-stream approximation. Equation 1 in the introduction is only valid for the two-stream approximation but not valid if, as in the present case, the emissivity is less than one. Another source of

error is that the transmittance values computed by the older Modtran version used in MILIA are not optimum. By using the modern Modtran6 package with the highest resolution settings, the transmittance values one obtains are ~2.7% in excess of the transmittance values obtained from MILIA as described above.

5. SUMMARY

The free online website "Modtran Infrared Light in the Atmosphere" (MILIA n.d.) was recently updated by Pease and Archer. MILIA is used extensively to aid in instructing non-science majors in basic physics of the environment courses. The present manuscript describes how the output of MILIA can be of use for instructing somewhat more advanced students in obtaining a numerical solution of SE. The OLI is obtained—using only a spreadsheet—for the case where 400 ppm CO_2 is the only GHG, and the result agrees with what is expected from SpectralCalc to within a relative error of ~4%, with the error on the high side.

I attempted to use the DF approximation to correct this error by using the maximum possible correction allowed according to Zhao and Shi. This procedure lowered the error to ~3.6% but did not bring the error to zero. The reason for this apparent violation of DF theory will be the subject of a future investigation.

6. REFERENCES

- Andrews, D. A., 2010: *An introduction to atmospheric physics* (2nd ed.). New York, NY: Cambridge University Press.
- Archer, D., 2006: *Global warming, understanding the forecast* (1st ed.). Chicago, IL: Wiley.
- Bohren, C., & Clothiaux, E. E., 2006: *Fundamentals of atmospheric radiation*. Chicago, IL: Wiley.
- Digital Dutch, n.d.: Double Dutch. <https://www.digitaldutch.com/atmoscalc/>
- Goody, R. M., & Yung, Y. L., 1989: *Atmospheric radiation theoretical basis* (2nd ed.). New York, NY: Oxford University Press.
- Houghton, J., 2007: *The physics of atmospheres* (3rd ed.). New York, NY: Cambridge University Press.
- Liou, K. N., 1980: *An introduction to atmospheric radiation*. Elsevier, *International Geophysics Series*, 34, xx–xx.
- Marshall, B. T., Gordley, L. L., & Chu, D. A., 1994: BANDPAK: Algorithms for modeling broadband transmission and radiance. *J. Quant. Spectrosc. R.A.*, 52(5), 581–599.
- Modtran Infrared Light in the Atmosphere, n.d.: Modtran Infrared Light in the Atmosphere. <http://climatemodels.uchicago.edu/modtran/>
- Petty, G., 2006: *A first course in atmospheric radiation*. Madison, WI: Sundog Publishing.
- Pierrehumbert, R. T., 2014: *Principles of planetary climate* (3rd printing). New York, NY: Cambridge University Press.
- SpectralCalc, n.d.: SpectralCalc. <http://www.spectralcalc.com>

- Taylor, F. W., 2014: *Elementary climate physics*. New York, NY: Oxford University Press.
- Wallace, J. M., & Hobbs, P. V., 2006: *Atmospheric science, an introductory survey*. Amsterdam, NL: Elsevier.
- Zhao, J. Q., & Shi, G. Y., 2013: An accurate approximation to the diffusivity factor. *Infrared Phys. Techn.*, 56, 21–24.