

## RC LACE Stay Report

Topic: Bug correction in the ACDIFV3 routine

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### 1 INTRODUCTION

TOUCANS (Third Order moments Unified Condensation Accounting and N-dependent Solver for turbulence and diffusion) is a compact turbulence parameterization, used in the ALARO-1 physical package [1], [2].

One of its features is the parameterization of third order moments, used to calculate their contribution to turbulent fluxes of moisture ( $\overline{w'q'_T}$ ) and static energy ( $\overline{w's'_{sL}}$ ). In the code, this calculation is done in the `ACDIFV3` routine. There are known bugs in this routine, which have already been investigated in previous stays [4], [5]. In these stays, some new bugs were also discovered. It was found out that all of these bugs, when corrected, have little impact on results and stability of the solver, except one. The problematic bug is in an auxiliary variable `ZZZ` of the `ACDIFV3` routine, which should not be divided by the time step (`TSPHY` in code). When this bug is corrected, the solver becomes unstable and crashes the model after two steps of forecast for all tried cases.

### 2 SOLVER STABILITY

Before the stay, I revised the theory leading to the solver Eqs. (249)-(256) in TOUCANS documentation [3]. Some minor inconsistencies were found, which should be investigated further, but should not influence the stability of the solver.

Comparing equations to the code, which was done in [5], the only thing that was not tried is the inclusion of the time term ( $A_t$  in the documentation), which is not implemented in the code, but is present in the equation in the documentation.

The time term can be eliminated theoretically if we assume  $s_{sL}^* = s_{sL}^+$ , as shown in [5]. The value of  $s_{sL}^*$ , a solution for the intermediate solver step, is not explicitly determined in

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TOUCANS documentation, so the mentioned assumption was taken to be true, and the code was left as is, without the time term.

After theory revision and discussion, we realized that the correct expression should be  $s_{sL}^* = s_{sL}^{loc}$ . This makes more sense, as  $s_{sL}^*$  is an intermediate solution of the solver, and  $s_{sL}^{loc}$  is the local downgradient solution calculated before inclusion of TOMs. This means that the equations in the documentation are correct, but the code is not (see [5]), so the time term should be implemented.

(Note: Wherever  $s_{sL}$  is mentioned, it is implied that the same reasoning applies also to  $q_T$  equations.)

The time term  $A_t$  (in the code, ZAT on full levels and ZATH on half-levels) is expressed as (see [3]):

$$A_t = - \overbrace{K_H'' T_H''}^{\hat{\quad}} \frac{1}{e_k},$$

where averaging to full and half levels is also taken into account (the "overbrace" operator ( $\overbrace{\quad}$ ) averages to full levels and the "hat" operator ( $\hat{\quad}$ ) to half levels).  $T_H''$  is a stability function obtained when TOMs are also taken into account (PTH\_FUN in the code).  $K_H''$  is the exchange coefficient in the moist case (ZKTROV in the code).

With already existing variables in the code, the time term was implemented as:

```
ZATH (JLON, JLEV) =
    (PAPHIF (JLON, JLEV) - PAPHIF (JLON, JLEV+1)) *
    ZKTROV (JLON, JLEV) * PTH_FUN (JLON, JLEV) * ZITKE (JLON, KLEV) /
    (RG * ZRHO (JLON, JLEV))

ZAT (JLON, JLEV) =
    PALPH (JLON, JLEV) * ZATH (JLON, JLEV-1) / PLNPR (JLON, JLEV) +
    (1.0_JPRB - PALPH (JLON, JLEV) / PLNPR (JLON, JLEV)) * ZATH (JLON, JLEV)
```

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To see if this term can help the stability of the solver, we first verified that it is everywhere positive. If we write expressions for elements of the  $j$ -th row of the tridiagonal solver matrix with variables from the code, including the time term, we get (see [5] for equations without time term):

$$\begin{aligned} a_j &= -Z_j K_{j-1} + P_j T_{j-1}^-, \\ b_j &= 1 + \frac{A_t}{\delta t} + Z_j (K_{j-1} + K_j) - P_j (T_j^- - T_j^+), \\ c_j &= -Z_j K_j - P_j T_{j+1}^+, \end{aligned}$$

where  $Z = \text{ZIPOI}$ ,  $K = \text{ZKTROV2}$ ,  $P = \text{PRDEL P}$ ,  $T^- = \text{ZXSTAM}$ ,  $T^+ = \text{ZXSTAP}$ ,  $A_t = \text{ZAT}$  and  $\delta t = \text{TSPHY}$ .  $b$  is the element of the main diagonal and  $a$  and  $c$  are the elements of the other two diagonals.

In order for the solver to be stable, the matrix has to be positive definite (diagonally dominant), so:

$$(1) \quad d_j = |b_j| - |a_j| - |c_j| > 0,$$

should hold for every  $j$ . As the time term is everywhere positive and only adds to the main diagonal ( $b_j$ ), it should increase the solver stability.

After running experiments with the time term included, the model still crashed, but ran for more timesteps. After more investigation, we discovered that the remaining instability was caused by terms  $\text{ZITKE} = \frac{1}{e_k}$  and  $\text{ZITAU2TKE} = \frac{\tau^2}{e_k}$  which have TKE ( $e_k$ ) in the denominator.

Since TKE is limited from below to  $10^{-8}$ , these terms can attain very large values which are then reflected in the variables present in the solver. These large values then cause big jumps in the diagonal dominance variable  $d$  in equation (1), which can drop below zero. To correct that, we limited TKE in the `ACDIFV3` to  $10^{-4}$ , by limiting the `ZFTKE` variable in the code.

If we ran experiments with both time term included and TKE values limited, the solve was numerically stable for 24 hours of forecast. It is important to note that both corrections have to be made to achieve stability, either one or the other correction alone is not enough.

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Experiments were performed on the same cases as the ones before the addition of the time term. One case is a predominantly dry case from 7 Sep 2023 with strong dry convection and the second a moist convective case from 24 June 2022. Both were numerically stable for 24 hours of forecast.

To illustrate the effect of the time term addition on solver's numerical stability, we drew a profile of minimums the  $d$  variable for each vertical level (Fig. 1) for: (i) the reference experiment with cleaned version of `ACDIFV3` from cycle 47t1 (A101), (ii) experiment with corrected bugs except for the `ZZZ` bug (A102) and (iii) experiment with all bugs corrected, added time term and stricter lower limit for TKE (A103). For experiment A103, a good stability behaviour can be seen, closer (but not too close to) zero in the PBL where turbulent fluxes have larger values, and 1 (a diagonal matrix), in the upper atmosphere, where turbulent fluxes are zero. The other experiments remain very close to 0 for most levels, which leads to an unstable situation. There is an anomaly on level 86, which does not seem to affect the overall stability, but should be investigated.

To see the impact, we can look at the distributions of values of TOMS contributions to static energy flux and values of the same flux before the `ACDIFV3` routine (the local value) (Fig. 2). TOMS contributions are a few percent of the whole flux, but are still about 50 times bigger than in the reference version (not shown). The contributions also have a systematic effect, which can be seen if we draw the difference of new and old TOMS contributions on the surface level (`KLEV`) after 15 hours of forecast (Fig. 3).

### 3 DIFFUSION OF CONSERVATIVE VARIABLES

During the investigation, it was noticed that in the calculations of diffusion of conservative variables under the `LDIFCONS` switch, which is present in the `ACDIFV3` routine, fluxes of static energy and moisture are not updated on the surface level. An experiment was prepared where the fluxes are also updated on the surface level, which includes also a section of code under the `LDIFCONS` switch in the `ARP_GROUND_PARAM` routine, but the impact was not yet properly investigated.

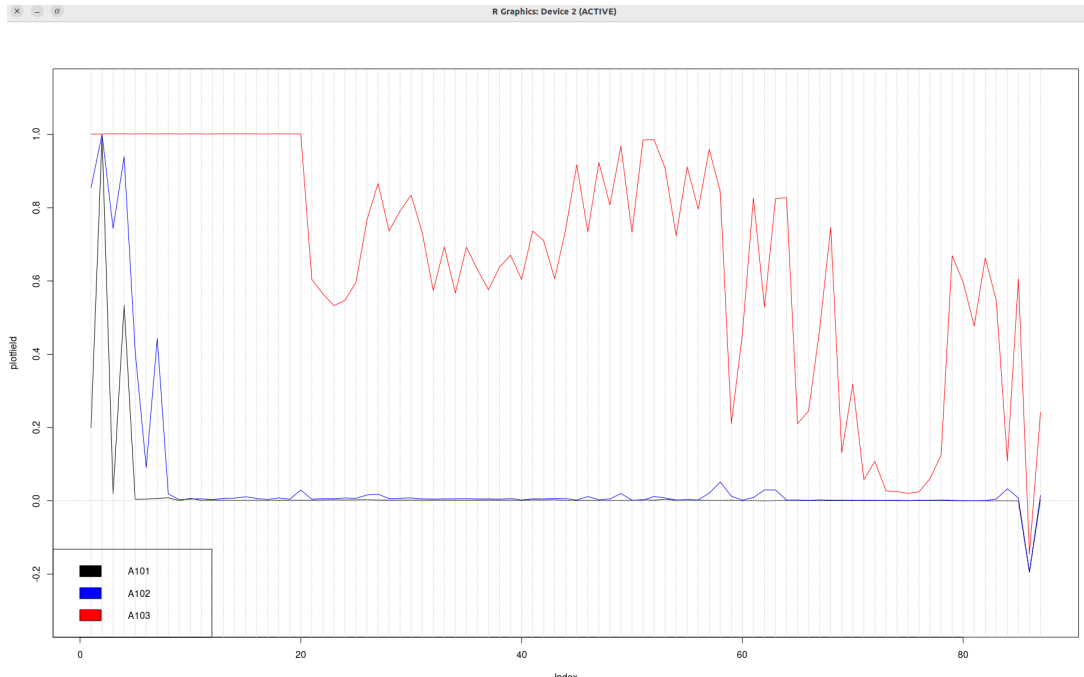


FIGURE 1. Solver stability on height levels after 1 hour of forecast of the dry case.

#### 4 FURTHER WORK

Further work to be done:

- Finish the revision of theory,
- Investigate the anomaly on level 86,
- Investigate the impact of updating of static energy and moisture fluxes on the surface level under LDIFCONS switch,
- Study of TOMs impact in the well mixed PBL below capping cloud layer, in order to check their ability to maintain turbulent transport in no-gradient conditions.
- Study of TOMs counter-gradient effects on an atmospherically stable case.

For great help and discussions during the stay I would like to thank J. Mašek and M. Hrastinski and the whole Czech team for making the stay a pleasant one.

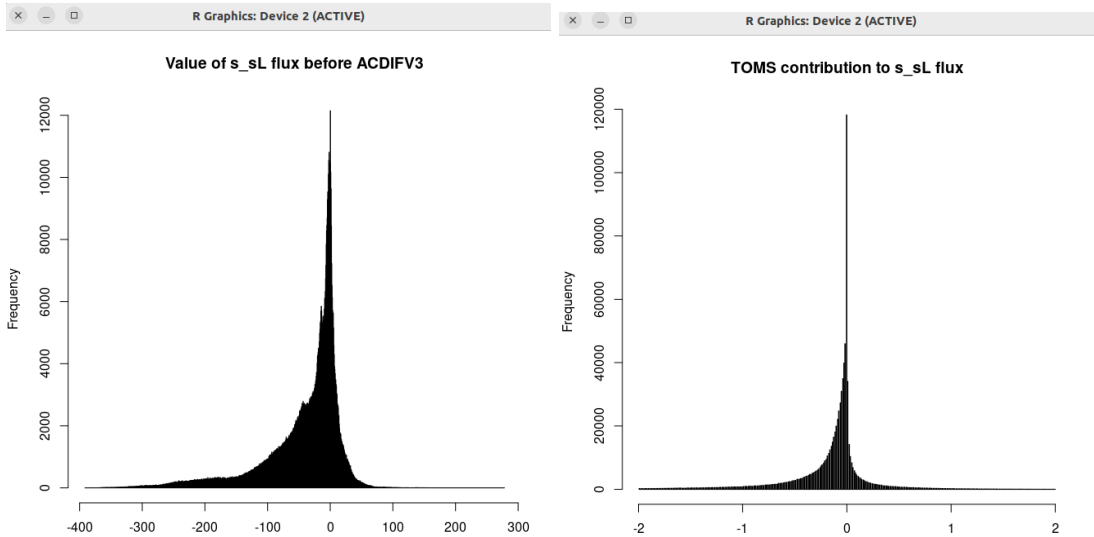


FIGURE 2. Distributions of values of local static energy flux (left) and TOMS contributions to static energy flux (right) in units of  $\frac{m^3}{s^3}$  after 15 hours of forecast of the dry case.

## REFERENCES

- [1] I.Bašták-Ďurán, J.-F.Geleyn, F.Vaña, *A compact model for the stability dependency of TKE production-destruction-conversion terms valid for the whole range of Richardson numbers.*, JAS, 71(8), 3004-3026 (2014).
- [2] I.Bašták-Ďurán, J.-F.Geleyn, F.Vaña, J.Schmidli, R.Brožkova, *A turbulence scheme with two prognostic energies.*, JAS, 75(10), 3381-3402 (2018).
- [3] I.Bašták-Ďurán, *TOUCANS documentation*, 15. July 2015.
- [4] P.Smerkol, *Debugging TOMs routine in TOUCANS.*, RC-LACE stay reports, 2016-2019.
- [5] P.Smerkol, *Derivation of TOMs solver.*, RC-LACE addendum to stay report, 2017.

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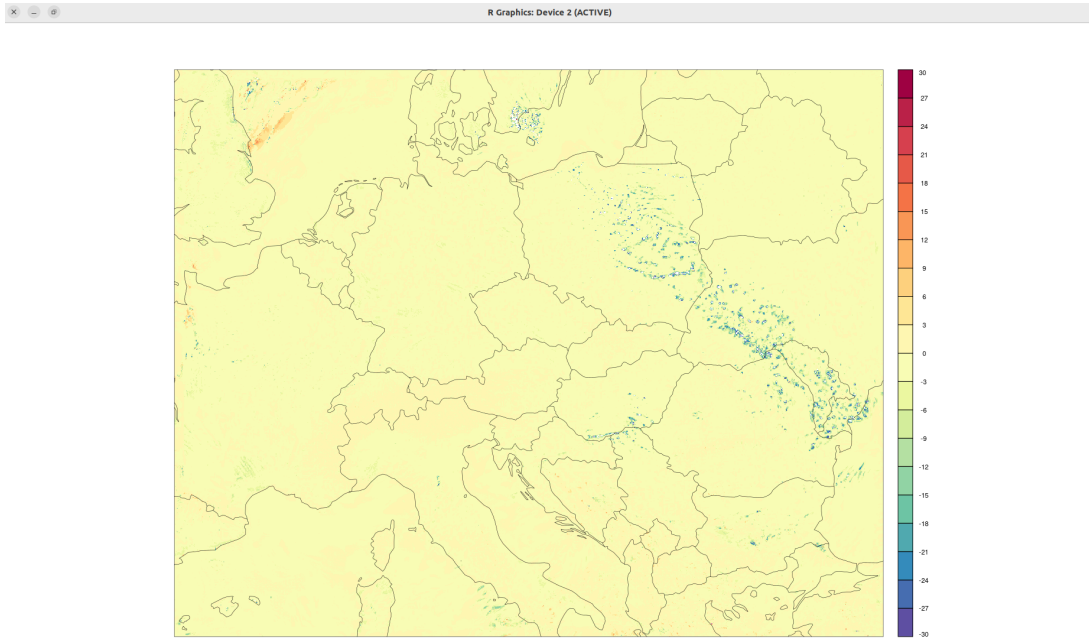


FIGURE 3. Difference of new and old TOMS contributions to static energy in units of  $\frac{m^2}{s^2}$  after 15 hours of forecast on KLEV.