Status report of work on gaseous transmission functions

Prague, 14/9/06

Alena Trojáková

Czech Hydrometeorological Institute
Na Šabatce 17, 143 06 Prague 4

Contents

1 Introduction

Current parameterization of radiation transfer used in ALADIN model is based on solution of the δ-two-stream version of the radiation transfer equations incorporating the effect of scattering, absorption and emission by cloud droplets and gases in each part of the spectrum (currently divided into two bands - solar (0.245 μm - 4.642 μm) and thermal (4.642 μm - 105.0 μm) one), for a descending diffusive flux $F^{\downarrow}$, an ascending diffusive flux $F^{\uparrow}$ and parallel solar flux S differential with respect to optical depth δ:

$$\begin{aligned} \frac{\partial F^{\uparrow}}{\partial \delta} &= \alpha_1 F^{\uparrow} - \alpha_2 F^{\downarrow} - \alpha_3 J \\ \frac{\partial F^{\downarrow}}{\partial \delta} &= \alpha_2 F^{\uparrow} - \alpha_1 F^{\downarrow} + \alpha_4 J \\ \frac{\partial S}{\partial \delta} &= -\frac{S}{\mu_0} \end{aligned} \tag{1}$$

where

$$\begin{aligned} \alpha_1 &= 2[1 - \overline{\omega}(1 - \beta_0)] \\ \alpha_2 &= 2\beta_0\overline{\omega} \\ \alpha_3 &= \begin{cases} \overline{\omega}\beta(\mu_0) & \text{solar} \\ 2(1-\overline{\omega}) & \text{thermal} \end{cases} \\ \alpha_4 &= \begin{cases} \overline{\omega}[1 - \beta(\mu_0)] & \text{solar} \\ \alpha_3 & \text{thermal} \end{cases} \\ J &= \begin{cases} \frac{S}{\mu_0} & \text{solar} \\ \pi B & \text{thermal} \end{cases} \end{aligned}$$

The simultaneous and consistent treatment if scattering and molecular absorption is possible, if we use the k-distribution method for describing the absorption properties of gases in wide spectral intervals. The simplest practical approach of this method is to calculate the average gaseous transmission function for a wide spectral interval, using a narrow-band model, and then fit this function of the absorber amount by series of exponentials.

$$\tau_\nu(u) \approx \sum_{i=1}^{I} \xi_i e^{-k_i u} \tag{2}$$

where k_i can be considered as a set of pseudo-monochromatic gaseous absorption coefficients of the gas in the spectral band, representing the ensemble of all monochromatic absorption coefficients. The weights ξ_i are constrained to sum one to ensure energy conservation.

This note doesn't intent to be detailed documentation of radiation scheme of ALADIN model, which is available in Gerard (2002) or Ritter and Geleyn (1992), but a short resume of studied subject dedicated to improvement of gaseous transmission function used in ACRANEB scheme, which has deficiencies with respect to RRTM scheme as was shown by Gwen Hello by 1-D inter comparison of the schemes, see Fig.1. Following sections describe at first computation of optical thickness by ACRANEB scheme and an attempt of revitalization of the fitting procedures to compute coefficients used in transmission functions computations.And an appendix contains a summary of available utilities and data sets.

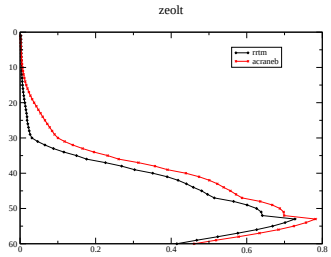

Fig. 1: ZEOLT.

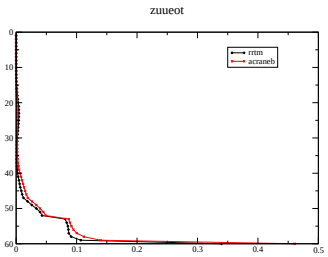

Fig. 2: ZUUEOT.

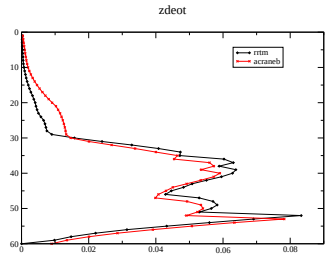

Fig. 3: ZDEOT.

2 Absorption and diffusion by gases in ACRANEB scheme

Following Gerard (2002) the formulation of optical depth $\triangle\delta$ to the gas quantity is highly non-linear and is defined as sum of optical depths of G different gases, which are individually calculated from equivalent widths $w^g_{\triangle\nu}$ by Padé formula:

$$\triangle\delta_{\triangle\nu} = \sum_{g=1}^{G} w^g_{\triangle\nu} \frac{1+\sum_{n=1}^{N_g}(w^g_{\triangle\nu})^n \mathrm{VNP}^n_{\triangle\nu}}{1+\sum_{n=1}^{N_g}(w^g_{\triangle\nu})^n \mathrm{VDP}^n_{\triangle\nu}} \tag{3}$$

The formula implies the development into N_g terms for gas g:

$$\begin{array}{llll} N_{H_2O}=5, & N_{CO_2}=5, & N_{O_3}=5 & \text{in short waves} \\ N_{H_2O}=5, & N_{CO_2}=5, & N_{O_3}=3 & \text{in long waves} \end{array}$$

Equivalent widths $w^g_{\triangle\nu}$ are evaluated by spectral integration including a continuum term and a Malkmus band model:

$$w^g_{\triangle\nu} = \frac{a}{b}\frac{q^g_{r\triangle\nu}}{q^g_{n\triangle\nu}}\left(\sqrt{1+4b\frac{(q^g_{n\triangle\nu})^2}{q^g_{r\triangle\nu}}}-1\right) + cq^g_{r\triangle\nu} \tag{4}$$

where
a, b and c depend on the spectral interval and the gas, integrate the information on width and intensity of spectral lines (α_0, S_0) and reference temperature and pressure. Coefficient a stands for the "weak line" part of the equivalent width, b for the "strong line" part and c for the "continuum" part.
$q^g_{n\triangle\nu}$ is linked to the crossed quantity of gas g: $u_g = 2\delta p q_g$, factor 2 comes from the isotropy hypothesis. For the solar descending flux it is necessary to take into account so that $q^g_{n\triangle\nu} = u_g/(2\mu_0^{'})$, while otherwise $q^g_{n\triangle\nu} = u_g$.
$q^g_{r\triangle\nu}$ is the same mass multiplied by different correction factors to take into account temperature and pressure dependency of (α and S), the grey-body diffusion and scattering and multiple absorption makes that crossed quantity of gas will be larger, leading to the introduction of the diffusivity factor $\beta = \sqrt{e}$. The expression are given below:

	$\downarrow O_3$	$\uparrow O_3$	$\downarrow H_2O$	$\uparrow H_2O$	$\downarrow CO_2$	$\uparrow CO_2$
q_n solar	$u_g/(2\mu_0^{'})$	u_g	$u_g/(2\mu_0^{'})$	u_g	$u_g/(2\mu_0^{'})$	u_g
q_r solar	$u_g/(2\mu_0^{'})p\sqrt{T}$	$u_g p\sqrt{T}\frac{\beta}{2}$	$u_g/(2\mu_0^{'})p\sqrt{T}$	$u_g p\sqrt{T}\frac{\beta}{2}$	$u_g/(2\mu_0^{'})pT$	$u_g pT\frac{\beta}{2}$
q_n thermal	$u_g T^2$	$u_g T^2$	$\frac{u_g}{T}$	$\frac{u_g}{T}$	u_g	u_g
q_r thermal	$u_g pT^4\frac{\beta}{2}$	$u_g pT^4\frac{\beta}{2}$	$u_g p\frac{1}{T}\frac{\beta}{2}$	$u_g p\frac{1}{T}\frac{\beta}{2}$	$u_g pT^2\frac{\beta}{2}$	$u_g pT^2\frac{\beta}{2}$

For water vapor in the thermal domain, it is necessary to introduce a more complex continuum term owing to the so-called e-type effect:

$$q_{c\triangle\nu} = \frac{q_{r\triangle\nu}}{T^4}(1 + d_1 q_{H_2O} T^{\frac{49}{2}} e^{\frac{d_2}{T}})$$

3 Transmission functions

3.1 SPLIDACO or TGASE

An input experimental data and program for computation of broad band transmission function for given spectral interval (with or without continuum term) via modified Malkmus model (5) and (6) were provided by Bodo Ritter. These are original data sets used to find current tuning of ACRANEB scheme. Inputs contain:

- solar insolation at the top of the model of Labs and Neckel, resp. Theakara and Drummond (for 410 spectral intervals)
- input data for "band model" the spectrally resolved narrow band model parameters required for the calculation of their spectrally integrated equivalents

The main computation of transmission function (so called modified Malkmus model) is following if continuum term is included

$$\tau = \sum \tau_i = \sum e^{-\frac{1}{2}\frac{p}{p_0}\sqrt{\frac{T_0}{T}}\frac{b_i}{a_{min}}\left(\sqrt{1+\frac{4a_i u}{\frac{p}{p_0}\sqrt{\frac{T_0}{T}}}}-1\right)-c_i u\frac{p}{p_0}\sqrt{\frac{T_0}{T}}} \tag{5}$$

and otherwise

$$\tau = \sum \tau_i = \sum e^{-\frac{1}{2}\frac{p}{p_0}\sqrt{\frac{T_0}{T}}\frac{b_i}{a_{min}}\left(\sqrt{1+\frac{4a_i b_i u}{bc_{min}\frac{p}{p_0}\sqrt{\frac{T_0}{T}}}}-1\right)} \tag{6}$$

where

$$a_{min} = max(a_i, eps)$$

$$bc_{min} = max((b_i - c_i\frac{p}{p_0}\sqrt{\frac{T_0}{T}}), eps)$$

and u is absorber amount

The output contains transmission function $\tau = \tau(u)$ for each gas at temperatures $T = 204.0, 229.9, 255.8, 281.7, 307.6K$ and $\frac{p}{p_0} = 1.000, 0.850, 0.750, 0.600, 0.500, 0.400, 0.300, 0.200, 0.100, 0.075, 0.050, 0.030, 0.020, 0.010, 0.005$. An example of transmission function for CO_2 at $T = 204.0K$ in thermal spectral interval is on Fig 4. And on Fig. 5. there are corresponding transmission functions from M1D ALADIN model simulations, what can be assumed as a validation of datasets with respect to current model settings.

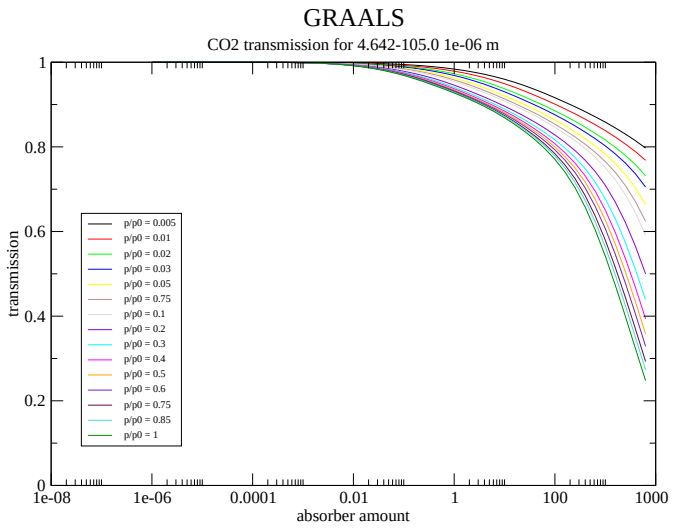

Fig. 4: $\tau(u_g)$ SPLIDACO in thermal sp. interval for CO2 with isothermal vertical profile T=204K.

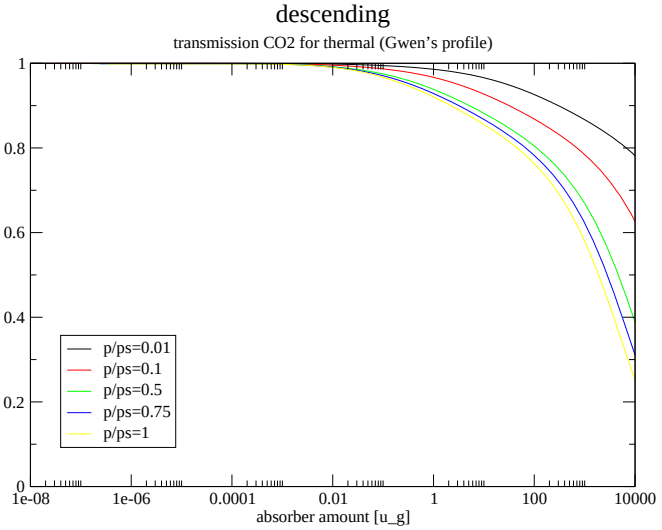

Fig. 5: $\tau(u_g)$ M1D model with non-isothermal vertical profile (descending)

3.2 LBLRTM

Line By Line Radiative Transfer Model (LBLRTM) is an accurate and efficient line-by-line radiative transfer model derived from the Fast Atmospheric Signature Code (FASTCODE). The HITRAN database provides the basis for the line parameters used in LBLRTM. These line parameters, as well as additional line parameters from other sources, are extracted for the use in LBLRTM by a line file creation program LNFL. A line parameters database build from HITRAN and suitable for use with LNFL is available from the AER RT web site (rtweb.aer.com).

LBLRTM outputs can be used as more accurate source of transmission functions for a new tuning and some of its examples are on Fig. 6. and Fig. 7 .

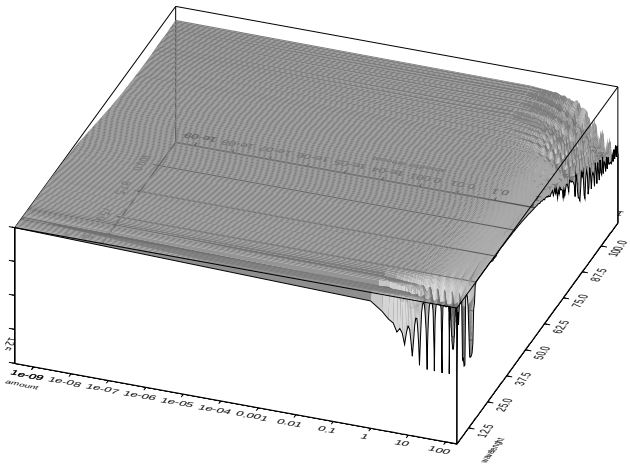

Fig. 6: $\tau(u_g, \lambda)$ for O3 in thermal sp. interval.

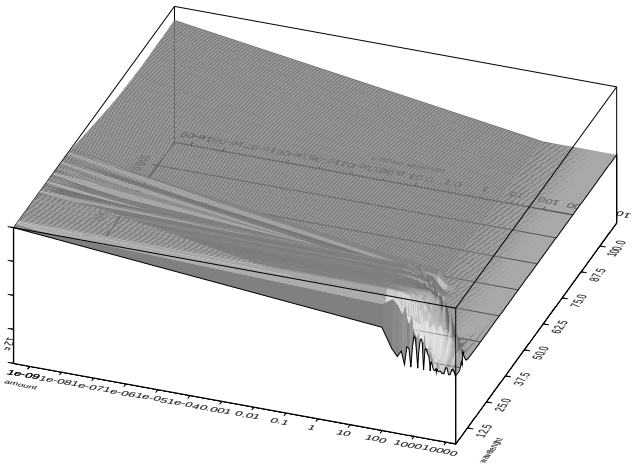

Fig. 7: $\tau(u_g, \lambda)$ for H2O in thermal sp. interval.

4 Fitting procedures

From the section 2 is clear a need to find Padé approximation of (3), coefficients of Malkmus model (4) and their temperature dependency.

4.1 Padé approximation

A Padé rational approximation to function $f(x)$ is quotient of two polynomials $P_M(x)$ and $Q_N(x)$ of degree m and n respectively. Let's denote nominator of (3) as $P(x) = x(1 + \sum_{k=1}^{M} p_k x^k)$ and denominator as $Q(x) = 1 + \sum_{j=1}^{N} q_j x^j$, thus we can write

$$f(x) = \frac{x(1 + \sum_{k=1}^{M} p_k x^k)}{1 + \sum_{j=1}^{N} q_j x^j} + \epsilon(x) \tag{7}$$

After multiplication of (7) by its denominator, one gets

$$f(x)(1 + \sum_{j=1}^{N} q_j x^j) = x(1 + \sum_{k=1}^{M} p_k x^k) + \epsilon(x)(1 + \sum_{j=1}^{N} q_j x^j) \tag{8}$$

Let's denote last term $\epsilon(x)(1 + \sum_{j=1}^{N} q_j x^j)$ as E(x) and using least square method to minimize $\sum_i E^2(x_i)$

$$\sum_i E^2(x_i) = \sum_i [f(x_i)(1 + \sum_{j=1}^{N} q_j x_i^j) - x_i(1 + \sum_{k=1}^{M} p_k x_i^k)]^2 \tag{9}$$

one obtains system of $N + M$ linear equations for unknown $p_k, k = 1..M$ and $q_j, j = 1..N$ coefficients, which can be solved easily. In some cases this approximation oscillates, as is shown in Fig. 8. So an iterative procedure was developed, following Geleyn (XXXX), which minimizes $\sum_i PP(x_i)E^2(x_i)$ where $PP_(x_i) = [\frac{1}{x_i(1+\sum_{k=1}^{M} p_k x_i^k)}]$ with p_k from previous iteration.

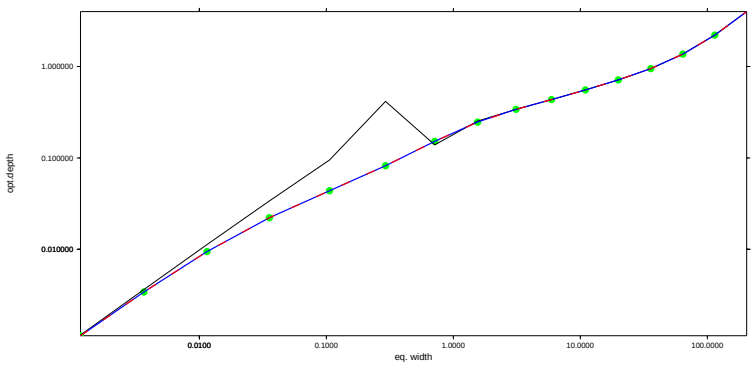

Fig. 8: Fitting of Padé approximation of an artificial $\delta(w)$ sample. Data as green points, Padé approximation in black (used as first guess for iteration) and in blue the solution after 2 iterations. As reference also coefficients from ACRANEB scheme as red dashed line.

4.2 Malkmus model coefficients

The integration of absorption over optical path is complicated by the dependency of absorption coefficients k_ν on both pressure and temperature. To overcome this problem we can assume that the absorption along nonhomogenous path can be approximated by the absorption along some homogeneous path with some appropriately adjusted values of p and absorber amount u_g. The approximation assumes that the absorption coefficient is separable into two factors: one depending only on ν and the other on p and T. Then equation (2) would read

$$\tau_\nu(u) \approx \sum_{i=1}^{I} \xi_i e^{-k_i(\frac{p}{p_0})^\alpha(\frac{T}{T_0})^\beta u} \tag{10}$$

I have assumed to have the transmission functions for various T and p from SPLIDACO as the only available input. I tried to develop "reverse engineering" method to diagnose temperature dependency of transmission functions $\tau = \tau(u, T, p)$ or $a = 1 - \tau$, which is simpler to fit by Padé approximation. At first the absorption dependency $a_{TR} = a(u_g)$ from SPLIDACO at reference temperature T=255.8 K is fitted, let's call it reference function. And afterwards α parameter is searched so to satisfy $a_T(\alpha u) = a_{TR}(u)$ for all temperatures. And the dependency $\alpha = \alpha(T)$ gives you searched temperature dependency, one can fit it by simple polynomial function $y = kT^m$.

This procedure works nicely for simple functions, but has problems with real data sets (from SPLIDACO), where is quite difficult to find a proper reference function on all definition interval. I obtained encouraging results from tests for O3 in both spectral interval, but more detailed work should be done on this part.

Last step should be to incorporate the temperature dependency in reduced absorber amount and with unreduced absorber amount and transmission function, as equivalent width $w = \int 1 - \tau(\nu)d\nu$, to fit the coefficients a, b and c of Malkmus band model (4). Unfortunately this item I was not able to tackle at all.

5 Summary

What was done:

- porting M1D as the main validation tool
- porting SPLIDACO and LBLRTM as sources of transmission functions
- development of Padé approximation procedure
- development of "reverse engineering" procedure to diagnose temperature dependency of transmission functions

Remaining work:

- development of fitting procedures for coefficients of Malkmus model and maybe also revisiting temperature dependency of these coefficients from transmission function. Or there is another way to fit the coefficients directly from line parameters (the width and intensity of lines (α_0, S_0)).

References

L. Gerard, 2000: Physical Parameterization for high resolution operational NWP model *PHD thesis*
B.Ritter and J.-F.Geleyn, 1992: A Comprehensive Radiation Scheme for Numerical Weather Prediction Model with Potential Application in Climate Simulation *Mon.Wea.Rev.*,**120**, 303-325
J.-F. Geleyn, XXXX: Procedure to generate gaseous absorption properties *notes*

Appendix

A List of Symbols

$F^{\downarrow}, F^{\uparrow}$	...	diffusive downward,upward flux
S	...	parallel solar flux with respect to a horizontal plane
S_0	...	solar constant
μ_0	...	cosine of solar zenith angle
δ	...	optical thickness
δ_0	...	optical thickness of gray constituents only
δ_i	...	optical thickness of gas, considering absorption coefficient i
f	...	fraction of radiation contained in the diffraction peak of the phase function
ω	...	single-scattering albedo
$\overline{\omega}$	...	$\frac{\omega(1-f)}{1-\omega f}$
T, T_s	...	temperature,earth's surface temperature
p	...	atmospheric pressure

B Various tools

Following tools and data sets are available, each contains README file with short description of compilation and running. Everything is stored on archive in mma153/voodoo/RAD/ as export.tar.

- **M1D - Single column model** contains 1-D model package with modification to allow comparison of radiation fluxes was provided by Gwen Hello. Original package is stored on archive mma153/M1D/M1D.alena.tar.gz and version ported at CHMI (Linux voodoo, compiled with lf95 - Lahey/Fujitsu Fortran 95 Compiler), is stored in export/M1D directory in previously mentioned archive export.tar.

- **SPLIDACO or TGASE** contains main source main.f90, where You have to define a gas H2O,CO2,O3 via $IGAS = 1, 2, 3$, with $FKONT$ if continuum is included or not, $NTEMPE$ is number of temperature included in computations, NU number of absorber amounts and NP is a number of pressure scaling. Program creates ASCII output fort.44, which could be processed by script proc_output.pl to create $\tau(u_g)$ dependency for each given temperature and pressure.

- **LBLRTM, LNFL** To run LBLRTM one needs special (binary file), which is created by LNFL program. LNFL uses line parameter database as input and one should define spectral interval and trace gasses to be used in its control file TAPE5. In directory LNFL there is an example of such file for solar and thermal part of ACRANEB calculation ($0.245 - 105\mu m$) only with CO2 H2O O3 molecules included. And LBLRTM/camex/ contains examples of scripts to obtain dependency $\tau(u_g, \lambda)$ in thermal spectral interval for H2O and O3, which are plotted (via plot.pl) on Fig. 6. and Fig. 7.

- **PADE** contains procedure find_coeff_pade.pl which finds corresponding Padé coefficients from $\delta(w)$ dependency.

- **T_dependency** contains procedure run_dep_T.pl to diagnose temperature dependency by "reverse engineering" method.