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Implementation of a positive definite mass-flux scheme and a method for removing the negative tracers in the NCEP GFS planetary boundary layer and cumulus convection schemes

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Abstract

A positive definite mass-flux transport scheme and a method for removing negative tracer mixing ratio values have been implemented into the NCEP GFS planetary boundary layer and cumulus convection schemes. The unrealistic negative values caused by either the discretization scheme or numerical artifacts have been successfully removed with no adverse impacts on the GFS weather forecasts.

1. Introduction

It has been known that discretization approaches based on central differencing in numerical advection schemes can produce negative values for positive definite tracer mixing ratios. To eliminate negative values for water vapor and cloud water in the operational National Centers for Environmental Prediction's (NCEP) global spectral weather forecast model, Yang et al. (2009a,b) adopted the total variation diminishing (TVD) flux-limited scheme (Thuburn, 1993; Van Leer, 1974) for vertical advection of tracers, replacing the central differencing scheme. With the TVD scheme, most of the negative mixing ratio values for water vapor and cloud water were removed in the NCEP Global Forecast System (GFS).

As Yang et al. (2009a) have pointed out, there are other sources of negative tracer values. One of them is the mass-flux (MF) scheme in the GFS cumulus convection for the convective transport by updraft and downdraft. Since central differencing has been used for the MF scheme, negative water vapor mixing ratios can be generated from cumulus convection. In the current (as of 2021) operational convection scheme (Han and Pan, 2011; Han et al., 2017), ozone and turbulent kinetic energy (TKE) as well as water vapor are vertically transported by cumulus convection and significant negative values occurred for TKE and ozone. In addition, the current operational GFS (GFSv16) adopts a TKE-based moist eddy-diffusivity mass-flux (EDMF) planetary boundary layer (PBL) scheme (hereafter TKE-EDMF PBL scheme; Han and Bretherton, 2019), which can produce negative values for TKE, ozone, water vapor and hydrometeors due to the central differencing MF scheme. This scheme can also produce negative aerosol mixing ratios when aerosol vertical transport is included in the GFS convection and PBL schemes.

In this study we replace the central differencing scheme with the positive definite TVD scheme in the GFS cumulus convection and PBL MF schemes. We have found that, although the TVD scheme largely reduces the magnitude of negative tracer values, a significant magnitude of negative values is still generated. In this study, therefore, we also develop a method for removing the remaining negative tracer mixing ratio values while conserving the column integrated total tracer mass.

2. Positive definite TVD flux-limited scheme

The TVD scheme is applied to the flux form of the advection term. The flux form of the vertical advection for a tracer mixing ratio, q, can be written as

$$\frac{\partial q}{\partial t} = -\omega \frac{\partial q}{\partial p} = -\left(\frac{\partial \omega q}{\partial p} - q \frac{\partial \omega}{\partial p} \right) \quad (1)$$

where p is the pressure, $\omega = - \rho g w$, ρ is the air density, g is the gravity, and w is the vertical velocity. The numerical discretization of the right-hand side of Eq. (1) for the k layer (denoted as A_k) can be written as

$$A_k = \frac{1}{\Delta p_k}\left(\omega_{k-1/2} q_{k-1/2} - \omega_{k+1/2} q_{k+1/2}\right) - \frac{1}{\Delta p_k} q_k \left(\omega_{k-1/2} - \omega_{k+1/2}\right)$$

and $$\Delta p_k = p_{k-1/2} - p_{k+1/2} \tag{2}$$

where k-1/2 and k+1/2 are respective lower and upper half levels (with k increasing upward). The q at the lower half level in the central differencing scheme is given by

$$q_{k-1/2} = \frac{1}{2}\left(q_{k-1} + q_k\right) \tag{3}$$

The q at the upper half level for the central differencing scheme is similarly obtained.

The q at the lower half level for the upwind scheme is given by

$$q_{k-1/2} = \begin{cases} q_{k-1} & if\, \omega_{k-1/2} < 0 \\ q_k & if\, \omega_{k-1/2} \geq 0 \end{cases} \tag{4}$$

The upwind scheme is a positive definite scheme, but it is too diffusive and has a lower numerical accuracy.

The positive definite TVD flux-limited scheme was developed to be less diffusive and more numerically accurate than the upwind scheme. For the upward vertical motion (i.e., $\omega_{k\text{-}1/2} < 0$), q at the lower half level for the TVD scheme (Thuburn, 1993) is given by

$$q_{k-1/2} = q_{k-1} + \Phi^{-}_{k-1}\left(q^{H}_{k-1/2} - q_{k-1}\right)$$

and $$q^{H}_{k-1/2} = \frac{1}{2}\left(q_k + q_{k-1}\right) \tag{5}$$

where the anti-diffusive flux-limited term (Van Leer, 1974) is given by

$$\Phi^{-}_{k-1} = \frac{r^{-}_{k-1} + |\, r^{-}_{k-1}\,|}{1 + |\, r^{-}_{k-1}\,|}$$

and $$r^{-}_{k-1} = \frac{q_{k-2} - q_{k-1}}{q_{k-1} - q_k} = \frac{\Delta q_{k-2}}{\Delta q_{k-1}} \tag{6}$$

For the downward vertical motion (i.e., $\omega_{k-1/2} > 0$),

$$q_{k-1/2} = q_k + \Phi_k^+ \left(q_{k-1/2}^H - q_k \right)$$

and $$q_{k-1/2}^H = \frac{1}{2}\left(q_k + q_{k-1} \right) \qquad (7)$$

where the anti-diffusive flux-limited term is given by

$$\Phi_k^+ = \frac{r_k^+ + |\, r_k^+ \,|}{1 + |\, r_k^+ \,|}$$

and $$r_k^+ = \frac{q_k - q_{k+1}}{q_{k-1} - q_k} = \frac{\Delta q_k}{\Delta q_{k-1}} \qquad (8)$$

Fig. 1 shows values of initially positive tracer mixing ratio after some time integration with different advection schemes for an idealized case. The central differencing advection scheme is clearly shown to generate a negative value. Both upwind and TVD schemes do not produce negative tracers, whereas the TVD scheme is less diffusive and more accurate than the upwind scheme.

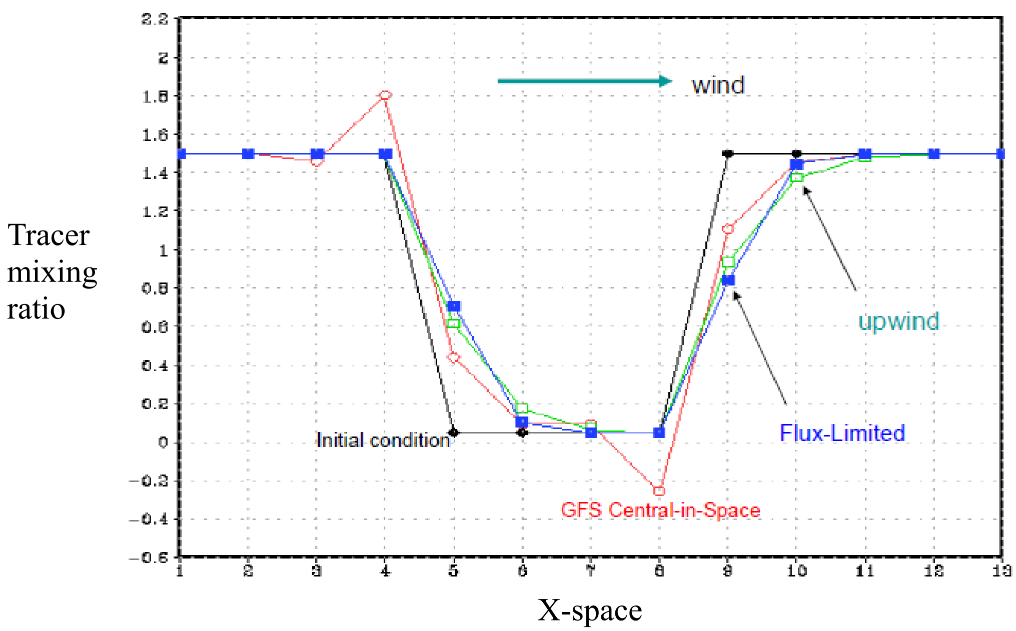

Fig. 1. Tracer mixing ratios after some time integration with different advection schemes for an idealized case. The black line represents the initial tracer mixing ratio with no negative value. The red, green, and blue lines mark results from the central differencing, upwind, and TVD advection schemes, respectively. [From Yang et al. (2009a).]

Assuming no external forcing, the change rate of a prognostic positive tracer variable due to turbulent diffusion and transport by updrafts and downdrafts in the PBL or convection schemes can be written as

$$\frac{\partial \overline{\phi}}{\partial t} = -\frac{\partial}{\partial z}\left(\overline{w'\phi'}\right) \quad (9a)$$

$$\overline{w'\phi'} = -K\frac{\partial \overline{\phi}}{\partial z} + M_u(\phi_u - \overline{\phi}) - M_d(\phi_d - \overline{\phi}) \quad (9b)$$

$$\frac{\partial \overline{\phi}}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial \overline{\phi}}{\partial z}\right) + \frac{\partial}{\partial z}\left((M_u - M_d)\overline{\phi}\right) + \frac{\partial}{\partial z}\left(-M_u\phi_u + M_d\phi_d\right) \quad (9c)$$

where ϕ is the positive definite tracer variable, w is the vertical velocity, overbars indicate horizontal averages across a grid cell, primes represent sub-grid scale fluctuations, K is the turbulent eddy diffusivity, M denotes the mass flux, and the subscript 'u' and 'd' refer to the updraft and downdraft properties, respectively. The first term in the right-hand side of Eq. (9c) is the turbulent diffusion term and exists only in the PBL scheme. The TVD scheme is applied to the second term in the right-hand side of Eq. (9c), which represents the vertical transport of the tracer by the MF. Note that one should use the combined updraft and downdraft MF for the TVD scheme where the half level value depends on the direction of the combined MF. The third term in the right-hand side of Eq. (9c) accounts for the divergence of parcel fluxes due to updrafts and downdrafts.

Fig. 2 displays the maximum and minimum values of the sub-grid TKE every 6 forecast hours over the globe from the GFS run using the TVD scheme compared to the control GFS run using the central differencing scheme.

Central		TVD	
max TKE	min TKE	max TKE	min TKE
37.01081	-2.91881	37.74255	-0.8153
63.64521	-2.188344	63.97289	-0.59283
84.49205	-2.677069	88.21877	-0.88441
147.0343	-2.362137	128.9055	-1.27692
166.4528	-2.26057	157.634	-0.67856
102.2713	-3.043875	98.10609	-1.97941

45.92924	-2.220357	47.97842	-0.87563
44.87528	-2.64257	45.23304	-0.88497
50.37382	-2.325083	60.52139	-0.98047
62.76791	-2.019215	73.22465	-0.4367
168.5564	-2.355599	61.29884	-0.75169
60.22577	-3.040793	71.64494	-0.7452
42.57714	-2.992054	41.48038	-3.09797
51.07372	-1.874743	40.58673	-0.72027
47.18581	-2.359504	33.16606	-0.52156
41.46842	-3.216556	56.3333	-0.66239
52.59673	-3.246931	42.22956	-0.80629
46.27276	-2.272117	51.83812	-0.5497

Fig. 2. Maximum and minimum values of sub-grid turbulent kinetic energy (TKE) every 6 forecast hours over the globe from the GFS run using the TVD scheme (right) compared to the control GFS run (left) using the central differencing scheme.

As shown in Fig. 2, the magnitude of the negative TKE is largely reduced with the TVD scheme, but small negative values still remained. It appears that the occurrence of small negative values is unavoidable even with the positive definite TVD MF scheme. This might be due to imbalances in the divergence of parcel fluxes [the third term in the right-hand side of Eq. (9c)] and vertically unequal grid sizes. Therefore, we develop a method of removing the remaining negative tracer values, which is described in the next session.

3. Development of a method for removing the negative tracers

Simply zeroing out the negative tracers can lead to mass conservation issues as it increases the total mass of the tracer with time (not shown). A method removing the negative tracer values while conserving the column integrated total tracer mass has been developed by borrowing tracer mass from other layers within the PBL or cumulus clouds after mass-flux transport. For each tracer, the amount of mass borrowed from a given layer is computed using the column-dependent ratio defined in Eq. (10):

$$Ratio = \frac{\int_{bot}^{top} \rho q_{neg} dz}{\int_{bot}^{top} \rho q_{pos} dz}, \quad Ratio < 0 \tag{10}$$

where 'bot' and 'top' denote bottom and top layers of the PBL or cumulus clouds, respectively, and the subscript 'pos' and 'neg' refer to the positive and negative values of the tracer mixing ratio (q), respectively. Then, the negative values are set to zero by borrowing the positive values from other layers as

do k=bot, top
  if (q(k) < 0), q(k)=0
  if (q(k) > 0), q(k)=(1+*Ratio*) * q(k)   (11)
enddo

where 'k' is the vertical index. In this way, the total tracer mass over the vertical column is conserved while removing the negative values. Note that for TKE the air density, ρ, is not multiplied in Eq. (10) because TKE is not a mixing ratio. Fig. 3 displays the maximum and minimum values of the sub-grid TKE every 6 forecast hours over the globe from the GFS run using both the TVD scheme and the method removing negative tracers [i.e., Eqs. (10) and (11)]. As shown in Fig. 3, the negative TKE values are now negligibly small and appear to be successfully removed.

Both TVD and	borrowing positive TKE
max TKE	min TKE
37.0415	-9.02E-17
64.40881	-6.59E-17
89.12389	-1.11E-16
151.9699	-2.08E-16
162.2496	-1.94E-16
105.492	-6.07E-17
46.84769	-1.98E-16
47.31166	-1.39E-16
58.40775	-1.13E-16
59.53362	-2.39E-16
49.4918	-1.80E-16
68.02324	-1.27E-16
46.55048	-1.07E-16
40.5466	-1.13E-16

68.66727	-2.19E-16
65.04642	-1.56E-16
52.83929	-1.04E-16
52.49757	-2.12E-16

Fig. 3. Maximum and minimum values of sub-grid turbulent kinetic energy (TKE) every 6 forecast hours over the globe from the GFS run using both the TVD scheme and the method removing negative tracers described in the text.

Although Eqs. (10) and (11) effectively remove negative tracer values, they also tend to reduce low cloud coverage when applied to the liquid water tracer because a portion of the liquid water contributing to low clouds is subtracted to compensate for the negative liquid water amounts in the lower layers below the low clouds. To address this issue, we first borrow liquid water from water vapor as

$$
\begin{aligned}
&\text{do k=bot, top}\\
&\quad \text{if } (q_l(\text{k}) < 0) \text{ then}\\
&\qquad tem = q_v(\text{k}) + q_l(\text{k})\\
&\qquad \text{if (tem>=0) then}\\
&\qquad\quad q_v(\text{k}) = tem\\
&\qquad\quad T(\text{k}) = T(\text{k}) - L_v/c_p * q_l(\text{k})\\
&\qquad\quad q_l(\text{k}) = 0\\
&\qquad \text{elseif } (q_v(\text{k}) > 0) \text{ then}\\
&\qquad\quad q_l(\text{k}) = tem\\
&\qquad\quad T(\text{k}) = T(\text{k}) + L_v/c_p * q_v(\text{k})\\
&\qquad\quad q_v(\text{k}) = 0\\
&\qquad \text{endif}\\
&\quad \text{endif}\\
&\text{enddo}
\end{aligned} \qquad (12)
$$

where q_v is the water vapor, q_l is the liquid water specific humidity, T is the temperature, c_p is the specific heat at constant pressure, and L_v is the latent heat of vaporization of water. Then, we borrow liquid water from the other layers if negative liquid water values are still present. With this method, the low cloud fields are similar to the control ones, while the negative water is removed. This method is also applied to negative rain water.

When mass-flux transport and eddy diffusion are simultaneously computed as in the current TKE-EDMF PBL scheme, the eddy diffusion process can leak the negative tracer values (which are caused by the MF scheme) out of the mass-flux transport layers. On the other hand, it has been found that small negative moisture values (order of -10^{-6}~-10^{-5} Kg/Kg) which are not related to the MF scheme occasionally occur mostly at the model 1st layers (and sometimes at the model 2nd and 3rd layers) under stable conditions. The negative values at the model 1st layers appear to be caused by downward surface latent heat fluxes slightly larger than downward moisture fluxes from the level just above during nighttime. Thus, in the final version of the TVD-based TKE-EDMF PBL scheme, negative tracer values produced by the mass-flux scheme are first removed by borrowing from the positive tracer values within the mass-flux transport layers, and additional negative tracers (leaked out of the mass-flux transport layers due to eddy diffusion or generated by downward surface flux imbalance during nighttime) are removed by borrowing from positive tracer values across the entire column layers. Negative liquid water and rain water are borrowed from the positive moisture at the same layers before borrowing from positive values at other model layers. In the operational GFS cumulus convection scheme, which has no MF transport for hydrometeors as well as no turbulent diffusion term, the TVD scheme and Eqs. (10) and (11) are applied only within the mass-flux transport layers to remove the negative tracer values. These methods, combined with the TVD scheme, allow to limit the magnitude of the generated negative tracer mixing ratios below 10^{-16}.

4. Medium-range forecast tests

To assess the impacts of the TVD scheme and the method removing negative tracer values on medium-range forecasts, 6-day forecasts at 00Z cycle every 5 days were conducted for the period of December 2, 2019 – February 29, 2020 using initial conditions from parallel runs performed with the operational GFSv16 model. The GFS used in this test has 127 vertical sigma-pressure hybrid layers with a model top of about 80 km and a horizontal grid spacing of about 13 km.

The control forecast is denoted by 'ccab07' and the experimental forecast using the TVD scheme and the method removing negative tracer values is denoted by 'ccab92'. Fig. 4 shows a comparison for the column integrated liquid and ice water path. Although the water path from the experimental forecasts is slightly smaller than that from the control forecasts, their distributions over the globe are very similar.

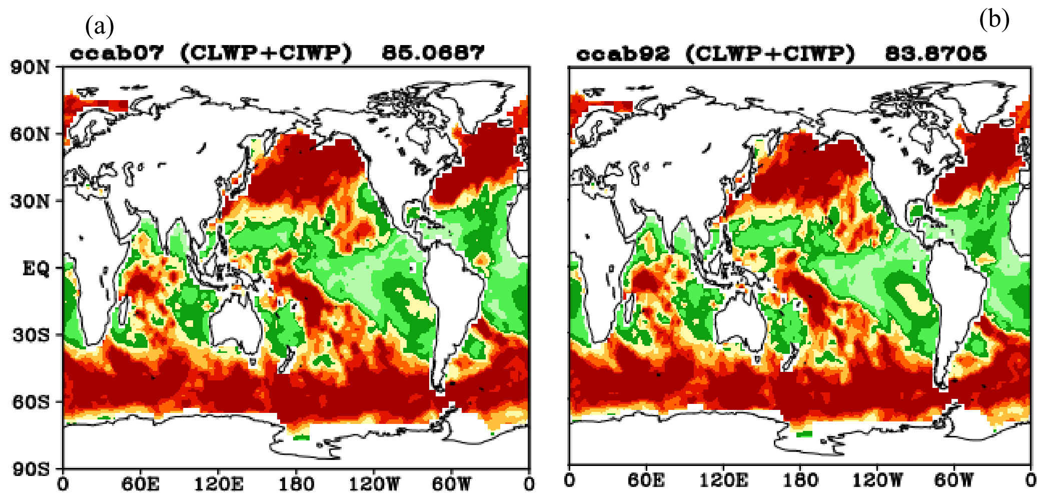

Fig. 4. Mean column integrated liquid and ice water path (g/m^2) for (a) the control forecasts and (b) the forecasts with the TVD scheme and method removing negative tracer values. The forecast period for the mean calculation is from 2 Dec 2019 to 29 Feb 2020, and the mean path is the average of 54, 60, 66, and 72 forecast hours.

Fig. 5 shows that the differences between the forecasts with the TVD scheme and method removing the negative tracer values (ccab92) and the control forecasts (ccab07) are generally very small, although the total cloud fraction is slightly smaller in ccab92 than in ccab07 while the surface downward short wave radiation flux is slightly larger in ccab92 than in ccab07.

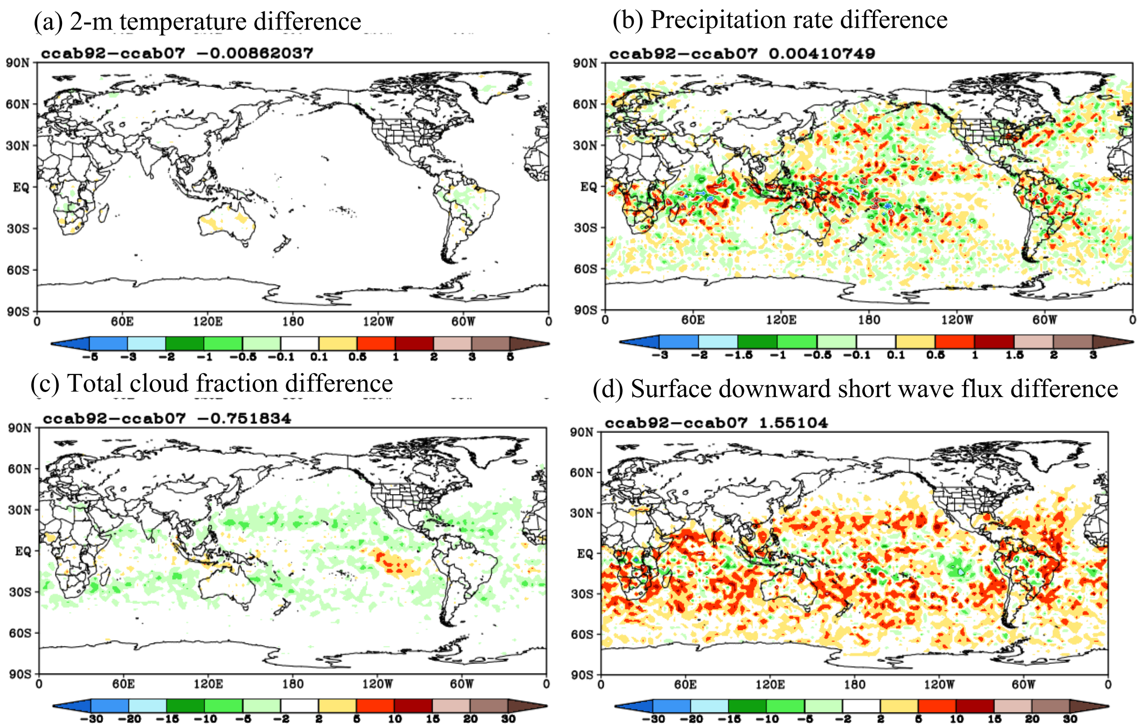

Fig. 5. As in Fig. 4, but for the mean differences between the forecasts with the TVD scheme and method removing the negative tracer values and the control forecasts of (a) 2-m temperature (K), (b) precipitation rate (mm/d), (c) total cloud fraction (%), and (d) surface downward short wave radiation flux (W/m^2).

A comparison of the 500 hPa height anomaly correlations – which illustrate how well synoptic scale systems are represented over the globe – is shown in Fig. 6 for northern (20ºN-80ºN) and southern (20ºS-80ºS) hemispheres. For both the northern and southern hemispheres, although the experimental forecasts display slightly better anomaly correlations than the corol forecasts, the improvements are statistically neutral.

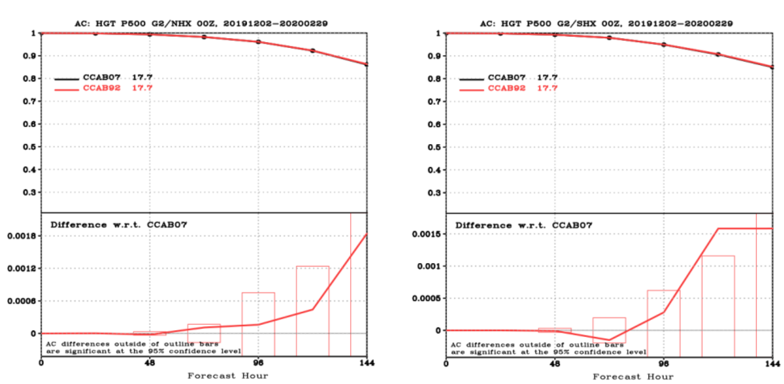

Fig. 6. Mean anomaly correlation of 500 hPa height and its difference (CCAB92 – CCAB07) for the forecasts with the TVD scheme and method removing negative tracer values (CCAB92) with respect to the control forecasts (CCAB07) in the (a) northern hemisphere (20º-80ºN) and (b) southern hemisphere (20º-

80ºS) from 2 Dec 2019 to 29 Feb 2020. The differences outside the rectangle bars are statistically significant at the 95% confidence level.

Fig. 7 displays the wind vector root mean square errors (RMSE) for the tropics (20ºS-20ºN) as a function of height and forecast hour. Compared to the control forecasts, the wind vector RMSE for the experimental forecasts is slightly increased in earlier forecast hours but slightly decreased in later forecast hours.

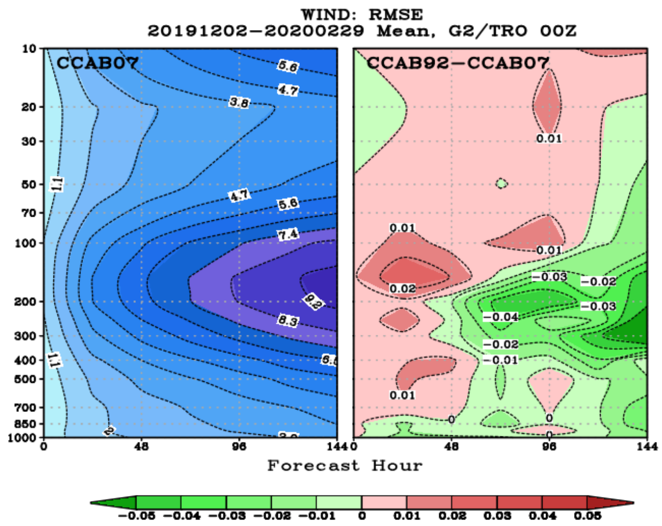

Fig. 7. Mean difference (CCAB92 – CCAB07) of wind vector RMSE over the tropics (20ºS-20ºN) for the forecasts with the TVD scheme and method removing negative tracer values (CCAB92) with respect to the control forecasts (CCAB07) from 2 Dec 2019 to 29 Feb 2020. Positive differences (red) are degradations and negative differences (green) are improvements.

Fig. 8 displays precipitation forecast skill comparison over the continental United States (CONUS), showing that the differences are very small also for the precipitation forecast skill. Figs. 4-8 indicate that the overall impacts of the TVD scheme and method removing the negative tracer values on the medium-range forecasts are very small.

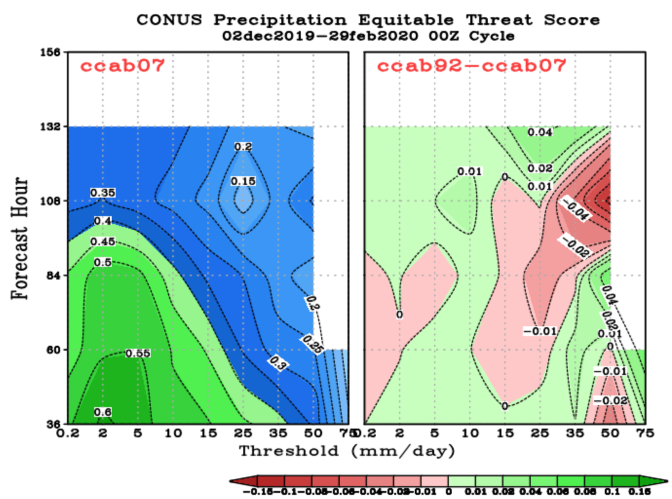

Fig. 8. Precipitation equitable threat score over the continental United States for the control forecasts (ccab07) and its difference (ccab92 – ccab07) for the forecasts with the TVD scheme and method removing

negative tracer values (ccab92) with respect to the control forecasts from 2 Dec 2019 to 29 Feb 2020. Positive differences (red) are degradations and negative differences (green) are improvements.

5. Summary

To eliminate the unrealistic negative tracer mixing ratios caused by the central differencing discretization in the MF schemes of the NCEP GFS PBL and cumulus convection schemes, a positive definite TVD scheme has been applied for the mass-flux transport of tracers including TKE, moisture and hydrometeors. Despite largely reducing the magnitude of negative tracer values, it appears that the occurrence of small negative values is unavoidable even with the positive definite TVD mass-flux scheme. This might be due to imbalances in the divergence of parcel fluxes and vertically unequal grid sizes. Simply zeroing out the negative tracers is not recommended because it can affect mass conservation, increasing the total tracer amount with time.

A method for removing negative tracer values has been developed by borrowing from positive tracer values at other layers within PBL or cumulus clouds after mass-flux transport. This method, however, tended to reduce low cloud coverage as liquid water mass is subtracted to compensate for the negative tracer values. Therefore, the method was updated for the liquid and rain water tracers to borrow from water vapor at the same layer first, then from other layers. Additional negative tracer values (leaked out of the mass-flux transport layers due to eddy diffusion or generated by unbalanced downward surface fluxes in stable conditions) are removed by borrowing positive tracer values across the entire column layers.

Medium-range forecasts using the TVD scheme and the method for removing negative tracers have been conducted. Their impacts on the GFS weather forecasts were small with no adverse impacts on the forecast skills.

Acknowledgments

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