Identification/impact/rectification of a bug in radiation code pre-processing and spectral files

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1) Identification

A long-standing error has been identified in the calculation of Rayleigh scattering coefficients within the Edwards and Slingo (1996) radiation code which means that the Rayleigh scattering coefficients are in error in all spectral files. The error arises in the routine scatter_rayleigh.f , which is part of the pre-processing software used to generate the spectral files containing information on the radiative properties of atmospheric constituents. The version of Edlen’s formula (Edlen, 1953), for the refractive index of air was incorrectly coded. This error was found whilst identifying discrepancies between aircraft measurements of radiance/irradiance and radiative transfer modelling with the Edwards and Slingo (1996) radiation code. The source of the error is described in Appendix 1, and a correction to rayleigh_scatter.f is provided in Appendix 2.

In practice, this means that all the Rayleigh coefficients in the spectral files will be too small by approximately 20% (see inset of Figure 1 in Appendix 1), leading to a planet that is too dark by a global annual average of about 1.5Wm^{-2} and the surface irradiance will be too high by approximately 1.5Wm^{-2}.

2) Impact

An initial assessment of the impact of this bug upon the top of atmosphere and surface fluxes may be made using the parameterisation of Lacis and Hansen (1974):-

$$R_{Ray} = \frac{0.28}{(1+6.43\mu_o)}$$

Where R$_{Ray}$ is the effective planetary albedo due to Rayleigh scattering and μ_o is the cosine of the solar zenith angle. For an ‘average’ solar zenith angle of 60degrees, R$_{Ray}$=0.066. If we assume an average top of the atmosphere insolation of 340Wm^{-2} then approximately 22.4Wm^{-2} would be reflected owing to Rayleigh scattering. An error of 20% in the Rayleigh scattering coefficients therefore roughly translates to an error of approximately 4.5Wm^{-2} at the top of the atmosphere. If one considers that the error will only be manifest in cloud-free areas where the Rayleigh optical depth is significant when compared to the cloud optical depth, then one can multiply this error by (1-cloud fraction) where the global mean cloud fraction is around 0.7 (e.g. Haywood and Shine, 1995), then an error of approximately 1.4Wm^{-2} is estimated. The error in the surface radiation budget would be of similar magnitude to the top of the atmosphere error owing to the conservative nature of Rayleigh scattering. The sign of the error is to make the planetary albedo too dark; correcting the error will lead to a brightening of the planet and a reduction of down-welling irradiance at the surface.

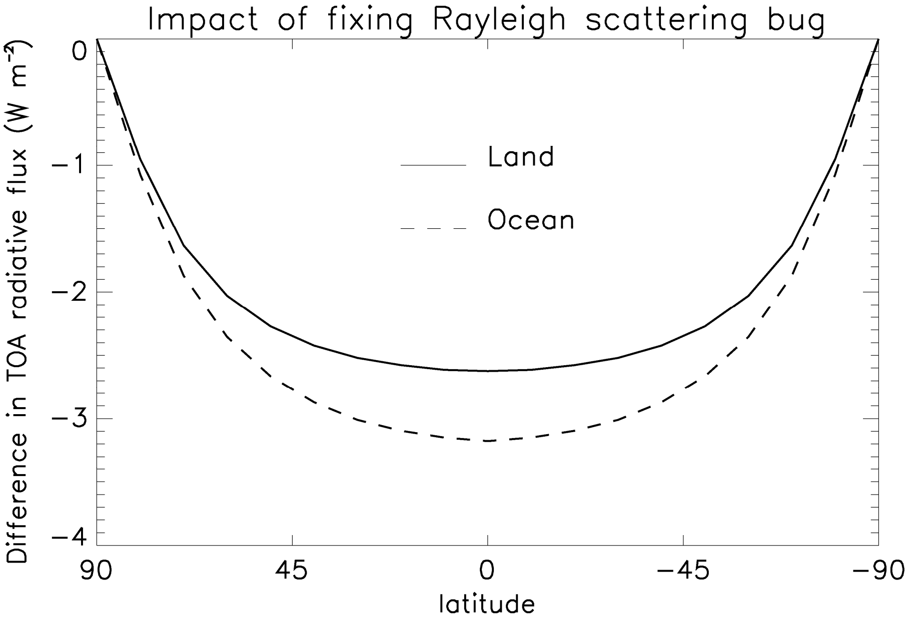

Figure 1. Calculations of the difference in the top of the atmosphere fluxes excluding clouds for land (surface reflectance = 0.15), and for ocean areas. A mid-latitude summer is used for the calculations. The calculations diurnally averaged and are for the Equinox and a TOA solar constant of 1370Wm^{-2}.

Figure 1 shows a more robust estimate may be obtained from running the Edwards and Slingo (1996) code off-line with and without the error in the Rayleigh scattering coefficients and diagnosing the difference in the top of the atmosphere and surface fluxes. The results are shown over land and ocean surfaces. These results show that the TOA clear-sky error is unlikely to exceed 3Wm^{-2}.

Further diagnosis of the magnitude of the error is possible by investigating the top of the atmosphere and surface radiation budget from two parallel runs using HADGEM2. Note that the cleanest way to investigate the magnitude of the error would be to run a single model with a double call to the radiation code, but this would require some significant recoding. In the analysis that we present, there will therefore be some influence of weather on the results, particularly as the integrations are for only 3 years. However, the important point is to highlight the approximate magnitude of the error in surface and top of the atmosphere and to correct it rather than to make an in depth study of the effects of an error, so it is judged that the model results presented here provide a broad estimate of the magnitude of the error.

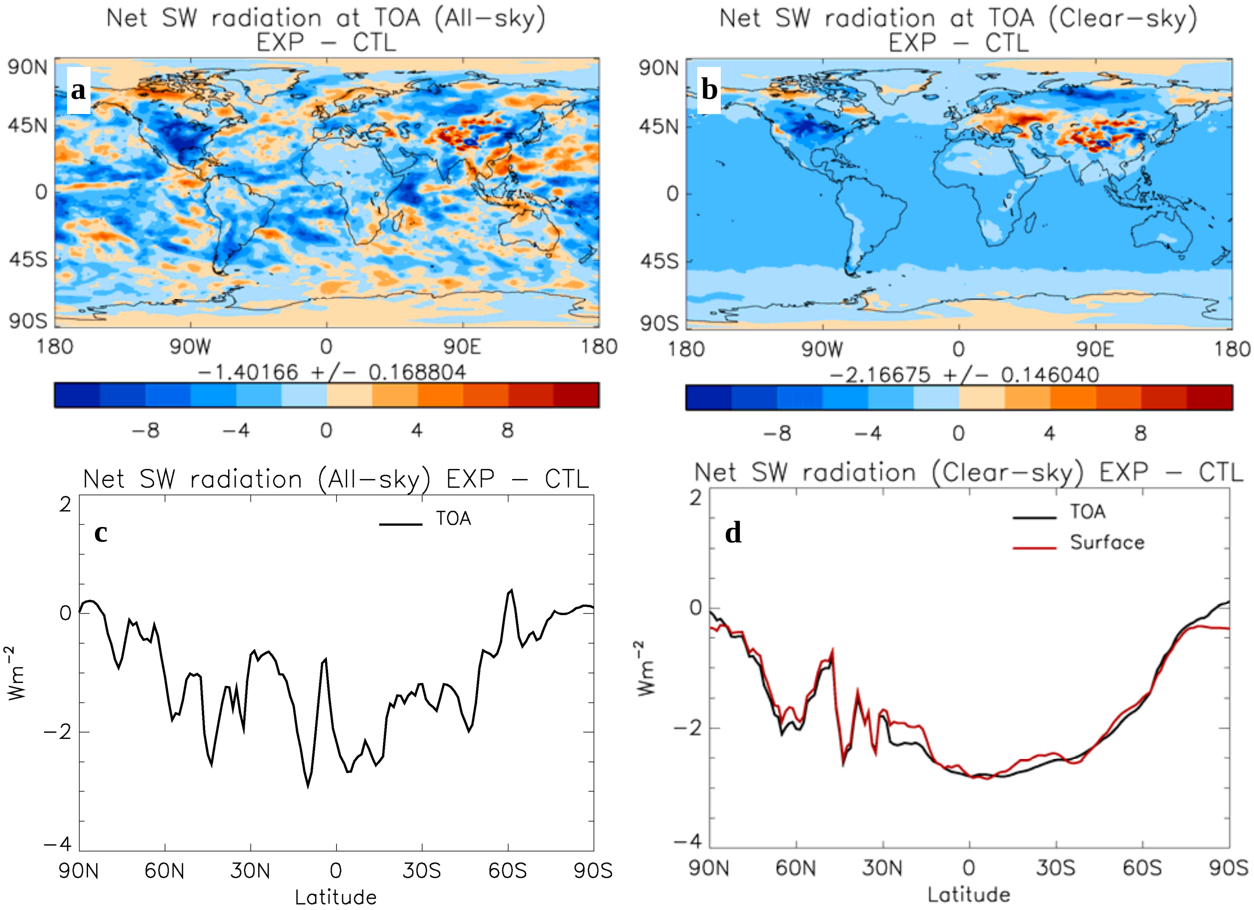

Figure 2. Results from 3-year model integrations described above showing a) the error in the top of the atmosphere solar flux including clouds, b) the error in the top of the atmosphere flux excluding clouds, c) the error in the zonal mean of the TOA solar flux, d) the error in the TOA and surface fluxes in the absence of clouds. The ± values represent the standard deviations in the three years.

While figure 2a and 2c show the obvious effects of weather (particularly differences in cloud fields), figures 2b and 2d where clouds are excluded from the radiative transfer calculations show far less influence. Two things are worthy of note. Firstly, the error in the top of the atmosphere radiation budget when clouds are included appears to be around -1.4Wm^{-2} which is in agreement with that derived from the simplified Lacis and Hansen (1974) model. Secondly, the agreement between the zonal mean plot shown in Figure 1 from the off-line radiative transfer calculations is in very good agreement with that obtained from the 3-years model integrations.

3) Rectification

While rectification of rayleigh_scatter.f is straightforward (appendix 2), a co-ordinated approach is strongly recommended because it has been used widely throughout the Met Office in all versions of the UM including HADCM3, HADGEM2, HADGEM3, etc, and in the NWP global, NAE, and 4km models, and in the LEM. The code has been distributed widely to the scientific research and meteorological forecasting communities including the Australia, Norway, and South African weather services. Corrected spectral file could be generated for all commonly used spectral configurations (e.g. 220band spectral file, HADGEM2 spectral file etc), and distributed as a single tar file to the relevant institutions.

NWP:

It is strongly recommended that this error be addressed in PS20, particularly because PS21 and PS22 will only allow very limited changes in physics.

Hadley Centre:
It is strongly recommended that this error be addressed in HADGEM3. It may be too late for this error to be addressed in HADGEM2, which is unfortunate because HADGEM2 runs will likely be submitted to the IPCC 5AR.

External customers:
APP holds details of all institutions that the radiative transfer code has been distributed to. In the UK these include the meteorology department and ESSC at the University of Reading. Internationally, all weather services that are using the UM should be informed of this model change. It would be best to provide updated spectral files to these institutions as they may not have the expertise in setting up the pre-processing routines for the Edwards and Slingo (1996) radiation code.

References:

Edwards, J. M., and A. Slingo, Studies with a flexible new radiation code, 1, Choosing a configuration for a large scale model, Q. J. R. Meteorol. Soc., 122, 689–720, 1996.

Haywood, J.M., and Shine, K.P., 1995. The effect of anthropogenic sulfate and soot aerosol on the clear sky planetary radiation budget. *Geophys. Res. Letts.*, 22, 5, 603-606.

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APPENDIX 1.

ANALYSIS BY JEAN-CLAUDE THELEN

1 Rayleigh Extinction Coefficients

A comparison of the Edward-Slingo radiation code (ES-Code) and SBDART shows that the Rayleigh extinction coefficients are different by roughly 20% (see figure 1). As a consequence clear-sky radiances in SBDART will be larger by 20% than in the ES-Code. Below we compare the algorithm used to compute the Rayleigh extinction coefficients in the ES-Code and SBDART in order to determine what causes this discrepancy.

The basic equation for the Rayleigh extinction coefficient is given by (see for example Froehlich and Shaw,1980):

$$k_R = 24\frac{\pi^3}{\lambda^4}\frac{1}{N}\frac{(m_r^2-1)^2}{(m_r^2+2)^2}f(\delta) \tag{1}$$

where k_R is the Rayleigh extinction coefficient (m^{-1}), λ is the wavelength (m), N is the molecular density of gas (m^{-3}), m_r is the real part of the refractive index of air, f is a correction factor to take into consideration the anisotropic property of molecules and δ is the anisotropic factor. The correction factor f is given by:

$$f(\delta) = \frac{6+3\delta}{6-7\delta} \tag{2}$$

In the ES-Code, the Rayleigh extinction coefficient is calculated using equations (1) and (2) where the refractive index of air m_r is given by the following fit (Edlen, 1953) :

$$10^8(m_r-1) = 6432.8 + \frac{2949810}{146-\lambda^{-2}} + \frac{25540}{41-\lambda^{-2}} \tag{3}$$

which is valid for "standard air", i.e. $T = 288.15$K and $P = 1023.25$hPa.

SBDART, on the other hand, uses a fit of the form

$$k_R = \frac{\nu^4}{a-b\nu^2} \tag{4}$$

where ν is expressed in wavenumbers (cm^{-1}) and k_r is given in km^{-1}. Shettle (1980) gives the values for a and b as $a = 9.26799\times10^{18}$ and $b = 1.07123\times10^9$ while SBDART actually uses $a = 9.38076\times10^{18}$ and $b = 1.08426\times10^9$. Both codes use a $\delta = 0.0279$ as the anisotropic factor.

According to Shettle (1980) the above approximation was obtained by doing a least squares fit to Penndorf's molecular scattering coefficients (Penndorf, 1957). However, as Penndorf (1957) used equation (1) and the refractive index of air from Edlen (1953) to calculate his scattering coefficients, equation (1) and the fit (4) should give approximately the same results.

A possible source of confusion is the definition of "standard temperature and pressure" (STP) which in Edlen (1953) is defined as $T = 288.15$ K, and $P = 1013.25$hPa, while the ES-Code and SBDART define STP as $T = 271.15$K and $P = 1013.25$ hPa. As a consequence the equation for refractive index of air, i.e. equation (3), needs to be rescaled in the ES-Code and SBDART for it to be valid at 271.15K.

In what follows we adopt Edlen's definition of STP, i.e. $T_{STP} = 288.15$K and $P_{STP} = 1013.25$hPA. The refractive index of air at non-standard temperature and pressure can then be normalised to that defined at standard temperature and pressure as follows (see Tomasi et al.,2005):

$$(m_r-1) = (m_{STP}-1) * \frac{\rho}{\rho_{STP}} \tag{5}$$

where m_{STP} denotes the real part of the refractive index of air at STP and the density ρ (kg/m^3) is given by:

$$\rho = \frac{MP}{RT} \tag{6}$$

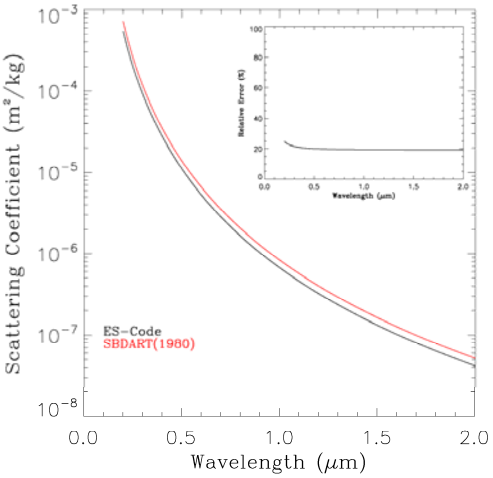

Figure 1: Rayleigh scattering coefficients versus wavelength for the ES-Code and SBDART at $T = 273.15$K and $P = 1013.25$hPa. The inset shows the relative error between the ES-Code and SBDART

Here M denotes the the mean molecular weight (kg/mole), P is the pressure (Pa), T is the temperature (K) and R is the universal gas constant (m^{3}Pa/K/mole). Substituting the expression for the density into equation (5) we find that the refractive index of air at non STP is given by:

$$(m_r - 1) = (m_{STP} - 1) * \frac{T_{STP}}{T} \tag{7}$$

where we assumed that pressure $P = P_{STD} = 1013.25$ hPA. Thus at $T = 273.15$ and $P = 1013.25$ the refractive index of air of Edlen (1953) becomes:

$$10^8(m_r - 1) = 6786.06 + \frac{3111800}{146 - \lambda^{-2}} + \frac{26942.5}{41 - \lambda^{-2}} \tag{8}$$

A quick comparison with the ES-Code shows that the scaling in the ES-Code has been done the wrong way round, resulting in a 20% difference when compared to SBDART. Substituting equation (8) into (1) gives the correct answer as can be seen from figure 2.

A Derivation of the Equation for the Rayleigh Mass Extinction Coefficient used in the ES-Code

The Rayleigh mass extinction coefficient $\hat{k}_R$ (m^2/kg) is given by:

$$\hat{k}_R = k_R/\rho \tag{9}$$

where k_R denotes the Rayleigh extinction coefficient given by equation (1), i.e.

$$k_R = 24\frac{\pi^3}{\lambda^4}\frac{1}{N}\frac{(m_r^2 - 1)^2}{(m_r^2 + 2)^2}f(\delta) \tag{10}$$

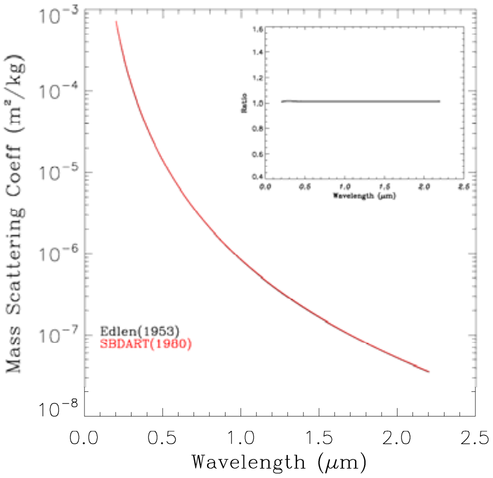

Figure 2: Rayleigh scattering coefficients versus wavelength for the ES-Code and SBDART at $T = 273.15$K and $P = 1013.25$hPa. The inset shows the ratio between the ES-Code and SBDART

The molecular density of gas N (molecules/m^3) is given by

$$N = nN_A \tag{11}$$

where N_A is Avogadro's number (molecules/mole) and n is the number of moles per gas. The number of moles n can be obtained from the ideal gas law:

$$PV = nRT \tag{12}$$

where P is the pressure (Pa), V is the volume in m^3, T is the temperature (K) and R is the universal gas constant. Combining these equations we obtain:

$$\hat{k}_R = 24\frac{\pi^3}{\lambda^4}\frac{(m_r^2-1)^2}{(m_r^2+2)^2}\frac{1}{\rho}\frac{RT}{PVN_A}f(\delta) \tag{13}$$

Assuming a unit volume, making use of the fact that $(m_r^2+2) \approx 3$ and substituting equation (6) into (13) we obtain:

$$\hat{k}_R = 8\frac{\pi^3}{\lambda^4}\frac{(m_r^2-1)^2}{3}\frac{1}{\rho^2}\frac{M_A}{N_A}f(\delta) \tag{14}$$

where M_A is the mean molecular weight of dry air (kg/mole). Finally, using equation (5) gives the expression for the mass extinction coefficient used in the ES-Code:

$$\hat{k}_R = 8\frac{\pi^3}{\lambda^4}\frac{(m_{STP}^2-1)^2}{3}\frac{1}{\rho_{STP}^2}\frac{M_A}{N_A}f(\delta) \tag{15}$$

B Summary of Constants

Values for the various constants that have been used in this note:

- Avogadro's number: $N_A = 6.0221367 \times 10^{23}$ molecules/mole
- Universal gas constant: $R = 8.31447$ m^{3}Pa/K/mole
- Molecular density of gas at 288.15 K and 1013.25 K: $N = 2.546899 \times 10^{25}$molecules/m^3
- Molecular density of gas at 273.15 K and 1013.25 K: $N = 2.686734 \times 10^{25}$molecules/m^3
- Molecular weight of dry air: $M_A = 28.9595 \times 10^{-3}$kg^3/mole

References

[1] B. Edlen. The Dispersion ofStandard Air. *J. Opt. Soc. Am.*, 43:339–344, 1953.

[2] C. Froehlich and G.E. Shaw. New Determination of Rayleigh Scattering in the Terrestrial Atmosphere. *Applied Optics*, 19:1173–1175, 1980.

[3] R. Penndorf. Tables of the Refractive Index for Standard Air and the Rayleigh Scattering Coefficient for the Spectral Region between 0.2 and 20.0 microns and their Application to Amospheric Optics. *J. Opt. Soc. AM.*, 47:176–182, 1957.

[4] E.P. Shettle, F.X. Kneizys, and W.O. Gallery. Suggested Modification to the Volume Molecular Scattering coefficient in LOWTRAN: Comment. *Applied Optics*, 19:2873–2874, 1980.

[5] C. Tomasi, V. Vitale, B. Petkov, A. Lupi, and A. Cacciari. Improved Algorith for Calculations of Rayleigh Scattering Optical Depth in Standard Atmospheres. *Applied Optics*, 44:3320–3341, 2005.

APPENDIX 2

Extract from scatter_Rayleigh.f

The erroneous verion of the fortran code is marked by !

```
!      refract_index_m1=6.09794e-05_RealK+2.79626e+10_RealK
!     &  /(1.46e+14_RealK-lambda_m2)
!     &  +2.42105e+08_RealK/(4.1e+13_RealK-lambda_m2)
!
       refract_index_m1=6.78606e-05_RealK+3.11180e+10_RealK
      &   /(1.46e+14_RealK-lambda_m2)
      &   +2.69425e+08_RealK/(4.1e+13_RealK-lambda_m2)
```