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*Supplement of*

## **A revised dry deposition scheme for land–atmosphere exchange of trace gases in ECHAM/MESSy v2.54**

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# Additional information: Overview of MESSy/E5VDIFF to MESSy/VERTEX adaptations

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## S1 Calculation of neutral transfer coefficients

The neutral transfer coefficients for vertical diffusion in E5VDIFF are calculated in a simplified way:

$$S_{NH} = 2.22 \cdot 0.22 \cdot \sqrt{2} \approx 0.690702, \quad (S1)$$

$$S_{NM} = S_{NH} \cdot 1.24 \cdot \frac{2.37}{3.69} \approx 0.550091. \quad (S2)$$

5 which yields wrong results. However, according to the original work by Mellor and Yamada (1982) it is implemented in VERTEX as follows:

$$S_{NH} = 3\sqrt{2}A_2\gamma_1, \quad (S3)$$

$$S_{NM} = S_{NH} \frac{A_1}{A_2} \left( \frac{\gamma_1 - C_1}{\gamma_1} \right), \quad (S4)$$

$$= 3\sqrt{2}A_1(\gamma_1 - C_1), \quad (S5)$$

10 with  $A_1 = 0.92$ ,  $A_2 = 0.74$ ,  $C_1 = 0.08$ ,  $\gamma_1 = \frac{1}{3} - 2\frac{A_1}{B_1}$ ,  $B_1 = 16.6$  which would yield  $S_{NH} \approx 0.698519$  and  $S_{NM} \approx 0.556171$ .

## S2 Latent heat of vaporisation/sublimation

The latent heat of vaporisation/sublimation  $L_{v,s}$  is only determined based on the interpolated absolute temperature ( $ztmitte$ ) in VERTEX (instead of being interpolated itself) :

$$15 \quad L_{int.} = \begin{cases} L_v, & T_{int.} \geq 273.15 \text{ K} \\ L_s, & T_{int.} < 273.15 \text{ K} \end{cases} .$$

## S3 Calculation of convective transfer coefficient

In E5VDIFF, the transfer coefficient for heat  $C_H$  is calculated in two ways: “zchl” and “zcdh\_2d”. The latter, which is provided to the basemodel interface layer for further usage in other submodels (e.g. TROPOP), however incorporates an incorrect

20 calculation of air density<sup>1</sup>. Hence in VERTEX, the channel object “zcdh\_2d” is set to “zchl” weighted for land/water/ice fractions.

#### S4 Stored friction velocity

In the original code of E5VDIFF, the friction velocity  $u_*$  is calculated per domain (land/water/ice) and then weighted,  $f_l u_{*,l} + f_w u_{*,w} + f_i u_{*,i}$ . However, since  $u_*$  is rather a quantification of the second-order moments ( $-\overline{u'w'}$ ), the weighting should be  
 25 applied to  $u_*^2$ . Thus, in VERTEX,  $u_*$  is calculated by  $u_* = \sqrt{f_l u_{*,l}^2 + f_w u_{*,w}^2 + f_i u_{*,i}^2}$ .

#### S5 Roughness lengths in transfer coefficients

The exchange coefficients are determined by the stability functions for momentum and heat,  $f_{m,h}$ , and the neutral exchange coefficients as

$$C_{m,h} = C_{N_{m,h}} f_{m,h}. \quad (S6)$$

30 According to Roeckner et al. (2003)  $C_{N_{m,h}}$  is calculated as:

$$C_{N_{m,h}} = C_N = \frac{\kappa^2}{\ln\left(\frac{z_L}{z_{0m}} + 1\right) \ln\left(\frac{z_L}{z_{0h}} + 1\right)} \quad (S7)$$

and in the E5VDIFF code it is:

$$C_{N_{m,h}} = \left( \frac{\kappa}{\ln\left(\frac{z_L}{z_{0m,h}} + 1\right)} \right)^2 \quad (S8)$$

over land. However, according to the general theory,

$$35 \quad C_{N_{m,h}} = \frac{\kappa^2}{\ln\left(\frac{z_L}{z_{0m}} + 1\right) \ln\left(\frac{z_L}{z_{0m,h}} + 1\right)}, \quad (S9)$$

which is also how it is applied in the E5VDIFF code over water. Over ice it does not matter, since there  $z_{0m} = z_{0h}$ .

Thus, in VERTEX,  $C_{N_{m,h}}$  over land is used as in Eq. S9.

#### S6 Asymptotic mixing length calculation

The asymptotic mixing length  $\lambda$  is used for the  $l$  which is taken at the interface between grid cells. However, in E5VDIFF  $\lambda$  is  
 40 calculated using the (geopotential) heights of the centres of the grid cells. This is made consistent in VERTEX

<sup>1</sup>Instead of  $\theta_v = \theta(1 + 0.61q - qt)$ , effectively  $\frac{\theta}{1+0.61q}$  is used.

## S7 Diffusion of momentum

Before in E5VDIFF the vertical diffusion is applied, the ocean's speed is used to "correct" the momentum at (physically) the lowest level:  $\text{zudif}(j1, klev) = \text{ztpfac2} * (\text{pum1}(j1, klev) - \text{pocu}(j1) * (1. \_dp - \text{pfrl}(j1)))$ . However, this is a non-physical way to account for the surface velocity and yields wrong results if current velocities are provided.

For example, considering a column over an ocean with wind and ocean velocity both set to  $(1, 0) \text{ ms}^{-1}$ . This would lead to a  $\text{zudif}(j1, klev)$  of 0, which will lead to unwarranted deceleration of the other levels due to the diffusion.

Instead, in VERTEX the ocean's velocity is properly taken into account as boundary condition for the applied Richtmeyer and Morton scheme, see e.g. Schulz et al. (2001).

## 50 S8 Calculation of roughness length over sea

Considering the updates of Sect. S7<sup>2</sup>, the roughness length over sea is calculated in E5VDIFF as

$$z_0 = \frac{0.018u_*^2}{g} \approx \frac{0.018C_M |U^{t-1} - U_{\text{ocean}}^{t-1}| |\tilde{U}|}{g}, \quad \tilde{U} = U^{t+1} + \frac{U^{t+1} - U^{t-1}}{2}, \quad (\text{S10})$$

where  $U = (u, v)$  is the wind velocity (vector) in the lowest grid cell, except for  $U_{\text{ocean}}$ , which is the ocean's surface velocity. However, to be consistent the absolute wind vector magnitude should always be considered compared to the surface, i.e.

55  $|U - U_{\text{ocean}}|$  instead of  $|U|$ , and the time of evaluation should be consistent. Therefore, in the code of VERTEX the roughness length is calculated as

$$z_0 = \frac{0.018u_*^2}{g} = \frac{0.018C_M |U^{t-1} - U_{\text{ocean}}^{t-1}|^2}{g}. \quad (\text{S11})$$

## S9 Calculation of momentum flux

Similar to Sect. S8, the momentum flux in E5VDIFF (i.e. wind stress) is calculated using inconsistent variables. For all surfaces

60 this is:

$$-\rho \overline{u'_i w'} = \rho C_M |U^{t-1} - U_{\text{surf}}^{t-1}| \tilde{u}_i, \quad (\text{S12})$$

$$= \rho \frac{u_*^2}{|U^{t-1} - U_{\text{surf}}^{t-1}|} \tilde{u}_i, \quad (\text{S13})$$

$$= \rho |\overline{U' w'}| \frac{\tilde{u}_i}{|U^{t-1} - U_{\text{surf}}^{t-1}|}. \quad (\text{S14})$$

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<sup>2</sup>Otherwise even more issues are present.

Here,  $U_{\text{surf}}$  is equal to  $0 \text{ m s}^{-1}$  over land and to  $U_{\text{ocean}}$  elsewhere (ocean/ice). However, to be consistent the wind stress should

65 be

$$-\rho \overline{u'_i w'} = \rho |\overline{U' w'}| \frac{u_i^{t-1} - u_{i,\text{surf}}^{t-1}}{|U^{t-1} - U_{\text{surf}}^{t-1}|}, \quad (\text{S15})$$

$$= \rho C_M |U^{t-1} - U_{\text{surf}}^{t-1}| (u_i^{t-1} - u_{i,\text{surf}}^{t-1}). \quad (\text{S16})$$

In the code of VERTEX, it is applied as such.

### S9.1 Kinematic heat and moisture fluxes

70 The kinematic heat fluxes are calculated like this:

$$\frac{LE}{\rho L_v} \neq \frac{L_v (f_l \overline{w' q'_l} + f_w \overline{w' q'_w} + f_i \overline{w' q'_i}) + L_s \overline{w' q'_{l,\text{sublimation}}}}{\rho L_v}, \quad (\text{S17})$$

which, however, contains two mistakes. First, the calculated density has similar shortcomings as those mentioned in Sect. S3.

Second, the kinematic moisture flux should be equal to  $\frac{LE}{\rho L_v}$ , which amounts to

$$\frac{LE}{\rho L_v} = \frac{f_l (L_v (\overline{w' q'_l} - \overline{w' q'_{l,\text{sublimation}}}) + L_s \overline{w' q'_{l,\text{sublimation}}}) + f_w L_v \overline{w' q'_w} + f_i L_s \overline{w' q'_i}}{\rho L_v}. \quad (\text{S18})$$

75 Like this the kinematic heat and moisture fluxes have been implemented in VERTEX.

### S9.2 Calculation of 2 m values

Due to the changes in Sect. S5, the calculation of the 2 m temperature and humidity are not valid any more over land. For the calculation  $\frac{\kappa}{\sqrt{C_{NH}(2\text{m})}}$  is used, which is calculated as

$$\frac{\kappa}{\sqrt{C_{NH}(2\text{m})}} = \ln \left( 1 + \left( e^{\sqrt{C_{NH}(z_{ref})}} - 1 \right) \frac{2}{z_{ref}} \right). \quad (\text{S19})$$

80 Originally (i.e. in E5VDIFF), this was right, as  $C_{NH}$  was defined as  $C_{NH} = \left( \frac{\kappa}{\ln\left(\frac{z_{ref}}{z_{0h}} + 1\right)} \right)^2$  (see Sect. S5), so that the right-hand side of Eq. S19 is equal to

$$\begin{aligned} \ln \left( 1 + \left( e^{\sqrt{C_{NH}(z_{ref})}} - 1 \right) \frac{2}{z_{ref}} \right) &= \ln \left( 1 + \left( e^{\ln\left(\frac{z_{ref}}{z_{0h}} + 1\right)} - 1 \right) \frac{2}{z_{ref}} \right) \\ &= \ln \left( 1 + \frac{2}{z_{0h}} \right) \\ &= \frac{\kappa}{\sqrt{C_{NH}(2\text{m})}}. \end{aligned}$$

85 However, since in VERTEX Eq. S9 is applied, this mathematical trick is no longer possible. Instead, in the updated code

$\frac{\kappa}{\sqrt{C_{NH}(2\text{m})}}$  over land is directly calculated as

$$\frac{\kappa}{\sqrt{C_{NH}(2\text{m})}} = \sqrt{\ln\left(\frac{2}{z_{0m}} + 1\right) \ln\left(\frac{2}{z_{0m,h}} + 1\right)}, \quad (\text{S20})$$

consistent with Eq. S9.

Note that for the calculation over water,  $\frac{\kappa}{\sqrt{C_{NM}(z)}}$  is used as basis (i.e.  $\ln\left(\frac{z}{z_{0m}} + 1\right)$  instead of  $\sqrt{\ln\left(\frac{z}{z_{0m}} + 1\right) \ln\left(\frac{z}{z_{0h}} + 1\right)}$ ),

90 so that this is not a problem there. Over ice,  $z_{0m} = z_{0h}$ .

## S10 Calculation of 10 m values

Unlike the variables in Sect S9.2, in E5VDIFF only momentum is evaluated at 10 m height, so that only  $C_M$  is used instead of  $C_H$ . However, (also over water and ice) the velocities at 10 m height are interpolated assuming a non-moving surface. In VERTEX, this has been corrected to account for the ocean's surface velocity.

### 95 S10.1 Place of calculation of heat transfer coefficients and friction velocity at 2 m

The heat transfer coefficients and friction velocity at 2 m are calculated in the subroutine '*e5vdifffvdiff2*' of E5VDIFF. As a result modules for e.g. emission and deposition made use of those values at the previous time step (just before applying vertical diffusion). In VERTEX this is remedied by moving the calculations to '*vertex\_vdiff1*'.

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