Comment

Comment on 'Shang S. 2012. Calculating actual crop evapotranspiration under soil water stress conditions with appropriate numerical methods and time step. *Hydrological Processes* 26: 3338–3343. DOI: 10.1002/hyp.8405'

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Abstract:

A previous study analyzed errors in the numerical calculation of actual crop evapotranspiration (ET_a) under soil water stress. Assuming no irrigation or precipitation, it constructed equations for ET_a over limited soil-water ranges in a root zone drying out due to evapotranspiration. It then used a single crop-soil composite to provide recommendations about the appropriate usage of numerical methods under different values of the time step and the maximum crop evapotranspiration (ET_c). This comment reformulates those ET_a equations for applicability over the full range of soil water values, revealing a dependence of the relative error in numerical ET_a on the initial soil water that was not seen in the previous study. It is shown that the recommendations based on a single crop-soil composite can be invalid for other crop-soil composites. Finally, a consideration of the numerical error in the time-cumulative value of ET_a is discussed besides the existing consideration of that error over individual time steps as done in the previous study. This cumulative ET_a is more relevant to the final crop yield. Published 2014. This article is a U.S. Government work and is in the public domain in the USA.

THE SHANG (2012) STUDY: ASSUMPTIONS, EQUATIONS AND RECOMMENDATIONS

Shang (2012) is herefoth denoted in this comment article as S12, whereas this article itself is denoted as YC for Yatheendradas (et al.) comment. Besides the original assumptions for calculating the actual crop evapotranspiration (ET_a) by Allen *et al.* (1998), S12 made important additional assumptions that are accordingly followed here as well:

1. Meteorological/atmospheric conditions were constant over multiple time steps (see Figure 3 by S12). This

means that the standard reference crop evapotranspiration (ET_o) from either grass or alfalfa was assumed constant.

2. Important source terms were neglected in the analytical and numerical formulations, where their inclusion may change the results and recommendations. One such term is the water input (irrigation or precipitation). This essentially slowly dried out the crop root zone because of evapotranspiration, starting from whichever considered instant in the crop phenology.

3. Another source term or key parameterization not considered but existing in reality and in practice is the time variation in the crop coefficient curve (Allen *et al.*, 1998). Typically, this curve assumes a low constant initial value phase, followed by a linear increase during a crop development phase, then a

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maximum constant value over a mid-season phase, and finally a linear decrease till harvest in a late-season phase. The instantaneous maximum crop evapotranspiration (ET_c) is obtained by multiplying ET_o by this crop coefficient. So for a constant ET_o from assumption 1 aforementioned, a constant ET_c over multiple time steps implies a corresponding enforced constancy in the crop coefficient. Figures 1–3 by S12 are obtained using this enforcement.

4. S12 neglected soil water flux through the bottom of root zone by assuming a 'deep groundwater level and in periods without heavy rain and irrigation'.

Following Allen *et al.* (1998), Equation (2) by S12 gave ET_a using ET_c and a water stress coefficient (K_s):

$$ET_a = K_s ET_c \qquad (1)$$

Equation (3) by S12 gave this piecewise linear K_s that increases with an increase in the soil water storage (W) from the wilting point (W_p) to the critical soil water storage for soil water stress (W_j):

$$K_s = \begin{cases} 0, & W \leq W_p \\ (W - W_p)/(W_j - W_p), & W_p < W < W_j \\ 1, & W \geq W_j \end{cases} \qquad (2)$$

Here, W_j was given by Equation (4) by S12 as lying between W_p and the soil water at field capacity (W_f):

$$W_j = pW_p + (1 - p)W_f, 0 < p < 1 \qquad (3)$$

where p is the depletable fraction of root zone water before water stress, and Equation (5) by S12 showed p depending both on the crop type through a p_{std} term and on the ET_c (mm/day):

$$p = p_{std} + 0.04(5 - ET_c) \qquad (4)$$

Finally, assuming that soil water stayed in the $W_p < W < W_j$ range in Equation (2) earlier for a time step, Equation (8) by S12 gave the following analytical solution (ET_b) of ET_a:

$$ET_b = (W_o - W_p)\left\{1 - e^{\left[-\frac{\overline{ET_c} \cdot \Delta t}{W_j - W_p}\right]}\right\}, W_p < W < W_j \quad (5)$$

where W_o is the initial soil water storage, Δt is the time step, and $\overline{ET_c}$ is the ET_c assumed constant (or 'representative') over the time step. Note that although ET_c is a rate, its analytical solution ET_b was formulated as a depth (mm).

For the same $W_p < W < W_j$ range, the Equations (9), (15) and (17) by S12 gave the following numerical solutions of the ET_a depth (mm), denoted by ET_{ee}, ET_{me} and ET_{H3} for the explicit Euler, the modified Euler and the Heun's third-order methods, respectively:

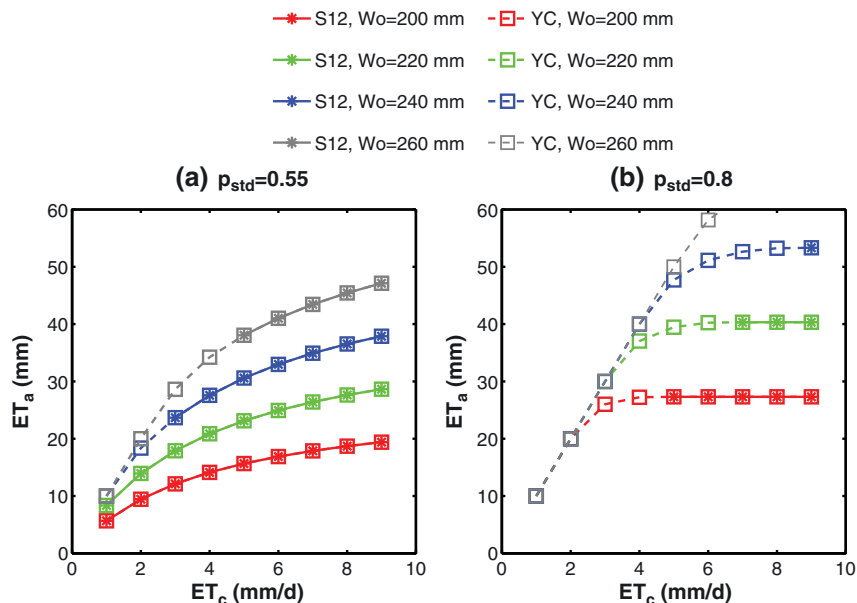$$ET_{ee} = \frac{W_o - W_p}{W_j - W_p}\overline{ET_c} \ \Delta t, \ \ W_p < W < W_j \qquad (6)$$

Figure 1. Analytical ET_a (i.e. ET_b) for different values of ET_c, W_o and p_{std}. In the legend, S12 and YC, respectively denote usage of equations from Shang (2012) and this comment article
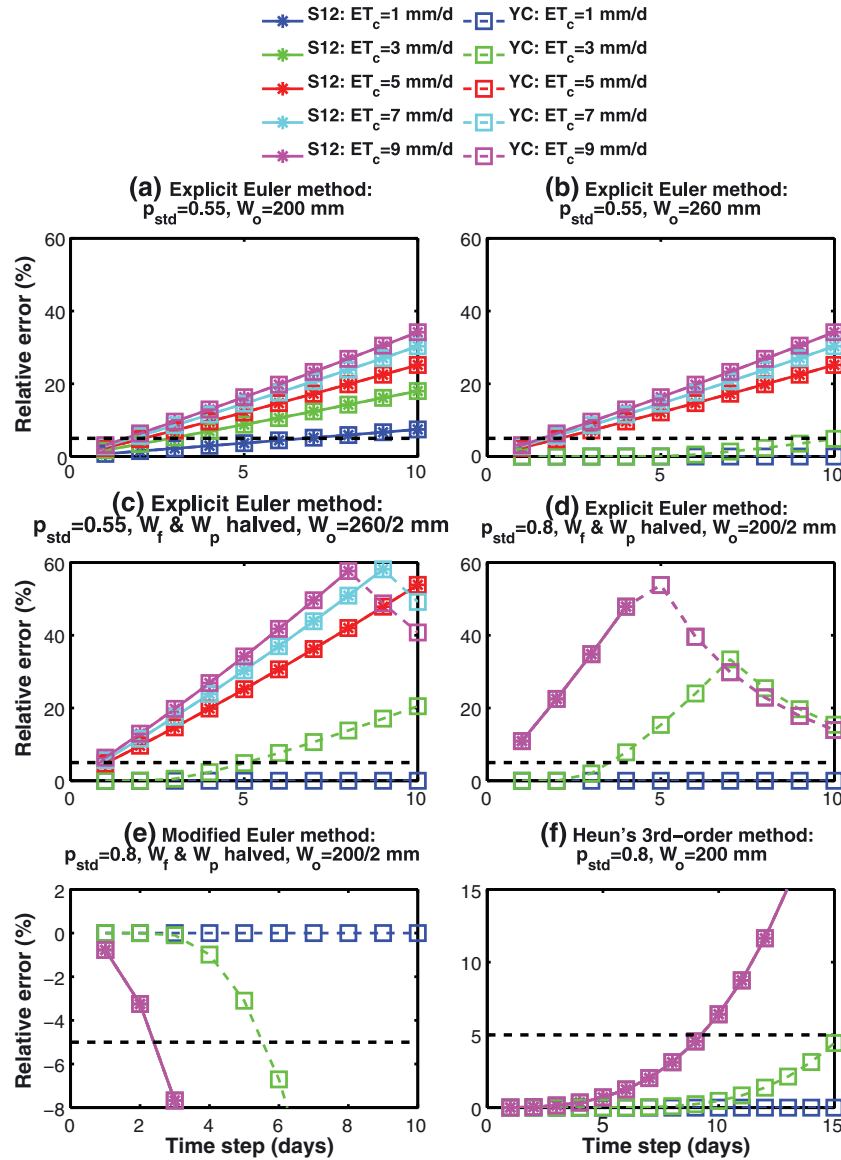
Figure 2. Relative error in ET_a for some numerical methods, crop-soil composites, initial conditions and ET_c values. In the legend, S12 and YC, respectively, denote the usage of equations from Shang (2012) and this comment article. Horizontal dashed line is the relative error threshold at 5% (or −5% as relevant)

$$ET_{me} = \frac{W_o - W_p}{W_j - W_p}\overline{ET_c}\Delta t\left(1 - \frac{1}{2}\frac{\overline{ET_c}\Delta t}{W_j - W_p}\right), W_p < W < W_j$$

(7)

$$ET_{H3} = \frac{W_o - W_p}{W_j - W_p}\overline{ET_c}\Delta t\left[1 - \frac{1}{2}\frac{\overline{ET_c}\Delta t}{W_j - W_p} + \frac{1}{6}\left(\frac{\overline{ET_c}\Delta t}{W_j - W_p}\right)^2\right], \quad (8)$$

$$W_p < W < W_j$$

S12 further used analytical Equation (5) in the previous texts as a benchmark to calculate the relative errors in the numerical ET_a from these Equations (6)–(8). Accordingly, S12 preferred less complex numerical methods for computational efficiency in making the following recommendations on their selection for calculating a satisfactorily accurate numerical ET_a:

A. If the time step is 1 day (d) and ET_c is any value, then use explicit Euler, else,

B. if the time step is up to 2 days and ET_c is below 5 mm/day, then use explicit Euler, else,

C. if the time step is up to 1 week and ET_c is any value, then use midpoint/modified Euler, else,

D. if the time step is up to 10 days and ET_c is below 5 mm/day, then use midpoint/modified Euler, else,

E. if the time step is up to 1 week and ET_c is any value, then use Heun's 3rd-order method.
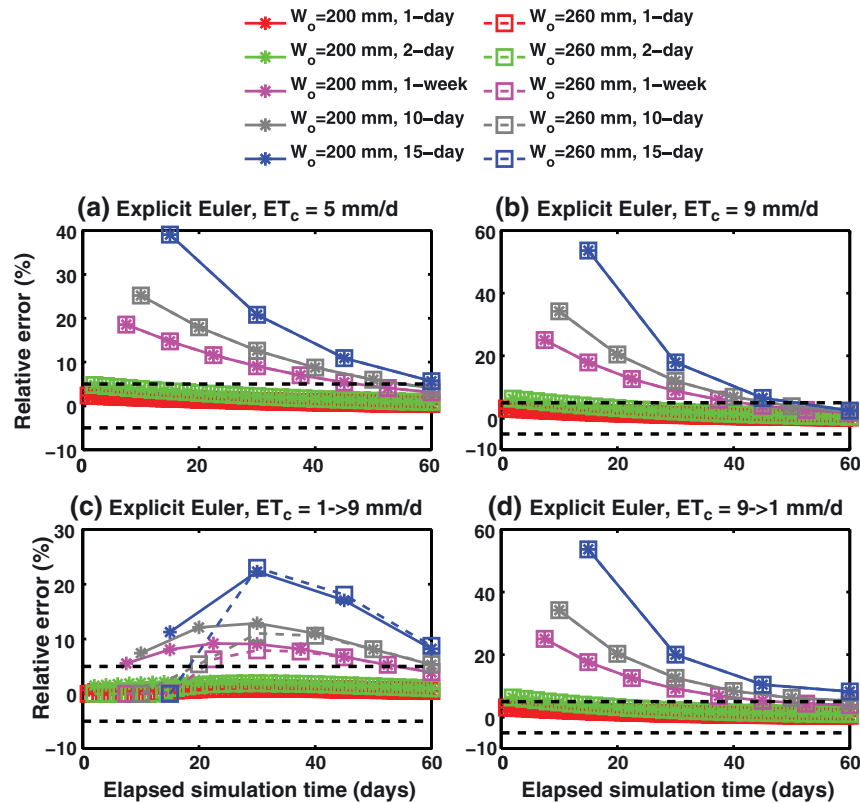
Figure 3. Relative error in cumulated ET_a of S12's crop-soil composite using the reformulated explicit Euler method for different ETc trends, initial conditions (Wo) and time step. Horizontal dashed lines are the relative error thresholds at ±5%

These recommendations were obviously made with practical applicability in mind. Hence, it is worth noting that following them for computational efficiency while attempting a realistic case of a non-constant ET_c over multiple time steps (i.e. by relaxing assumption 3 earlier) can mean continuously changing the numerical method during the simulation. For example, for a fixed time step of 2 days, a change in ET_c from 4 mm/day at a time step to 6 mm/day at the next would correspond to a change in the numerical method from the explicit Euler to the midpoint/modified Euler.

REFORMULATING THE S12 EQUATIONS: EFFECT ON RESULTS AND RECOMMENDATIONS

Figure 1 by S12 showed the analytical ET_b after a 10-day time step over a range of values for the ET_c (1 to 9 mm/day) and initial soil water (W_o from 200 to 260 mm). These ranges and the properties for crop ($p_{std} = 0.55$) and soil ($W_p = 158$ mm, $W_j = 396$ mm) are characteristic of their study site in North China. However, some combinations of ET_c and W_o actually move W_o out of the assumed $W_p < W < W_j$ range and into the $W > W_j$ range. For example, an ET_c of 1 mm/day gives a W_j of around 227 mm using Equations (3) and (4) earlier,

compared with which a W_o of 260 mm is greater and so outside the $W_p < W < W_j$ range. Such combinations of ET_c and W_o are omitted in Figure 1 by S12 and also in Figure 1a here wherein some asterisks derived using Equation (5) earlier are conspicuously absent at some square marker locations (these square markers are based on a reformulated ET_b to be presented further in the succeeding texts). These combinations of ET_c and W_o having $W_o > W_j$ tend to occur on the higher W_o curves at lower ET_c values. Note that at higher ET_c values on the same W_o curves, $W_p < W_o < W_j$ happens because of Equations (3) and (4) earlier that result in a W_j that increases with increasing ET_c.

For crop or soil properties different from the specific values considered by S12, such missing ET_b values due to the $W_p < W < W_j$ range constraint can occur for a significantly large number of combinations of ET_c and W_o. For example, see asterisks absent at more than half of the square marker locations in Figure 1b here, wherein the crop p_{std} value is now a higher-end value of 0.8 (Allen *et al.*, 1998).

Analytical and numerical formulations of ET_a specific to limited soil water ranges or not accounting for transition between such ranges would be limited in their applicability. For example, a formulation valid for soil

water in the $W \geq W_j$ range can be applied only if both W_o and the soil water at the end of a time step are in that range. Avoiding this limited applicability requires inclusion in the formulations of the transition between ranges by soil water during a time step, for example, from the $W \geq W_j$ range to the $W_p < W < W_j$ range. Also, the ET_b calculated using Equation (5) earlier for a W_o in the $W \geq W_j$ range can be overbiased near ET_c–W_o combinations where such transition occurs. As a

$$\Delta t_1 = (W_o - W_j)/\overline{ET}_c, \quad W_o \geq W_j \qquad (9)$$

Note that soil water hitting the lower threshold W_p during a time step is handled by enforcing this W_p constraint using 'min' functions.

Applying this time step and ET_a splitting and the W_p constraint gives the following generally applicable analytical solution ($ET_{b,C}$ in mm) of ET_a instead of the Equation (5) earlier by S12 that had a $W_p < W < W_j$ applicability only:

$$ET_{b,C} = \begin{cases} 0, & W_o \leq W_p \\[3mm] \min\left[(W_o - W_p)\left\{1 - e^{\left[-\frac{\overline{ET}_c \Delta t}{W_j - W_p}\right]}\right\}, (W_o - W_p)\right], & W_p < W_o < W_j \\[5mm] \min\left[\overline{ET}_c \; \Delta t_1 + (W_j - W_p)\left\{1 - e^{\left[-\frac{\overline{ET}_c(\Delta t - \Delta t_1)}{W_j - W_p}\right]}\right\}, (W_o - W_p)\right], & \\[3mm] & (W_o \geq W_j)\&\left([W_o - \overline{ET}_c \; \Delta t] < W_j\right) \\[2mm] \overline{ET}_c \; \Delta t, & (W_o \geq W_j)\&\left([W_o - \overline{ET}_c \; \Delta t] \geq W_j\right) \end{cases} \qquad (10)$$

benchmark to calculate the relative error in numerical ET_a, accurate ET_b is important. Hence, the analytical and numerical S12 equations are reformulated in the succeeding texts to avoid the aforementioned applicability constraints.

For a time step over which the soil water is above W_j throughout, the ET_a is constant at ET_c. For a time step that starts and ends with soil water values above and below W_j, respectively, the simpler ET_a equations due to the S12 assumptions enable splitting the ET_a into two terms. The initial term's corresponding portion of that time step when soil water is above W_j is:

These $ET_{b,C}$ values are the ones mentioned further earlier as being plotted in Figure 1 here using square markers. When $W_p < W < W_j$ over a time step, they coincide with asterisk markers derived using Equation (5) earlier by S12.

Similarly, the following are the numerical solutions of ET_a in millimetre (denoted by $ET_{ee, C}$, $ET_{me, C}$ and $ET_{H3, C}$ when using the explicit Euler, the modified Euler method and the Heun's third-order methods, respectively), instead of the Equations (6–8) earlier by S12 that had a $W_p < W < Wj$ applicability only:

$$ET_{ee,C} = \begin{cases} 0, & W_o \leq W_p \\[3mm] \min\left[\frac{W_o - W_p}{W_j - W_p}\overline{ET}_c \; \Delta t, (W_o - W_p)\right], & W_p < W_o < W_j \\[3mm] \min\left[\overline{ET}_c \; \Delta t, (W_o - W_p)\right], & (W_o \geq W_j)\&\left([W_o - \overline{ET}_c \; \Delta t] < W_j\right) \\[2mm] \overline{ET}_c \; \Delta t, & (W_o \geq W_j)\&\left([W_o - \overline{ET}_c \; \Delta t] \geq W_j\right) \end{cases} \qquad (11)$$

$$
ET_{me,C} = \begin{cases} 0, & W_o \leq W_p \\[2mm] \min\left[\dfrac{W_o - W_p}{W_j - W_p}\overline{ET_c}\ \Delta t\left(1 - \dfrac{1}{2}\dfrac{\overline{ET_c}\ \Delta t}{W_j - W_p}\right), (W_o - W_p)\right], & W_p < W_o < W_j \\[4mm] \min\left[\overline{ET_c}\ \Delta t_1 + \overline{ET_c}(\Delta t - \Delta t_1)\left(1 - \dfrac{1}{2}\dfrac{\overline{ET_c}(\Delta t - \Delta t_1)}{W_j - W_p}\right), (W_o - W_p)\right] \\[3mm] & \left(W_o \geq W_j\right) \& \left(\left[W_o - \overline{ET_c}\ \Delta t\right] < W_j\right) \\[3mm] \overline{ET_c}\ \Delta t, & \left(W_o \geq W_j\right) \& \left(\left[W_o - \overline{ET_c}\ \Delta t\right] \geq W_j\right) \end{cases} \tag{12}
$$

$$
ET_{H3,C} = \begin{cases} 0, & W_o \leq W_p \\[2mm] \min\left[\dfrac{W_o - W_p}{W_j - W_p}\overline{ET_c}\Delta t\left(1 - \dfrac{1}{2}\dfrac{\overline{ET_c}\Delta t}{W_j - W_p} + \dfrac{1}{6}\left(\dfrac{\overline{ET_c}\Delta t}{W_j - W_p}\right)^2\right), (W_o - W_p)\right], \\[4mm] & W_p < W_o < W_j \\[4mm] \min\left[\overline{ET_c}\Delta t_1 + \overline{ET_c}(\Delta t - \Delta t_1)\left(1 - \dfrac{1}{2}\dfrac{\overline{ET_c}(\Delta t - \Delta t_1)}{W_j - W_p} + \dfrac{1}{6}\left(\dfrac{\overline{ET_c}(\Delta t - \Delta t_1)}{W_j - W_p}\right)^2\right), (W_o - W_p)\right], \\[3mm] & \left(W_o \geq W_j\right) \& \left(\left[W_o - \overline{ET_c}\Delta t\right] < W_j\right) \\[3mm] \overline{ET_c}\Delta t, & \left(W_o \geq W_j\right) \& \left(\left[W_o - \overline{ET_c}\Delta t\right] \geq W_j\right) \end{cases} \tag{13}
$$

Note that in Equation (11) earlier, the apparently missing Δt_1 term for the $\left[\left(W_o \geq W_j\right) \& \left(\left[W_o - \overline{ET_c}\Delta t\right] < W_j\right)\right]$ case is because the original expression $\left[\overline{ET_c}\Delta t_1 + \overline{ET_c}(\Delta t - \Delta t_1)\right]$ reduces to $\overline{ET_c}\Delta t$.

When formulating the relative error in the numerical ET_a, S12 noticed that the common $(W_o - W_p)$ term in the analytical Equation (5) earlier and the numerical Equations (6–8) earlier cancelled out. S12 duly asserted that 'relative errors of ET_a calculated with numerical methods in one time step are independent of the initial soil water storage in the range of soil water stress', and any mention of the initial soil water (W_o) is correspondingly absent in the S12 recommendations. However, this supposed independence from W_o is erroneous as seen from the analytical Equation (10) and numerical Equations (11–13) earlier, where the $(W_o - W_p)$ term need not cancel out while formulating this relative error. This is also illustrated by the example contrast of this reformulation-derived relative error (denoted by square markers) between Figure 2a ($W_o = 200$ mm) and 2b ($W_o = 260$ mm) here that use the explicit Euler method, for the lower ET_c curves. Also, asterisk markers in Figure 2a here plotted using the S12 equations are same as the markers in Figure 2a by S12; it is evident that the latter plot should actually have been impossible with some W_o values, because an example $W_o = 260$ mm should reveal missing markers for the lower ET_c curves as shown by the missing asterisk markers in Figure 2b here. This was missed out on by the S12 study because its relative error formulation that was independent of W_o did not reveal any missing markers.

In Figure 2c–2d here, the original field capacity (W_f) and wilting point (W_p) values for a soil type closer to clay as considered by S12 are halved towards a soil type closer to loam (Walker, 1989), with W_o also correspondingly halved; this effectively decreases the soil water storage capacity and hence the water availability for evapotranspiration. The relative error for the explicit Euler method is now seen to decrease after some time step (reflecting the numerical water content value reaching W_p) and decreases earlier with an increase in p_{std} (0.55 for Figure 2c *vs* 0.8 for Figure 2d). This contradicts the trend from the equations and Figure 2 of the S12 study where the relative error seemed to monotonically increase with an increasing time step.

The high p_{std} value of 0.8 in Figure 2d here collapses the relative error value curves for ET_c of 5–9 mm/day into

a single one (not visually discernible) that is distinct from the ET_c curves of 1–3 mm/day. This also happens for the example plots for the modified Euler (Figure 2e) and the Heun's third-order methods (Figure 2f) having this same p_{std}. Note that the usage of the original equations by S12, where occurrence of soil moisture values outside the valid range were ignored, would have collapsed all the ET_c curves of 1–9 mm/day into this single curve. Hence, the reformulated equations accurately and better resolve the behaviour in relative error for such high p_{std} values.

A comparison between Figure 2b–2d here shows the relative error curves starting out steeper for lower soil water storage capacities (i.e. lower W_f and W_p) and higher p_{std} values. This aspect was not highlighted by S12; although the properties of the specific crop-soil composite used were specified, the absence of a caveat about the validity of those results regarding relative error for that specific composite clearly gave an erroneous impression that those results and consequent recommendations were valid for all crop-soil composites.

Using the same relative error threshold of 5% by S12 and a time step of 1 day, Figure 2c–2d here show that the explicit Euler method can only be used for these crop-soil composites if ET_c is some respective specific value less than 5 mm/day. This contrasts with the recommendation 'A' earlier by S12 that this method can be used for any ET_c for a 1-day time step. Similarly, for a 2-day time step, the explicit Euler method is supposedly invalid if ET_c is above 5 mm/day as per the recommendation 'B' above by S12, but Figure 2c–2d here show this method becoming invalid above some lower respective specific value of ET_c between 3 and 5 mm/day and dependent on the crop-soil composite and its initial condition.

Similarly, for the modified Euler method, the respective recommendations 'C' and 'D' earlier by S12 state that the method can be respectively used for any ET_c in case of a 1-week time step and for an ET_c of 5 mm/day or less in case of a 10-day time step. However, for the specific crop-soil composite and initial condition in Figure 2e here, this method can be used only when ET_c is below some respective specific value between 1 and 3 mm/day for both time steps. Finally, the recommendation 'E' earlier by S12 states that the Heun's 3rd-order method can be used for up to a 15-day time step for any ET_c. However, this recommendation becomes invalid when ET_c is above 3 mm/day for the specific crop-soil composite and initial condition in Figure 2f here (note that its *x*-axis extends out to 15 days).

CONSIDERING THE RELATIVE ERROR IN CUMULATIVE ET_A

The cumulated ET_a at the end of the crop season (or harvest) is more relevant to the crop yield than the ET_a over any single time step and is a common metric used in drought early warning systems (e.g., Senay and Verdin, 2002). In providing recommendations, S12 considered only single time-step simulations, with the largest time step being 15 days. For considering multiple time-step simulations, a simulation period of 60 days (approximately 2 months) is used here.

Crop seasons are typically quite longer than 60 days, with some individual crop growth phases possibly spanning up to 60 days or even more (Allen *et al.*, 1998). The assumption 3 earlier of a constant ET_c even over multiple time steps as shown in Figure 3 by S12 is now relaxed here to allow a different ET_c for each time step in a simulation. This allows a piecewise linear increase/decrease of ET_c over a simulation and correspondingly a characterization of linearly increasing/decreasing portions of the crop coefficient curve. Any desired temporal combination of these portions with constant ET_c portions enables an assessment of the relative error in the cumulated ET_a over the relevant crop phenology simulation.

For the specific crop-soil composite used by S12, the 60-day evolution of the relative error in cumulated ET_a using the reformulated equations for the explicit Euler method is shown here for the following: a constant ET_c at 5 mm/day appearing in the S12 recommendations (Figure 3a), a constant ET_c at constant upper limit of 9 mm/day considered by S12 (Figure 3b), an ET_c linearly increasing from 1 mm/day to 9 mm/day during the simulation (Figure 3c), and an ET_c linearly decreasing from 9 mm/day to 1 mm/day (Figure 3d). Figures 3a–3d show that each relative error is actually near or below 5% at 60 days for a time step of up to 10 days with a projected decreasing trend beyond 60 days, meaning that the relative error for their piecewise linear combination over time should also be within 5% at 60 days and beyond. Also note the relative error at 60 days for an ET_c of 9 mm/day is actually lower than that for an ET_c of 5 mm/day, due to a faster decrease in its relative error over time (Figures 3a–3b).

SUMMARY

The S12 assumptions included (i) ignoring water input resulting in a root zone that eventually dries out as with rain-fed crops in water-scarce regions, (ii) constant ET_c over multiple time steps and (iii) deep groundwater implying negligible soil water flux through the bottom of root zone. This latter flux is significant in many regions (e.g. Schmid and Hanson, 2009; Schmid *et al.*, 2009). The assumption of no water input is specifically restrictive against a practical application of its equations for estimating ET_a. This essentially means that this model is inapplicable when water input becomes available. The S12 analytical and numerical formulations of ET_a over limited soil water ranges without accounting for transition

between the ranges restrict their applicability and accuracy. Also, the erroneous impression of a general validity of the S12 recommendations could have been avoided through exercising more rigour in either checking results for other crop-soil composites or specifying relevant caveats.

Although conforming to the S12 assumptions, a reformulation of its equations here towards applicability over the entire soil water range reveals a dependence of the relative error in numerical ET_a on the initial soil water. This relative error is also shown to be greatly dependent on the crop-soil composite. The consequently more complicated actual nature of this relative error now shows that crop and soil properties and the initial soil water also have to be considered in making recommendations regarding an appropriate numerical method.

Finally, any such recommendation can also consider the simulation setup and goal. For example, instead of considering the error in numerical ET_a at every time step, one can alternatively consider the error in cumulative ET_a for calculating crop yield.

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