Comment on "Improved ray tracing air mass numbers model"

Siebren Y. van der Werf
Kernfysisch Versneller Instituut, University of Groningen, Zernikelaan 25, 9747 AA, Groningen, The Netherlands
vdwerf@kvi.nl

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Air mass numbers have traditionally been obtained by techniques that use height as the integration variable. This introduces an inherent singularity at the horizon, and *ad hoc* solutions have been invented to cope with it. A survey of the possible options including integration by height, zenith angle, and horizontal distance or path length is presented. Ray tracing by path length is shown to avoid singularities both at the horizon and in the zenith. A fourth-order Runge–Kutta numerical integration scheme is presented, which treats refraction and air mass as path integrals. The latter may optionally be split out into separate contributions of the atmosphere's constituents. © 2008 Optical Society of America

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1. Introduction

Air mass numbers have traditionally been obtained via air mass integrals [1–3]. A recent publication by Kivalov [4] is, to our knowledge, the first-ever study to calculate air masses by ray tracing. His method introduces ray curvature explicitly by modeling path elements as circle segments. In doing so, the notorious singularity at the horizon ($z = 90°$) that has plagued earlier investigations [1–3] is avoided. In the end these circle segments are replaced by their chords, hence by their derivative at mid-interval. The intrinsic accuracy of the method is therefore of second order; i.e., truncation errors scale as the cube of the integration step size.

The curious aspect of Kivalov's work is that the need to remedy this horizon singularity does only exist by his own choice to use height above ground (or sea level) as the integration variable. In doing so, he follows a tradition in air mass studies: Kasten [1], Link and Neužil [2], and Kasten and Young [3] made the same choice and had to devise a special treatment for the horizon region. Studies on refraction and mirages, on the other hand, have mostly been performed in schemes where the horizon region is regular but where a singularity in the zenith itself ($z = 0°$) may exist.

In this Comment I review shortly the possible integration schemes and the strategies that have been put into practice. I point out that (1) choosing path length as the integration variable naturally avoids all singularities; (2) standard higher-order Runge–Kutta integration provides a natural solution strategy, wherein refraction and air masses may be taken along as path integrals; and (3) since all integrations are performed in parallel, mass integrals for different constituents such as dry air, water vapor, ozone, NO_2, CO_2, and aerosols may be obtained separately if density profile models are available.

2. Elements of Ray Tracing

Figure 1 illustrates the (increments of) variables of the light ray: φ is the polar angle measured from the Earth's center, $x = R_0\phi$ is the distance along the Earth's surface, and β is the tilt angle measured from the local horizontal. Its complement is the local zenith angle: $z = 90° - \beta$, and Δs is the length of the trajectory element. These describe the geometry of the path. The aim of ray tracing is usually to determine path integrals, such as the refraction integral $\xi = \int(d\beta - d\phi)$ (actually, when counted as positive, the refraction is $-\xi$) and the air mass integral

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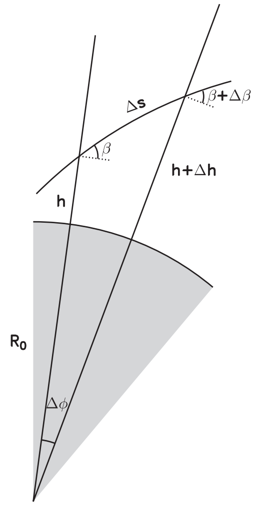

Fig. 1. Ray segment and explanation of its parameters.

$M = \int \rho \mathrm{d}s$, where ρ is the density. For any path the following differential equations govern its geometry:

$$\frac{\mathrm{d}h}{\mathrm{d}\phi} = (R_0 + h)\tan(\beta), \tag{1a}$$

$$\frac{\mathrm{d}\beta}{\mathrm{d}\phi} = 1 + \frac{(R_0 + h)}{r\cos(\beta)}, \tag{1b}$$

$$\frac{\mathrm{d}s}{\mathrm{d}\phi} = \frac{(R_0 + h)}{\cos(\beta)}. \tag{1c}$$

In these equations, $1/r$ is the local curvature of the ray, and it is here that the physics enters. For a spherically symmetric atmosphere the refractive index n does not depend on ϕ. Snell's law gives $n(R_0 + h)\cos(\beta) = $ constant along the ray, from which follows its curvature:

$$\frac{1}{r} = \cos(\beta)\frac{1}{n}\frac{\mathrm{d}n}{\mathrm{d}h}. \tag{2a}$$

More generally, when the characteristics of the atmosphere vary not only with height but in addition with distance along the Earth's surface, the curvature is

$$\frac{1}{r} = \frac{1}{n}\left[\cos(\beta)\frac{\partial n}{\partial h} - \frac{\sin(\beta)}{(R_0 + h)}\frac{\partial n}{\partial \phi}\right]. \tag{2b}$$

Ray tracing requires following the path backward from the observer by use of Eqs. (1) and using any of the four geometric variables, h, β, ϕ, or s, as the integration variable. Refraction and air mass may conveniently be viewed as path integrals in this procedure. Integration is usually carried out up till a height where the contributions to the refraction and air mass integrals become negligible. In practice a height of 85 km is sufficient.

Table 1 lists for each of the four integration schemes the sets of coupled linear differential equations that are to be solved in parallel. The most widely used method for such schemes is fourth-order Runge–Kutta integration, a family of procedures that dates back to 1895 [5] and to which numerous refinements have since been made, which are to be found in textbooks on numerical methods.

Table 1. Ray Tracing Integration Schemes

Integration Variable = h	Integration Variable = β	Integration Variable = ϕ	Integration Variable = s
$\mathrm{d}\beta = \dfrac{\left[1 + \dfrac{(R_0+h)}{r\cos(\beta)}\right]}{(R_0+h)\tan(\beta)}\mathrm{d}h$	$\mathrm{d}h = \dfrac{(R_0+h)\tan(\beta)}{\left[1 + \dfrac{(R_0+h)}{r\cos(\beta)}\right]}\mathrm{d}\beta$	$\mathrm{d}h = (R_0 + h)\tan(\beta)\mathrm{d}\phi$	$\mathrm{d}h = \sin(\beta)\mathrm{d}s$
$\mathrm{d}\phi = \dfrac{1}{(R_0+h)\tan(\beta)}\mathrm{d}h$	$\mathrm{d}\phi = \dfrac{1}{\left[1 + \dfrac{(R_0+h)}{r\cos(\beta)}\right]}\mathrm{d}\beta$	$\mathrm{d}\beta = \left[1 + \dfrac{(R_0+h)}{r\cos(\beta)}\right]\mathrm{d}\phi$	$\mathrm{d}\beta = \left[\dfrac{\cos(\beta)}{(R_0+h)} + \dfrac{1}{r}\right]\mathrm{d}s$
$\mathrm{d}s = \dfrac{1}{\sin(\beta)}\mathrm{d}h$	$\mathrm{d}s = \dfrac{\dfrac{(R_0+h)}{\cos(\beta)}}{\left[1 + \dfrac{(R_0+h)}{r\cos(\beta)}\right]}\mathrm{d}\beta$	$\mathrm{d}s = \dfrac{(R_0+h)}{\cos(\beta)}\mathrm{d}\phi$	$\mathrm{d}\phi = \dfrac{\cos(\beta)}{(R_0+h)}\mathrm{d}s$
$\mathrm{d}\xi = \dfrac{1}{r\sin(\beta)}\mathrm{d}h$	$\mathrm{d}\xi = \dfrac{\dfrac{(R_0+h)}{r\cos(\beta)}}{\left[1 + \dfrac{(R_0+h)}{r\cos(\beta)}\right]}\mathrm{d}\beta$	$\mathrm{d}\xi = \dfrac{(R_0+h)}{r\cos(\beta)}\mathrm{d}\phi$	$\mathrm{d}\xi = \mathrm{d}\beta - \mathrm{d}\phi = \dfrac{1}{r}\mathrm{d}s$
$\mathrm{d}M = \dfrac{\rho}{\sin(\beta)}\mathrm{d}h$	$\mathrm{d}M = \dfrac{\rho\dfrac{(R_0+h)}{\cos(\beta)}}{\left[1 + \dfrac{(R_0+h)}{r\cos(\beta)}\right]}\mathrm{d}\beta$	$\mathrm{d}M = \rho\dfrac{(R_0+h)}{\cos(\beta)}\mathrm{d}\phi$	$\mathrm{d}M = \rho\,\mathrm{d}s$

A. Integration by Height (h)

Choosing h as the integration variable (Table 1, column 1) introduces a $1/\tan(\beta)$ dependence in $d\beta$ and $d\phi$ and a $1/\sin(\beta)$ dependence in ds, $d\xi$, and dM, which makes them explode at the horizon: $\beta = 0°$. Older work on refraction, see, e.g., Smart [6], uses this method through the implicit dependence on h of the refraction index. The well-known result is a divergent series expansion in $\tan(z)$.

Kasten [1] and Link and Neužil [2] remedied their air mass integrals by making, in a limited region above ground or sea level, a coordinate transformation and by retaining higher powers of h. Kivalov [4] cured the problem by modeling ray elements as circle segments, thus explicitly bringing in the necessary curvature of the ray by which the singularity is avoided.

Integration by height has some further limitations: For an observer at some height above ground or sea level, the horizon and the region just above it are seen at negative angles. A corresponding light ray must then be followed in two steps: first from the observer to its lowest point and second from this lowest point upwards till typically 85 km above the Earth. In the presence of a temperature inversion the ray may exhibit one or more oscillations, making it necessary to cut the path in even more parts. Integration by h is therefore less suitable for the study of low-Sun phenomena and mirages.

B. Integration by Altitude (β)

Choosing β as the integration variable (Table 1, column 2) makes ds, dh, and dM singular in the zenith ($\beta = 90°$). Usually this is not a real problem: in the zenith s and h are trivially just the vertical distance over which one chooses to integrate. Further, the air mass is just the ratio of the atmospheric pressure over the acceleration of gravity: $M = P/g$, at least when the dependence of g on height is ignored. The celebrated Auer–Standish [7] approach uses this method: For a spherically symmetric atmosphere one obtains, upon using Eq. (2a),

$$d\xi = \frac{(R_0 + h)dn/dh}{n + (R_0 + h)dn/dh}\, d\beta, \tag{3}$$

which is usually integrated by Simpson's rule, finding h at each step by Newton–Raphson iteration. This method has been described in detail by Hohenkerk and Sinclair [8] and by Seidelmann [9]. For each integration step the ray's horizontal displacement follows trivially from $\Delta\phi = \Delta\beta - \Delta\xi$, thus in principle making this method suitable for ray tracing.

For sunsets and in particular for mirages, ray paths may be multiple-valued in β: They may have alternating positive and negative slopes. As above, for integration by h, one must then subdivide the ray in parts of monotonic slope and perform the integration separately in each of these. This method has been used by Young [10]. To our knowledge, integration by zenith angle has never been used for air masses.

C. Integration by Distance along the Earth ($x = R_0\phi$)

Whereas trajectories of near-horizontal rays may have alternating slopes, the horizontal distance from the observer is monotonic: rays go either to the right or to the left. There is no need to subdivide a trajectory into parts with either positive or negative slope. Therefore, integration by $x = R_0\phi$, the horizontal distance away from the observer, or by the polar angle ϕ itself (Table 1, column 3) is especially appropriate for near-horizontal rays and in particular for the study of mirages. It has been used extensively by Lehn [11], who modeled ray elements as parabolic segments. The same method was used by Bruton [12]. Van der Werf *et al.* [13,14] have used this scheme in combination with fourth-order Runge–Kutta integration. Choosing x (or ϕ) as the integration variable makes ds, dh, and dM singular in the zenith ($\beta = 90°$), which is not a real problem, as mentioned above. I do not know of any study on air masses that uses this scheme.

D. Integration by Path Length (s)

Choosing path length s itself as the integration variable (Table 1, column 4) avoids all singularities because dh/ds, $d\beta/ds$, $d\phi/ds$, $d\xi/ds$, and dM/ds are well behaved everywhere, including the notorious cases: the horizon and the zenith. Path length increases monotonically and there is no need for splitting trajectories in up- and down-sloping intervals. Integration by s has been used by Gutierrez *et al.* [15] in a study of mirages. Their set of differential equations was derived from Fermat's principle and differs in form (not in physics) from the ones that I use in this Comment.

3. Conclusion and Recommendation

The choice of h as the integration variable, which has become the traditional scheme in air mass studies, seems to be the least-fortunate option, and it has given rise to elaborate efforts to cope with a singularity at the horizon that does not exist in other schemes. Instead, I consider integration by path length as the most universally suitable and problem-free method. The study of our atmosphere and the distribution of its constituents and pollutants is of immediate interest, and many more studies on air masses and extinction integrals may be anticipated in near future. Standard methods of proven robustness and accuracy are naturally preferred. As an example, a solution scheme that is based on the classic fourth-order Runge–Kutta method, known for short as RK4, is given below in the Appendix A. In this scheme, refraction ξ, air mass M, and of course path length s itself are path integrals. The integrations are all performed in parallel. It is therefore trivial to add more equations for path integrals. In particular, if models are available, air masses for dry air, water vapor, ozone, NO_2, CO_2, and aerosols may be obtained separately.

Appendix A: RK4 Integration Scheme

With reference to Fig. 1, the result for a single integration step is

$$s_2 = s_1 + \Delta s, \tag{A1a}$$

$$h_2 = h_1 + (k_{h,1} + 2k_{h,2} + 2k_{h,3} + k_{h,4})\Delta s/6, \tag{A1b}$$

$$\beta_2 = \beta_1 + (k_{\beta,1} + 2k_{\beta,2} + 2k_{\beta,3} + k_{\beta,4})\Delta s/6, \tag{A1c}$$

$$\phi_2 = \phi_1 + (k_{\phi,1} + 2k_{\phi,2} + 2k_{\phi,3} + k_{\phi,4})\Delta s/6, \tag{A1d}$$

$$\xi_2 = \xi_1 + (k_{\xi,1} + 2k_{\xi,2} + 2k_{\xi,3} + k_{\xi,4})\Delta s/6, \tag{A1e}$$

$$M_2 = M_1 + (k_{M,1} + 2k_{M,2} + 2k_{M,3} + k_{M,4})\Delta s/6, \tag{A1f}$$

where for each quantity $X = h$, β, ϕ, ξ, M the k coefficients are stepwise evaluated as

$$k_{X,1} = \left.\frac{\mathrm{d}X}{\mathrm{d}s}\right|_{s_1, h_1, \beta_1, \phi_1}, \tag{A2a}$$

$$k_{X,2} = \left.\frac{\mathrm{d}X}{\mathrm{d}s}\right|_{s_1+\frac{1}{2}\Delta s, h_1+\frac{1}{2}k_{h,1}\Delta s, \beta_1+\frac{1}{2}k_{\beta,1}\Delta s, \phi_1+\frac{1}{2}k_{\phi,1}\Delta s}, \tag{A2b}$$

$$k_{X,3} = \left.\frac{\mathrm{d}X}{\mathrm{d}s}\right|_{s_1+\frac{1}{2}\Delta s, h_1+\frac{1}{2}k_{h,2}\Delta s, \beta_1+\frac{1}{2}k_{\beta,2}\Delta s, \phi_1+\frac{1}{2}k_{\phi,2}\Delta s}, \tag{A2c}$$

$$k_{X,4} = \left.\frac{\mathrm{d}X}{\mathrm{d}s}\right|_{s_1+\Delta s, h_1+k_{h,3}\Delta s, \beta_1+k_{\beta,3}\Delta s, \phi_1+k_{\phi,3}\Delta s}. \tag{A2d}$$

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