

Gridsize induced error in the discretization of exchange processes at the tropopause

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RESUMEN

Estudiamos el error introducido por el método de las diferencias finitas en la discretización de un modelo global simplificado 2-D de transporte de gases traza, para casos en que los coeficientes de difusión, que relacionan el flujo con el gradiente de la razón de mezcla, tienen discontinuidades de salto en la tropopausa. Analizamos el método convencional de celdas tanto para el caso de un flujo ascendente típico, como también para el caso de un flujo descendente típico con reacciones químicas, comparando las aproximaciones de las soluciones correspondientes para diferentes tamaños de paso de discretización. Para el flujo descendente típico resulta que si la rejilla no es suficientemente fina se pueden generar grandes errores; estos se propagan fundamentalmente en la troposfera. En cambio, el flujo típicamente ascendente resulta ser relativamente insensible al tamaño de paso de la discretización.

ABSTRACT

We study the accuracy of the finite differences discretization scheme for a 2-D simplified model of global tracer transport, in the case that the diffusion coefficients relating flux to the gradient of the mixing ratio have discontinuity jumps at the tropopause. We analyze the conventional box method for a typical downward flow with chemical reaction and for a typical upward flow, comparing the approximations of the solutions, for different discretization gridsizes. It turns out that the jumps may introduce remarkable errors in the discrete solutions, in the case of a typical downward flow; these errors propagate mainly into the troposphere. A noticeable improvement is achieved by reducing the gridsize. However, a typical upward flow is rather insensitive to the chosen gridsizes.

Keywords: Global tracer transport model, finite differences discretization scheme, tropopause discontinuity jumps, discretization errors.

1. Introduction

The earth's atmosphere is divided into several layers. Of particular interest for the global transport of tracers are the *troposphere* (from ground up to about 8 km height near the poles, about 18 km height near the equator) and the *stratosphere* (the next higher level). There results a rather sharp boundary between the two layers, the so-called *tropopause*, below of which vertical exchange coefficients are large, whereas above it they are small (Birner *et al.*, 2002; 2003; Schneider, 2004; Wirth, 2004).

Therefore, in 1-D and 2-D models of global tracer transport, the eddy diffusion coefficient tensor, relating flux to the gradient of the mixing ratio of some tracer has a discontinuity jump at the tropopause and also contains non-diagonal matrix elements in the lower stratosphere (Gidel *et al.*, 1983; Brühl and Crutzen, 1988). The question arises whether in numerical models a significant error is introduced by the numerical schemes, due to the tropopause jump. This question seems to be especially relevant if we consider the increasing interest in recent years of the atmospheric science community to understand stratosphere-troposphere exchange processes and also, to understand the impact of aircraft emissions on atmospheric chemistry. Both issues were analyzed in many model studies (Ko and Douglass, 1993; Brühl *et al.*, 1998; Groâ *et al.*, 1998; Rondanelli *et al.*, 2002; Gallardo *et al.*, 2004); in almost all of them the effect of the jump discontinuity of the coefficients, on the accuracy of the numerical scheme, is not considered.

In this paper we show the error behavior of the conventional box method, for the 2-D case (Gidel *et al.*, 1983; Brühl, 1987), with simplified numerical examples.

The basic equation for the time evolution of the concentration X of a particular tracer species in the atmosphere is given by

$$\frac{\partial X}{\partial t} + \text{div } F = Q \quad (1)$$

where F is the flux density vector of this quantity and Q is its net chemical production per volume unit. With $u = X/M_{air}$ denoting the mixing ratio of this tracer, M_{air} being the air concentration,

$$F = X \vec{v} - M_{air} IK \text{grad } u \quad (2)$$

consists of an advective term with \vec{v} being the velocity vector of an averaged motion, and of a second term describing eddy diffusion with IK being the symmetric positive definite tensor of eddy diffusion coefficients.

Since our emphasis is on the effects of the jump in the diffusion coefficients with the conventional box method, we adopt a very simple model which only mimics diffusion and a chemical reaction,

thereby neglecting advection and the effects of spherical geometry. Also spatial variations in the coefficients are not taken into account, besides of the variations resulting from the preferentially isentropic diffusion in the stratosphere which is closely connected to the shape of the tropopause. This does not mean that the neglected effects are not significant, but we want to clarify the numerical effects of the jumps without mixing in many different phenomena.

We restrict the chemistry term to a simple first order reaction:

$$Q = -\kappa X \quad (3)$$

with constant reaction rate κ . Furthermore we treat the air density as a constant such that equation (1) reduces to

$$\frac{\partial u}{\partial t} - \text{div}(IK \text{ grad } u) = -\kappa u \quad (4)$$

In addition, suitable boundary conditions have to be stated.

2. The simplified 2-D case

We consider the continuous model for a simplified cartesian case without advection and with constant air density. The corresponding differential equation for the mixing ratio u of a tracer species is

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial y} F_y - \frac{\partial}{\partial z} F_z - \kappa u, \quad 0 \leq y \leq Y, \quad 0 \leq z \leq Z \quad (5)$$

with

$$F_y = -K \frac{\partial u}{\partial y} - L \frac{\partial u}{\partial z}, \quad F_z = -L \frac{\partial u}{\partial y} - M \frac{\partial u}{\partial z} \quad (6)$$

and initial condition

$$u(y, z, 0) = u_0(y, z), \quad 0 \leq y \leq Y, \quad 0 \leq z \leq Z \quad (7)$$

K , L and M are the space dependent exchange coefficients, i.e. the “eddy diffusion coefficients”, and satisfy the condition

$$KM > L^2 \quad (8)$$

for the sake of positive definiteness of IK with

$$IK = \begin{bmatrix} K & L \\ L & M \end{bmatrix}$$

The chemical reaction rate κ is considered constant. We suppose that at the lateral boundary the flux is purely vertical, i.e. the normal flux F_y is zero; but since we further assume that the off-diagonal diffusion coefficient L is zero at the boundaries we have

$$\frac{\partial u}{\partial t}(0, z) = \frac{\partial u}{\partial y}(Y, z) = 0, \quad 0 \leq z \leq Z \quad (9)$$

at the lateral boundary. Therefore the boundary conditions are given by (9) and either in the case

$$F_z|_{z=0} = F_B, \quad F_z|_{z=Z} = k_z u; \quad k_z, F_B > 0, \quad (10)$$

of tracers characterized by an ‘‘upward flow’’ (e.g. the CFC-family), or in the case of tracers

$$F_z|_{z=0} = K_B u, \quad F_z|_{z=Z} = F_z; \quad k_B, F_z < 0, \quad (11)$$

characterized by a ‘‘downward flow’’ (e.g. the ClO_x family). The matching conditions at the jump line are well known (Marchuk and Skiba, 1976; 1992), i.e. at the tropopause these conditions are now given by

$$u|_S = u|_T \quad (12)$$

and

$$(M - \tau L) \frac{\partial u}{\partial z} \Big|_S + (L - \tau K) \frac{\partial u}{\partial y} \Big|_S = (M - \tau L) \frac{\partial u}{\partial z} \Big|_T + (L - \tau K) \frac{\partial u}{\partial y} \Big|_T \quad (13)$$

where τ is the slope of the tropopause and the notations $w|_S$ and $w|_T$ denote the limit values of w taken from the stratospheric and the tropospheric side, respectively. Condition (12) is a continuity

condition for the mixing ratio u at the tropopause and condition (13) is a continuity condition for the transverse flux component. We further suppose that the altitude z_{TP} of the tropopause is a piecewise continuously differentiable function of y , i.e. $z_{TP} = \Phi(y)$ for $0 \leq y \leq Y$.

3. The conventional box discretization

Several investigations in air chemistry (McRae *et al.*, 1982; Gidel *et al.*, 1983; Brühl, 1987) solve equation (1) numerically by applying a splitting method (Marchuk, 1975) where the transport step uses Euler's forward method as time discretization and for concentrations and fluxes centered difference methods are used as spatial discretization (Fiebig-Wittmaack and Börsch-Supan, 1994). This conventional method uses discretizations based on cells, or boxes, defined by the inequalities

$$(j-1)\Delta y \leq y \leq j\Delta y \quad \text{and} \quad (i-1)\Delta z \leq z \leq i\Delta z, \quad i = 1, \dots, n; \quad j = 1, \dots, m,$$

with $\Delta y = Y/m$ and $\Delta z = Z/n$. The grid G is given by

$$G = \{(y_j, z_i) / y_j = (j-1/2)\Delta y, z_i = (i-1/2)\Delta z, i = 1, \dots, n; j = 1, \dots, m\}$$

and the discrete values $u_{j,i}$ of the mixing ratio are given at the midpoint of the cell. In order to improve the discrete boundary conditions in our simplified case, we introduce additional fictive outer points. We denote by $F_y^{j,i}$ the discrete value of F_y calculated at the midpoint of the right boundary of j, i -th cell and by $F_z^{j,i}$ the discrete value of F_z calculated at the midpoint of the upper boundary of the j, i -th cell. Therefore, we obtain the following discrete equation for the j, i -th cell:

$$u_{j,i}(t + \Delta t) = u_{j,i}(t) - \Delta t \left[\frac{F_y^{j,i} - F_y^{j-1,i}}{\Delta y} + \frac{F_z^{j,i} - F_z^{j,i-1}}{\Delta z} + \kappa u_{j,i} \right] \quad (14)$$

The values at the fictive outer points must be calculated at every time step from the discretized boundary conditions. In order to ensure D-stability the inequality must hold; otherwise small errors

$$\Delta t \left[\frac{K}{(\Delta y)^2} + \frac{M}{(\Delta z)^2} \right] \leq \frac{1}{2} \quad (15)$$

would propagate exponentially in time, the faster the smaller the time step is.

4. Numerical example

We use simplified data taken from the distributions employed in the 2-D box model of the MPI Mainz (Brühl, 1987; Fiebig-Wittmaack and Börsch-Supan, 1994). Because of symmetry with respect to the equator we consider only one half sphere with $y = 0$ corresponding to the equator and $y = Y = 9990$ km corresponding to the north pole; $z = 0$ and $z = Z$ correspond to altitudes of 2 km altitude above ground (just above the planetary boundary layer) and 23.6 km altitude (near the ozone layer), respectively. We introduce the altitude above sea level $\bar{z} = z + 2$. In agreement with the MPI model our basic gridsizes are $\Delta z = 1.8$ km, $\Delta y = 1110$ km (i.e. for the latitude φ we take $\Delta\varphi = 10^\circ$), and the time step is $\Delta t = 2$ hours. The eddy diffusion coefficients are given by

$$K = 6 \times 10^3 \text{ km}^2/\text{h};$$

$$L = \begin{cases} 0, & \text{in the troposphere,} \\ K\alpha_y(\varphi)\alpha_z(\bar{z}), & \text{in the stratosphere,} \end{cases}$$

$$M = \begin{cases} 3 \times 10^{-2} \text{ km}^2/\text{h}, & \text{in the troposphere,} \\ K[\alpha_y(\varphi)\alpha_z(\bar{z})]^2 + 1.5 \times 10^{-3} \text{ km}^2/\text{h}, & \text{in the stratosphere,} \end{cases}$$

with

$$\alpha_y(\varphi) = \begin{cases} -0.05(\varphi - 25) & \text{if } 25^\circ \leq \varphi \leq 45^\circ, \\ -1 & \text{if } 45^\circ \leq \varphi \leq 55^\circ, \\ -0.05(75 - \varphi) & \text{if } 55^\circ \leq \varphi \leq 75^\circ, \\ 0, & \text{otherwise} \end{cases}$$

$$\alpha_z(\bar{z}) = \begin{cases} 8 \times 10^{-4} [1 - (17.3 - \bar{z})/10] & \text{if } \bar{z} \leq 17.3 \text{ km,} \\ 8 \times 10^{-4} & \text{if } 17.3 \text{ km} \leq \bar{z} \leq 19.1 \text{ km,} \\ 8 \times 10^{-4} [1 - (\bar{z} - 19.1)/3.6] & \text{if } 19.1 \text{ km} \leq \bar{z} \leq 22.7 \text{ km,} \\ 0, & \text{otherwise} \end{cases}$$

Here $\alpha = \alpha_y(\varphi) a_z(\bar{z})$ may be interpreted as the slope of the main diffusion direction; thus this deviates from the horizontal in the stratosphere between 25° and 75° latitude. Note that $\alpha = 0$ near the upper boundary has been introduced artificially in order to simplify the upper boundary conditions.

The tropopause $\bar{z} = \bar{\Phi}(\varphi)$ is approximated by the following description

$$\bar{\Phi} = \begin{cases} 15.501 & \text{if } \varphi \leq 15^\circ \\ 15.501 - 0.18(\varphi - 15) & \text{if } 15^\circ \leq \varphi \leq 35^\circ \\ 11.901 - 0.06(\varphi - 35) & \text{if } 35^\circ \leq \varphi \leq 75^\circ \\ 9.501 & \text{if } 75^\circ \leq \varphi \end{cases}$$

The shape of the tropopause and the eddy diffusion coefficients L and M are plotted in Figure 1 and Figure 2 respectively.

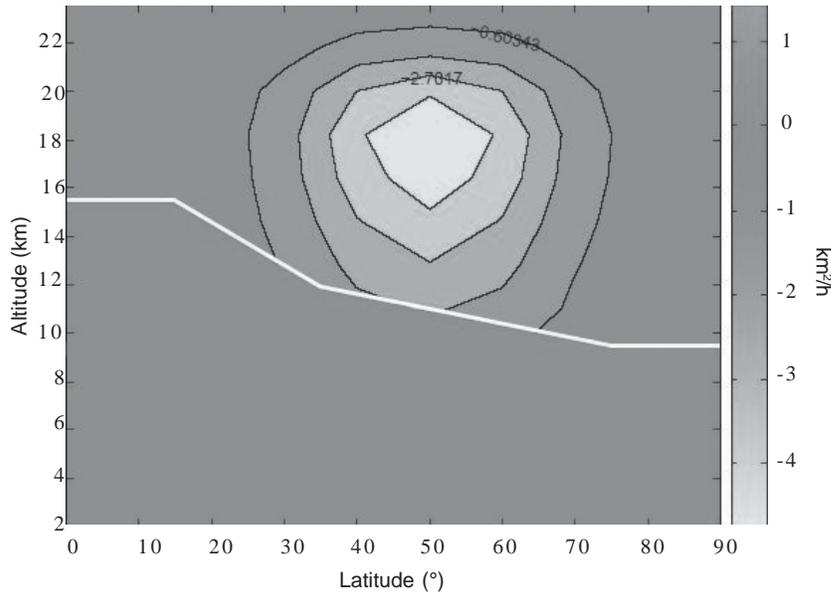


Fig. 1. The eddy diffusion coefficient L in km^2/h . The white line represents the tropopause.

We concentrate in two cases, namely an upward flow with $\kappa = 0$ and the boundary conditions (9) and (10) with $k_z = 5 \times 10^{-4} \text{ km/h}$ (modeling CFC flow) and a downward flow with $\kappa = 4 \times 10^{-4} \text{ h}^{-1}$ and boundary conditions (9) and (11) with the “absorption” coefficient at the lower boundary $k_b = -3.5 \times 10^{-3} \text{ km/h}$ (modeling ClO_x flow). In both cases the prescribed boundary flux density is normalized to ± 1 .

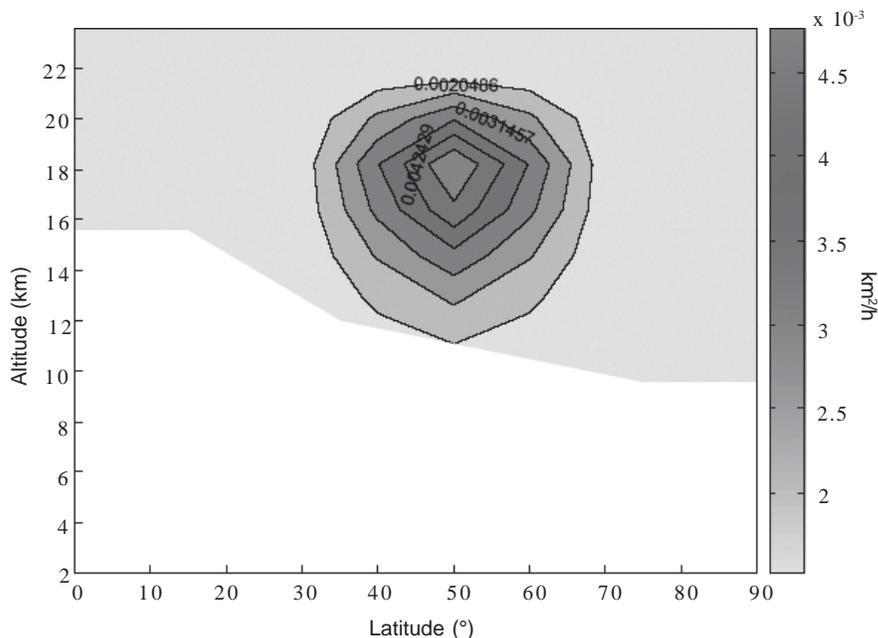


Fig. 2. The eddy diffusion coefficient M in km^2/h ; the white colour represents the value 3×10^2 .

Stationarity is achieved by applying (14) over a sufficiently large time interval, until the computed values do no longer change significantly in time (nearly 19,000 iterations were needed in the “CFC case” and nearly 30,000 iterations were needed in the “ ClO_x case”). We shortly describe how the discrete solutions look like: In the “CFC case”, along vertical lines, the mixing ratio decays upwards in a nearly piecewise linear fashion, from values near 9 units at the lower boundary to values near 2 units at the upper boundary, with rather small differential quotients in the troposphere (0.05 units per km near the equator to 0.04 units near the pole), and larger ones in the stratosphere (from 0.8 to 0.5 units per km); along horizontal levels one sees a maximum of the mixing ratio at the tropopause. In the “ ClO_x case” there is an exponential decay downwards of the tracer’s mixing ratio by factors between 0.5 per km (near the equator) and 0.6 per km (near the pole). In the troposphere the decay is much smaller (from 0.85 to 0.9 per km); along horizontal levels one sees a minimum of the mixing ratio at the tropopause.

Since the exact solutions are not known, we improve the numerical approximations by reducing the step sizes to $\Delta y/3$ and $\Delta z/3$ first and to $\Delta y/9$ and $\Delta z/9$ then, and estimate errors by comparison to the next more accurate case. Differences in percentage from the discrete solutions for the downward flow are shown in Figure 3 and Figure 4, and for the upward flow in Figure 5.

In observing the errors shown in Figures 3, 4 and 5, it should be kept in mind that these are global errors as propagated from their source points to the point considered in the figure and do not simply reflect the local errors at the points of the grid. In the 1-D case, by evaluating Green’s function and relating it to the solution, in the “ ClO_x case”, one can show also theoretically (see Appendix), that

locally generated relative errors are propagated essentially downwards whereas the influence upwards decreases exponentially. In the “CFC case” the relative influence is rather constant downwards and weakly decreasing upwards. We observe a similar behavior in the 2-D case.

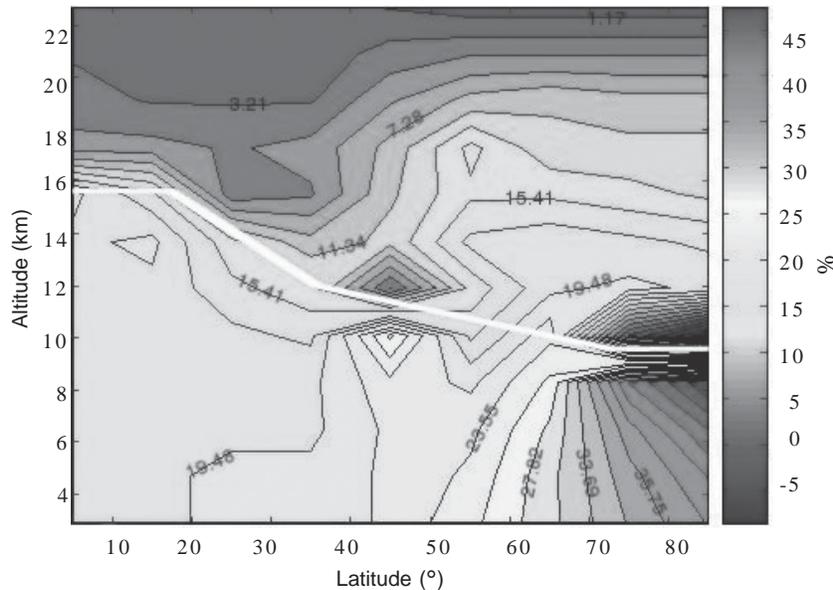


Fig. 3. Difference in percentage from the approximations of the stationary solutions of equations (5), (9) and (11) (ClO_x -case) computed with stepsizes $\Delta\phi = 10^\circ$, $\Delta z = 1.8$ km versus the case with $\Delta\phi = 10^\circ/3$ and $\Delta z = 0.6$ km. The white line represents the tropopause.

A consequence of this behavior is that, in spite of the fact that relative local errors are much larger in the stratosphere than in the troposphere because of larger variability of the solution there, the maximum of relative global errors lies in the troposphere where all errors propagated into.

5. Conclusions

The examples treated with our simplified model suggest that an upward flow without chemical reactions as typical for CFC, is rather insensitive to the large gridsize of the conventional treatment of the tropopause region (Fig. 5).

For a downward flow with reaction, as typical for ClO_x , large relative errors will occur already in the lower stratosphere (Fig. 3), since the equilibrium between diffusion and chemical destruction leads to a nearly exponential distribution of the mixing ratio in which the values in vertically neighboring cells differ by a factor between 2 and 4, in our example. If this is to be avoided, shortening of the meshsize is necessary (Fig. 4).

We conclude that for some tracers the jump of the coefficients at the tropopause can introduce remarkable errors in the discretizations, which propagate mainly into the troposphere.

In order to study the exchange processes at the tropopause, or, the impact of aircraft emissions, a careful numerical treatment of the jump effects near the tropopause must be achieved in the models; either shortening of the meshsize, or, a completely consistent treatment as in the Ritz-Galerkin finite element solution, eventually with triangular elements, may be the better way.

Finally, we conclude that even if we agree that important uncertainties of air chemistry models stem from the performance of the underlying dynamical model (Austin *et al.*, 2003), it must also be kept in mind, that the numerical treatment itself can introduce significant errors in the models output if the gridsize is not chosen adequately.

Further work should treat extensions of our simple model by introducing advection with a realistic meridional circulation, including spherical geometry and variable air density. Also the spatial-seasonal variation of eddy diffusion has to be taken into account in order to achieve a realistic picture.

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Appendix: The 1-D case

The only dimension considered here is the altitude z . The vertical exchange coefficient M is called K in this case. The subscript S refers to the stratosphere, whereas T refers to the troposphere. The lower boundary of the domain is $z = 0$ or $z = 2$ km respectively, the tropopause is assumed to be at $\bar{z} = \bar{z}_{Tp} = 9$ km or $\bar{z} = \bar{z}_{Tp} = 11$ km, and the upper boundary of the domain is at $z = Z = 21.6$ km or $z = 23.6$ km. The values used for the exchange coefficients are $K_S = 1.5 \times 10^{-3}$ km²/h and $K_T = 3 \times 10^{-2}$ km²/h.

We further introduce the thicknesses of the stratosphere and of the troposphere: $H_S = Z - z_{Tp} = 12.6$ km and $H_T = z_{Tp} = 9$ km. The chemical reaction constant is $\kappa = 4 \times 10^{-4}$ /h in the ClO_x case (as with 2-D), and $\kappa = 0$ in the CFC case. The upper and lower boundary conditions are the same as in the 2-D case. From the differential equation there result the exponential coefficients for the solution: $\mu_S = \sqrt{\kappa/K_S} = 0.516$ and $\mu_T = \sqrt{\kappa/K_T} = 0.1155$. The boundary value problem can be solved exactly.

For the mixing ratio u we obtain in the ‘‘ClO_x case’’ the following solution:

$$u(z) = \begin{cases} A_S \exp(\mu_S (z - z_{Tp})) + B_S \exp(-\mu_S (z - z_{Tp})) & \text{if } z \geq z_{Tp} \\ A_T \exp(\mu_T (z - z_{Tp})) + B_T \exp(-\mu_T (z - z_{Tp})) & \text{if } z \leq z_{Tp} \end{cases}$$

The constants are given by $A_S = 1.938$, $B_S = -1.231$, $A_T = 0.707$, $B_T = -4.42 \times 10^{-4}$. At the upper boundary, the B_S -term can be neglected and we obtain $u(Z) = 1.291 \times 10^3$. Going downward we observe a fast decline of the solution corresponding to the A_S -term until near the tropopause where the B_S -term comes into play. At the tropopause we have $u(z_{Tp}) = 0.707$, and then a slow decline until we reach $u(0) = 0.248$ at the lower boundary.

We now proceed to the Green's influence function $G(z; \zeta)$ from a unit source at $z = z_{Tp} + \zeta$. If the source is in the troposphere (i.e. $\zeta < 0$) we obtain

$$G(z, \zeta) = \begin{cases} A_S \exp(\mu_S (z - z_{Tp})) + B_S \exp(-\mu_S (z - z_{Tp})) & \text{if } z \geq z_{Tp} \\ A_{To} \exp(\mu_T (z - z_{Tp})) + B_{To} \exp(-\mu_T (z - z_{Tp})) & \text{if } z_{Tp} \geq z \geq z_{Tp} + \zeta \\ A_{Tu} \exp(\mu_T (z - z_{Tp})) + B_{Tu} \exp(-\mu_T (z - z_{Tp})) & \text{if } z - z_{Tp} + \zeta \end{cases}$$

with

$$A_S = \varepsilon_S B_S, A_{To} = 0.3883 * B_S,$$

$$B_{To} = 0.6117 B_S, B_{Tu} = \varepsilon A_{Tu}, \varepsilon = -6.25 \times 10^{-4}, \varepsilon_S = 2.25 \times 10^{-6}, B_S = D_1 A_{Tu} / C_1,$$

$$C_1 = 0.3883 \exp(\mu_T \zeta) + 0.6117 \exp(-\mu_T \zeta), D_1 = \exp(\mu_T \zeta) + \varepsilon \exp(-\mu_T \zeta),$$

$$A_{Tu} = 2.89 \times 10^2 / (D_2 + D_1 C_2 / C_1),$$

$$C_2 = -0.3883 \exp(\mu_T \zeta) + 0.6117 \exp(-\mu_T \zeta), D_2 = \exp(\mu_T \zeta) - \varepsilon \exp(-\mu_T \zeta)$$

Due to the dependence on ζ a further simplification is not possible. Note, however that $1 \geq \exp(\mu_T \zeta) \geq 0.353$ and $1 \leq \exp(-\mu_T \zeta) \leq 2.83$.

We observe that at the upper boundary the two terms are equal. Going downwards the B_S -term dominates and grows down to the tropopause. Also in the troposphere above the source point, the B_{To} -term dominates the A_{To} -term such that we have further growth there. Below the source point, however, the A_{Tu} -term is dominating causing a decrease of the function G downwards. This shows that the influence of an error in the troposphere relative to the solution remains about constant in the downwards direction whereas it declines in the upwards direction.

If the source is in the stratosphere (i.e. $\zeta > 0$) we obtain

$$G(z; \zeta) = \begin{cases} A_{So} \exp(\mu_S (z - z_{Tp})) + B_{So} \exp(-\mu_S (z - z_{Tp})) & \text{if } z \geq z_{Tp} + \zeta \\ A_{Su} \exp(\mu_S (z - z_{Tp})) + B_{Su} \exp(-\mu_S (z - z_{Tp})) & \text{if } z_{Tp} + \zeta \geq z \geq z_{Tp} \\ A_T \exp(\mu_T (z - z_{Tp})) + B_T \exp(-\mu_T (z - z_{Tp})) & \text{if } z \leq z_{Tp} \end{cases}$$

with

$$\begin{aligned} A_{So} &= \varepsilon_s B_{So}, B_T = \varepsilon A_T, A_{Su} = 4.476 \gamma_1 A_T, \\ B_{Su} &= -4.476 \gamma_2 A_T, \gamma_1 = 0.6119, \gamma_2 = 0.3887, \\ B_{So} &= 0.646 \times 10^3 \exp(\mu_s \zeta) - 0.410 \times 10^3 \exp(-\mu_s \zeta) \\ A_T &= 0.2358 \times 10^3 (\exp(-\mu_s \zeta) + \varepsilon_s \exp(\mu_s \zeta)). \end{aligned}$$

Again, a further simplification is not possible, but note that

$$1 \leq \exp(\mu_s \zeta) \leq 6.66 \times 10^2, \quad 1 \geq \exp(-\mu_s \zeta) \geq 1.50 \times 10^{-3}.$$

We have a similar behavior as in the case of the source point in the troposphere, but between the source point and the tropopause the function G is decreasing downwards. The statement about the relative error remains unchanged.

In the special case $\zeta = 0$ we can simplify:

$$G(z, 0) = \begin{cases} A_s \exp(\mu_s (z - z_{Tp})) + B_s \exp(-\mu_s (z - z_{Tp})) & \text{if } z \geq z_{Tp} \\ A_T \exp(\mu_T (z - z_{Tp})) + B_T \exp(-\mu_T (z - z_{Tp})) & \text{if } z \leq z_{Tp} \end{cases}$$

with

$$A_s = 5.31 \times 10^{-4}, \quad B_s = 2.36 \times 10^2 = A_T, \quad B_T = -0.1475.$$

This function declines from the tropopause height z_{Tp} to both sides exponentially. Relative to the solution of the original problem this means that the influence of an error at the tropopause remains constant down to the lower boundary whereas it declines very fast in the upward direction.

In the ‘‘CFC case’’, because of missing chemical reaction, the solution is piecewise linear. We have

$$u(z) = \begin{cases} A_s + B_s (z - z_{Tp}), & \text{if } z \geq z_{Tp} \\ A_T + B_T (z - z_{Tp}), & \text{if } z \leq z_{Tp} \end{cases}$$

From the simple differential equation, and the boundary and matching conditions we obtain $A_s = A_T = 1.04 \times 10^4$, $B_s = -6.67 \times 10^2$, $B_T = -3.33 \times 10^1$

and hence,

$$u(z=0) = 1.07 \times 10^4, u(z=z_{Tp}) = 1.04 \times 10^4, u(z=Z) = 0.2 \times 10^4.$$

The Green's function for this problem is treated with a similar ansatz, however splitted at the source point:

If $\zeta > 0$ then

$$G(z, \zeta) = \begin{cases} A_{So} + B_{So}(z - z_{Tp}), & \text{if } z \geq z_{Tp} + \zeta \\ A_{Su} + B_{Su}(z - z_{Tp}), & \text{if } z_{Tp} + \zeta \geq z \geq z_{Tp} \\ A_T + B_T(z - z_{Tp}), & \text{if } z \leq z_{Tp} \end{cases}$$

with

$$A_{So} = 1.04 \times 10^4, B_{So} = -6.67 \times 10^2, A_{Su} = 10.4 \times 10^3 - 0.667 \times 10^3 \times \zeta = A_T, B_{Su} = B_T = 0,$$

hence

$$G(0; \zeta) = G(z_{Tp}; \zeta) = G(z_{Tp} + \zeta; \zeta) = 10.4 \times 10^3 - 0.667 \times 10^3 \times \zeta, G(Z; \zeta) = 2.0 \times 10^3.$$

Relative to the above solution one sees that below the source point the influence of an error is reduced, the more the larger ζ , whereas above the source point it remains constant.

If $\zeta < 0$ then

$$G(z, \zeta) = \begin{cases} A_S + B_S(z - z_{Tp}), & \text{if } z \geq z_{Tp} \\ A_{To} + B_{To}(z - z_{Tp}), & \text{if } z_{Tp} + \zeta \geq z \geq z_{Tp} \\ A_{Tu} + B_{Tu}(z - z_{Tp}), & \text{if } z \leq z_{Tp} + \zeta \end{cases}$$

with

$$A_S = 10.4 \times 10^3 = A_{To}, B_S = -6.67 \times 10^2, B_{To} = -3.33 \times 10^1, A_{Tu} = 10.4 \times 10^3 - 0.033 \times 10^3 \times \zeta, B_{Tu} = 0,$$

hence

$$G(0; \zeta) = G(z_{Tp} + \zeta; \zeta) = 10.4 \times 10^3 - 0.033 \times 10^3 \times \zeta, G(z_{Tp}; \zeta) = 10.4 \times 10^3, G(Z; 0) = 2.0 \times 10^3.$$

Relative errors behave analogously to the case $\zeta > 0$, but the dependence on ζ is weaker. Eventually, for $z = 0$, we obtain

$$G(z, \zeta) = \begin{cases} A_S + B_S(z - z_{Tp}), & \text{if } z \geq z_{Tp} \\ A_T + B_T(z - z_{Tp}), & \text{if } z \leq z_{Tp} \end{cases}$$

with

$$A_S = 10.4 \times 10^3 = B_S = -6.67 \times 10^2, A_T = 10.4 \times 10^3, B_T = 0,$$

hence

$$G(0; 0) = G(z_{Tp}; 0) = 10.4 \times 10^3, G(Z; 0) = 2.0 \times 10^3.$$

We see that the relative error remains nearly constant over the whole domain.

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