



# Modeling surface residue decomposition and N release using the Cover Crop Nitrogen Calculator (CC-NCALC)

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**Abstract** Optimal utilization of cover crop (CC) residues in conservation tillage systems require fast-running crop-soil simulation models that can accurately predict surface residue decomposition through time, which in turn determines both nitrogen (N) availability for subsequent cash crop and the longevity of residue cover for effective soil protection, soil moisture conservation, and weed suppression. However, existing models either have long execution times or do not consider environmental variables to which surface residues are exposed. As a result, these models are not practical as a decision support tool used by producers. An improved surface residue water potential ( $\psi_{\text{residue}}$ ) module that provides fast estimates of hourly  $\psi_{\text{residue}}$  using easily available weather information was developed and integrated into the existing ‘Cover Crop Nitrogen Calculator (CC-NCALC)’.

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Specific dynamics of surface residue decomposition were accounted for by adjusting decomposition rates based on  $\psi_{\text{residue}}$  and temperature dynamics, N limitations, and fractional residue mass in contact with the soil. The modified CC-NCALC tool was calibrated and validated using on-farm litter bag decomposition data collected across 99 site-years during 2017–2019 from conservation tillage-based corn (*Zea mays* L.) systems in the mid-Atlantic and southeastern USA. Both residue mass [calibration: root mean square error (RMSE)=403 kg ha<sup>-1</sup>, relative RMSE (rRMSE)=27%, Willmott’s index of agreement (d)=0.98; validation: RMSE=483 kg ha<sup>-1</sup>, rRMSE=33%, d=0.97] and N (calibration: RMSE=9.1 kg ha<sup>-1</sup>, rRMSE=34%, d=0.93; validation: RMSE=15 kg N ha<sup>-1</sup>, rRMSE=48%, d=0.93) remaining on the soil surface over time were simulated reasonably well by the modified CC-NCALC tool. Accurate accounting of leaching and gaseous losses from high-quality CC residues (i.e., >5% N) and initial N

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immobilization from poor-quality CC residues could further improve model estimates. We propose that the modified CC-NCALC tool can be used as a decision support tool to help inform farmers and land managers regarding their residue and N management decisions in CC-based conservation tillage systems.

**Keywords** Cover crops · Decomposition and N release · Conservation tillage · CERES-N · Decision support tools

## Abbreviations

|                   |                                       |
|-------------------|---------------------------------------|
| CC                | Cover crops                           |
| CC-NCALC          | Cover Crop N Calculator               |
| CERES             | Crop Environment REsource Synthesis   |
| CARB              | Carbohydrates                         |
| CELL              | Holo-cellulose                        |
| LIGN              | Lignin                                |
| $k_{POOL}$        | Decay rate constants                  |
| $\psi_{residue}$  | Residue water potential               |
| $\psi_{air}$      | Air water potential                   |
| $\psi_{gradient}$ | Water potential gradient              |
| MTRF              | Moisture-temperature reduction factor |
| CNRF              | C:N ratio factor                      |
| $RM_{decomposed}$ | Residue mass decomposed               |
| $RN_{min}$        | Residue N mineralized                 |
| $N_{im}$          | N immobilized                         |

## Introduction

Cover crops (CCs) are non-marketed crops planted during the winter or summer fallow period to provide continuous soil cover and a myriad of agroecosystem services. Cover crops reduce soil erosion, improve soil water storage via increased infiltration and reduced evaporation, improve nutrient cycling, suppress weeds, break pest and disease cycles, increase soil organic matter, improve soil health, and stabilize crop yields (Blanco-Canqui et al. 2015; Daryanto et al. 2018; Marcillo and Miguez 2017; Meisinger et al. 1991). Moreover, CCs play an important role in nitrogen (N) management for cropping systems by scavenging residual soil mineral N or fixing atmospheric  $N_2$  and releasing N back to the soil after termination (Poffenbarger et al. 2015; Thapa et al. 2018a, b). Therefore, CC-based conservation tillage grain production systems, in which the subsequent cash crop is planted into the mulch of previous CC residues,

are increasingly adopted in the mid-Atlantic and southeastern US regions (Mirsky et al. 2012).

The efficacy of surface CC residues to protect soil, conserve water, and suppress weeds depends on the mass and thickness of the mulch layer, which in turn is influenced by the rate at which residue decomposes. Decomposition also regulates the amount and timing of N mineralized or immobilized from CC residues. The potential of CC residues to supply N is of great value in cereal crop production systems because they rely on large external N inputs to sustain yields. On the other hand, slow decomposing CC residues that have a high C:N often immobilize N and hence, increase N fertilizer needs for subsequent cash crops. The ability to accurately predict N mineralized or immobilized from decomposing CC residues with site-specific models will allow farmers and land managers to effectively manage N in crop production systems and hence, avoid environmental impacts of N losses from over-fertilization and yield losses from under-fertilization, and ensure ecosystem services are optimized in CC-based conservation tillage systems.

The CERES (Crop Environment REsource Synthesis) models are a group of crop-soil simulation models that include a common decomposition and N transformation sub-model (hereafter, referred as CERES-N) that simulates mineralization-immobilization of N associated with the decomposition of crop residues on a daily time step (Godwin and Jones 1991). The CERES-N sub-model has been used to simulate decomposition and N release from CC residues (Quemada et al. 1997; Schomberg and Cabrera 2001; Woodruff et al. 2018). The CERES-N sub-model is very accessible and broadly applicable as it requires a minimum set of input data. When properly calibrated and validated, the model can be used as a powerful tool for making informed decisions by farmers and land managers which in turn will help them reduce N management costs, increase farm profitability, and achieve long-term sustainability via optimized usage of CC residues in their fields.

To date, various modifications have been made to the original CERES-N sub-model to improve predictions of field-measured data. For example, Vigil et al. (1991) reduced the critical C:N above which the decomposition rate is reduced from the original value of 25 to 13. As compared to the original CERES-N sub-model where residue C pools were assumed to be in fixed proportions [i.e., 20% soluble carbohydrates (CARB), 70% holo-cellulose (CELL), and 10% lignin (LIGN)], modifying the sub-model to allow users to

input values for residue C pools provided better estimates of decomposition and N mineralized or immobilized from CC residues (Quemada and Cabrera 1995; Quemada et al. 1997; Schomberg and Cabrera 2001; Woodruff et al. 2018). The daily first-order decay rate constants were reduced from the original value of 0.8 to 0.14 d<sup>-1</sup> for *CARB* by Quemada and Cabrera (1995) and from 0.0095 to 0.00095 d<sup>-1</sup> for *LIGN* by Vigil et al. (1991). Similarly, the daily first-order decay rate constant for *CELL* was expressed as a function of lignin content in residues by Woodruff et al. (2018). In the original CERES-N sub-model, 20% of N mineralized from decomposing residues is synthesized back to soil organic matter pool. To improve simulations, Woodruff et al. (2018) changed this value to 25% for incorporated and 12.5% for surface residues, respectively.

The CERES-N sub-model with these modifications simulated decomposition, and N mineralized or immobilized, of incorporated residues reasonably well with predictions in good agreement with measured data (Woodruff et al. 2018). Because of its efficacy, the CERES-N sub-model has been publicly deployed as a web-based, decision support tool referred to as the *Cover Crop Nitrogen Calculator* (CC-NCALC). The CC-NCALC tool is used by farmers and land managers to estimate N released from incorporated CC residues and hence, adjust N fertilizer needs for subsequent cash crops (Gaskin et al. 2019). In the case of conservation tillage systems, however, the CC-NCALC tool consistently overpredicted decomposition of surface CC residues (Woodruff et al. 2018). This indicates that factors influencing surface residue decomposition are not adequately addressed. For example, soil water ( $\theta_g$ ) and soil temperature (T) are used as drivers of surface residue decomposition in the CC-NCALC tool even though they do not reflect the true state of environmental conditions for surface residues. Recent studies have advocated the use of residue water potential ( $\psi_{residue}$ ) and T to adjust decomposition rates of surface CC residues in process-based models (Melkonian et al. 2017; Thapa et al. 2021a, b; Woodruff et al. 2018). Moreover, despite evidence that the rate of surface residue decomposition decreased as biomass increased (Steiner et al. 1999; Stott et al. 1990; Thapa et al. 2022; Thorburn et al. 2001), residue mass effects on the microenvironment are not considered in the CC-NCALC tool.

Therefore, accuracy in CC-NCALC tool predictions of N mineralized or immobilized from surface CC residues in conservation tillage systems can be improved if factors affecting surface residue decomposition, such as, residue moisture and temperature dynamics, N limitations, and fractional soil-residue contact or residue mass effects are properly addressed.

In our previous work, a surface  $\psi_{residue}$  module was developed, calibrated, and validated to estimate  $\psi_{residue}$  of surface CC residues at a 1-h time step using hourly data on air relative humidity (RH), air T, and rain (Dann et al. 2021). Similarly, a two-dimensional response surface equation to calculate residue moisture-temperature reduction factor (*MTRF*) was also developed (Thapa et al. 2021a). In this study, we integrate the surface  $\psi_{residue}$  module and implement *MTRF* into the CC-NCALC tool to adjust surface residue decomposition rates based on residue environment (i.e.,  $\psi_{residue}$  and T). We also introduce a soil-residue contacting factor that adjusts surface residue decomposition rates based on residue mass since residues in contact with the soil surface decompose more rapidly. We finally calibrate and validate the modified CC-NCALC model using on-farm litter bag decomposition data collected across 99 site-years during 2017–2019 in conservation tillage-based corn (*Zea Mays L.*) systems in the mid-Atlantic and South-eastern USA.

## Materials and methods

### Adaptation of the CC-NCALC tool for surface residue decomposition

As described earlier, the existing CC-NCALC tool worked effectively for incorporated residues. In this work, the CC-NCALC tool was adapted for surface residue decomposition by considering the effects of residue moisture and temperature dynamics, N limitations, and soil-residue contact on residue decay rates.

### Surface residue water potential module

For residue moisture dynamics, an original surface  $\psi_{residue}$  module was developed and integrated into the existing CC-NCALC tool. The detailed structure of

the surface  $\psi_{residue}$  module was provided in Dann et al. (2021). Briefly, the module requires the initial residue water content ( $\theta_g$ ) at the start of simulation ( $t_0$ ) and computes hourly changes in  $\theta_g$  accounting for hourly air  $RH$ , air T, and rain. The fundamental principle governing transfer of water into and out of surface CC residues is the existing water potential gradient at the residue-air interface (i.e.,  $\psi_{gradient} = \psi_{air} - \psi_{residue}$ ). Surface residues gain moisture from the atmosphere typically during nighttime and early morning hours when air RH increases due to a positive change in the  $\psi_{gradient}$  ( $\psi_{air} > \psi_{residue}$ ). The surface  $\psi_{residue}$  module also considers gain in residue  $\theta_g$  via dewfall and rain. As  $RH$  decreases in late morning and into the afternoon hours ( $\Delta RH < 0$ ), residue drying occurs as a function of air T and residue  $\theta_g$ . In model development studies, Dann et al. (2021) further observed that exchange of water at the soil-residue interface was negligible and hence, omitted the effect of soil  $\theta_g$ . At any given time ‘ $t$ ’,  $\psi_{residue}$  is calculated from residue  $\theta_g$  using a characteristic water release curve function ( $\psi_{residue} = a \cdot (residue\theta_g)^b$ ) in which the parameters ‘ $a$ ’ and ‘ $b$ ’ are determined as a function of residue lignin concentrations.

#### *Underlying model structure of the modified CC-NCALC tool*

The CC-NCALC tool divides crop residues into three pools that differ in their rates of decomposition: *CARB*, *CELL*, and *LIGN*. All three pools decompose simultaneously using first-order decay rate kinetics. The hourly amount of residue mass decomposed ( $RM_{decomposed}$ , kg ha<sup>-1</sup> h<sup>-1</sup>) and gross N mineralized ( $GrossRN_{min}$ , kg N ha<sup>-1</sup> h<sup>-1</sup>) from surface CC residues are determined as the product of adjusted hourly decay rate constants and the corresponding size of individual pools.

$$\left\{ \begin{array}{l} RM_{decomposed} = \sum_{POOL=1}^3 (k_{POOL} \cdot MTRF \cdot CNRF \cdot ContactFactor \cdot RM_{POOL}) \\ Gross RN_{min} = \sum_{POOL=1}^3 (k_{POOL} \cdot MTRF \cdot CNRF \cdot ContactFactor \cdot RN_{POOL}) \end{array} \right. \quad (1)$$

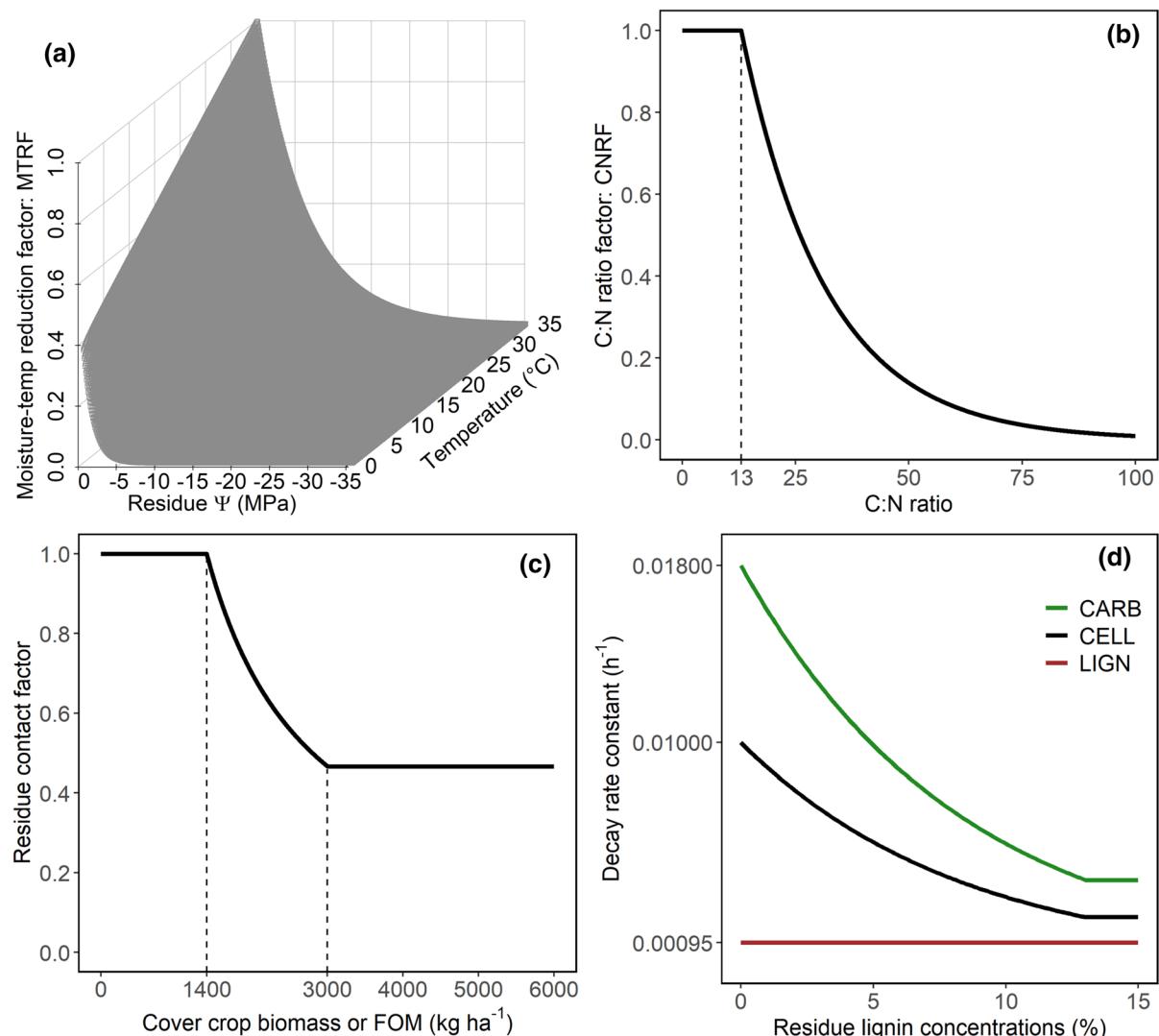
where,  $RM_{POOL}$  and  $RN_{POOL}$  are residue mass and N sizes for individual components (i.e., 1=*CARB*, 2=*CELL*, and 3=*LIGN* in kg ha<sup>-1</sup>),  $k_{POOL}$  is the optimum (or maximum) hourly decay rate constants for each pool under non-limiting conditions (i.e.,  $k_{CARB}$ ,  $k_{CELL}$ , and  $k_{LIGN}$  in h<sup>-1</sup>), and *MTRF*, *CNRF*, and *ContactFactor* are residue moisture-temperature reduction factor, C:N ratio factor, and residue contact factor, respectively (Fig. 1a-d). While  $k_{LIGN}$  is assumed to be constant,  $k_{CARB}$  and  $k_{CELL}$  are determined as functions of residue lignin concentrations, as shown in Eq. (2).

$$\left\{ \begin{array}{l} k_{CARB} = K_{CARB} \cdot \exp\left(-12 \cdot \frac{\% LIGN}{100}\right) \\ k_{CELL} = K_{CELL} \cdot \exp\left(-12 \cdot \frac{\% LIGN}{100}\right) \\ k_{LIGN} = K_{LIGN} \end{array} \right. \quad (2)$$

where,  $K_{CARB}$ ,  $K_{CELL}$ , and  $K_{LIGN}$  are empirical coefficients. *MTRF*, *CNRF*, and *ContactFactor* are unitless factors, scaled from 0 to 1, to adjust surface residue decomposition for limitations imposed by residue environment ( $\psi_{residue}$  and T), N availability, and soil-residue contact, respectively.

$$\left\{ \begin{array}{l} MTRF = \begin{cases} (0.384 + 0.018 \cdot T) \cdot \exp^{(0.142+0.628 \cdot T^{-1}) \cdot \psi_{residue}}, & T > 0^\circ C \\ 0, & T \leq 0^\circ C \end{cases} \\ CNRF = \begin{cases} \exp^{(-0.693 \cdot \frac{(CNR-13)}{13})}, & CNR \geq 13 \\ 1, & CNR < 13 \end{cases} \\ Contact Factor = \begin{cases} 1, & RM_t \leq RM_{min} \\ \frac{RM_{min}}{RM_t}, & RM_{min} < RM_t < RM_{max} \\ \frac{RM_{max}}{RM_t}, & RM_t \geq RM_{max} \end{cases} \end{array} \right. \quad (3)$$

where,  $\psi_{residue}$  is the hourly surface residue water potential as estimated by the surface  $\psi_{residue}$  module (MPa),  $T$  is the hourly air temperature at 2-m height



**Fig. 1** The default functions for the adjustment factors (Eq. 3) that limits surface residue decomposition under sub-optimal conditions in the modified CC-NCALC tool due to: **a** moisture and temperature limitations (moisture-temperature reduction factor: *MTRF*), **b** N limitations (C:N ratio factor: *CNRF*),

and **c** fractional soil-residue contact (*ContactFactor*). Panel **d** represents the hourly decay rate constants for different residue pools ( $k_{POOL}$ ) as a function of residue lignin concentrations (Eq. 2)

(°C), *CNR* represents the overall C:N ratio of the whole soil-residue mulch layer ( $CNR = \frac{0.426 \cdot RM_t}{(RN_t + N_{inorg})}$ ;

$N_{inorg}$  is the soil inorganic N pool in the surface soil layer),  $RM_t$  and  $RN_t$  are residue mass and N remaining at time ‘t’,  $RM_{min}$  represents residue mass below which surface residue decomposition is independent of the mass, and  $RM_{max}$  is the residue mass above which surface residue decomposition is no longer impacted by residue mass. The use of *MTRF* and

*ContactFactor* to adjust  $k_{POOL}$  in the modified CC-NCALC tool is a major departure from its earlier version. The *MTRF* function was developed by Thapa et al. (2021a) in a 150-d laboratory-controlled experiment aimed at modeling interactive effects of  $\psi_{residue}$  and T on C mineralization from surface CC residues. Similarly, the function for *ContactFactor* used here is adopted from Thorburn et al. (2001) after slight modifications.

In the modified CC-NCALC tool, 12.5% of gross N mineralized from surface CC residues is synthesized back into soil organic matter or to the more stable pool (i.e., *FractionSynthesized*) and the rest enters the soil inorganic N pool (Woodruff et al. 2018). This fraction accounts for the N that is incorporated into microbial biomass. The tool operates on an hourly time step, so that decomposition of fresh residue inputs and soil organic matter are happening simultaneously. The rate of N mineralization from the soil organic matter pool was estimated using a relationship developed by Egelkraut et al. (2003). Nitrogen immobilization is calculated in a similar manner to that of the original CERES-N sub-model, but is now set to occur when microbial N demand during residue decomposition is not fulfilled from gross N mineralized and is estimated using the following equation:

$$N_{im} = \text{Minimum}[(RM_{decomposed} \cdot 0.0213 - Gross RN_{min}), N_{inorg}] \quad (4)$$

where, 0.0213 is the microbial N demand (g N required per g *RM* decomposed) and is calculated by multiplying the fraction of C in residues (i.e., 0.426 g g<sup>-1</sup>) by the microbial C use efficiency (i.e., 0.4 g C assimilated per g C *FOM* decomposed) and dividing by the microbial biomass C:N (i.e., 8). The immobilized N transferred from surface soil to residue mulch is primarily stored back into the readily decomposable carbohydrate N pool (i.e., *RN<sub>CARB</sub>*) and is readily available for microbes to decompose high C:N surface CC residues. Net N mineralized from surface CC residues (*NetRN<sub>min</sub>*) was estimated as below:

$$\text{Net RN}_{min} = \text{Gross RN}_{min} \cdot (1 - \text{FractionSynthesized}) - N_{im} \quad (5)$$

At a given time '*t*', the amount of residue mass (*RM<sub>t</sub>*, kg ha<sup>-1</sup>) and N (*RN<sub>t</sub>*, kg N ha<sup>-1</sup>) remaining on the soil surface are estimated using the following equations:

$$\left\{ \begin{array}{l} \text{Simulated RM}_t = \text{RM}_{(t-1)} - RM_{decomposed} \\ \text{Simulated RN}_t = RN_{(t-1)} + N_{im} - \text{Gross RN}_{min} \end{array} \right. \quad (6)$$

#### On-farm cover crop decomposition studies

We used data from the PSA (Precision Sustainable Agriculture) project to calibrate and validate the

modified CC-NCALC tool for simulating decomposition and N release from surface CC residues in conservation tillage-based corn systems in the mid-Atlantic and southeastern USA (Fig. S1). A detailed description of the experimental approach and measured variables in the PSA project is provided in Thapa et al. (2022). In total, litter bag decomposition data collected from 99 site-years during 2017–2019 were used (calibration: 50 site-years; validation: 49 site-years). The dataset allowed model evaluation across a wide range of soils, weather, and management scenarios.

In brief, on-farm experiments were conducted in farmers' fields under their management. Farmers either broadcasted or drilled CC seeds between September and November, after the harvest of previous summer cash crops. The most popular CCs among

farmers were grasses planted in monocultures or in mixtures with legumes and broadleaves. Just prior to CC termination the following spring (March–May), aboveground CC biomass samples were destructively collected by clipping two separate 1 m<sup>2</sup> areas in each of the two subplots. The CC biomass samples from each subplot were first mixed to form a composite sample and then distributed among 12 nylon mesh litter bags (0.26 by 0.6 m dimensions). Initial fresh weights of CC residues placed in each litter bag were recorded. In total, 24 litter bags were prepared at each farm site providing four sets of six litter bags. Cover crop residue  $\theta_g$  at termination was based on fresh and dry weights of time '0' litter bags. Residue  $\theta_g$  was then used to calculate the dry weight equivalent of fresh CC residues placed in each litter bag. Prior to litter bag installation, pre-existing residues were removed from the soil surface to facilitate direct contact between litter bags and the underlying soil. Litter bags were collected at approximately 0, 14, 30, 60, between 90 and 120 days after CC termination, and at corn physiological maturity. After each retrieval period, litter bags were oven-dried at 60 °C for at least a week before recording dry weights.

Residue samples from each litter bag were ground to pass through a 1-mm sieve and analyzed for C and N concentrations using dry combustion via Leco Tru-Mac CN Analyzer (LECO Corporation, St. Joseph,

MI). To account for soil contamination, 1-g of ground residue samples from each litter bag was ashed at 550 °C for 4 h. Residue mass remaining in the litter bags were corrected for ash contents to determine ‘Final ash-free residue dry weights’. Similarly, ‘Initial ash-free residue dry weights’ were calculated for each litter bag using ash content values for time ‘0’ residue samples. Measured amount of residue mass ( $RM_t$ ) and N content ( $RN_t$ ) remaining in litter bags over time were calculated using the following equations:

$$\begin{cases} \text{Measured } RM_t = \frac{(\text{Final ash-free residue dry weight})_t}{(\text{Initial ash-free residue dry weight})_0} \cdot RM_0 \\ \text{Measured } RN_t = \frac{(\text{Final ash-free residue dry weight})_t \cdot N_t}{(\text{Initial ash-free residue dry weight})_0 \cdot N_0} \cdot RN_0 \end{cases} \quad (7)$$

where,  $N_0$  and  $N_t$  represents residue N concentrations in litter bags collected at time ‘0’ and ‘ $t$ ’ hours, respectively.

#### Model input data

The modified CC-NCALC tool operates at 1-h time steps and requires data on CC dry biomass ( $RM_0; kg ha^{-1}$ ), initial residue  $\theta_g$  (g water g<sup>-1</sup> dry residue), residue N concentrations (%N), and residue C chemistry (%CARB, %CELL, and %LIGN) as input variables. Cover crop residue C chemistry was determined on time ‘0’ litter bag samples via near infrared reflectance spectroscopy (NIRS) using a scanning monochrometer (model 6500; FOSS NIRSystems, Silver Spring, MD; Gaskin et al. 2019). The CC-NCALC tool also requires hourly data on air RH and T at 2-m height and rain to simulate diurnal changes in the  $\psi_{residue}$  of surface CC residues throughout the decomposition period. We obtained hourly weather data from the in-house weather API (Application Programming Interface) built for the PSA project (<https://api.precisionustainableag.org/weather/>). Our weather API imports hourly air RH and T data from the North American Land Data Assimilation System Phase-2 (NLDAS-2; Xia et al. 2012) and hourly rain data from the Multi-Radar Multi-Sensor System (MRMS; Zhang et al. 2016).

#### Model calibration and validation: data analysis

The overall performance of the modified CC-NCALC tool during calibration and validation phases were evaluated by including all simulated versus measured

data on residue mass ( $RM_t$ ) and N ( $RN_t$ ) remaining across all site-years. We further evaluated the modified CC-NCALC tool for individual site-years. In both cases, we excluded the initial time ‘0’ values from analysis.

Performance evaluation metrics included slope and  $R^2$  obtained from simple linear regression analysis between simulated vs. measured data on residue mass ( $RM_t$ ) and N ( $RN_t$ ) remaining on the soil surface as well as model fit statistics such as the root mean square error ( $RMSE$ ), relative root mean square error ( $rRMSE$ ), and index of agreement ( $d$  Addiscott and Whitmore 1987; Whitmore 1991; Willmott 1981).

$$\left\{ \begin{array}{l} RMSE = \sqrt{\frac{\sum_{i=1}^n (S_i - M_i)^2}{n}} \\ rRMSE = \frac{RMSE}{\bar{M}} \cdot 100\% \\ d = 1 - \left[ \frac{\sum_{i=1}^n (M_i - S_i)^2}{\sum_{i=1}^n (|S_i - \bar{M}| + |M_i - \bar{M}|)^2} \right], 0 \leq d \leq 1 \end{array} \right. \quad (8)$$

where,  $M_i$  and  $S_i$  are the  $i^{th}$  measured and simulated data ( $RM_t$  or  $RN_t$  remaining),  $\bar{M}$  is the mean of the measured data, and  $n$  is the total number of observations. The  $RMSE$  represents average differences between simulated and measured data and has the same unit as that of the measured parameter (Eq. (8)). However,  $RMSE$  is more sensitive to extreme values due to squared differences. The  $rRMSE$  is calculated by dividing  $RMSE$  by the mean of the measured data and hence, represents the relative difference between simulated and measured data. In both cases, values of  $RMSE$  and  $rRMSE$  closer to 0 indicates better model performance. The  $d$  represents the ratio of the mean square error and potential error and varies between 0 and 1 (Willmott 1981). For  $d$ , a value of 1 indicates perfect match and a value of 0 indicates no agreement at all. Model fit statistics were calculated using the *hydroGOF* package in R (Zambrano-Bigiarini 2020).

## Results

### Overview of the calibration and validation dataset

The calibration and validation dataset consisted of 99 site-years of on-farm litter bag data collected across the mid-Atlantic and southeastern USA encompassing

**Table 1** Ranges of soils, climates, and management (cover crop quantity and quality) variables across 99 site-years used for calibration and validation of the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool

| Variables   | Units                 | Calibration dataset <sup>†</sup> | Validation dataset <sup>†</sup> |
|---|-----------------------|----------------------------------|---------------------------------|
| Total site-years                                    |                       | 50                               | 49                              |
| Latitude  |                       | 32.6–40.7                        | 32.6–40.7                       |
| Soil texture  |                       |                                  |                                 |
| Sand  | %                     | 7.7–86.8                         | 8.0–88.4                        |
| Clay  | %                     | 4.2–38.2                         | 4.2–30.2                        |
| Weather <sup>‡</sup>                                |                       |                                  |                                 |
| Mean daily air temperature ( <i>T</i> )             | °C                    | 20.0–25.4                        | 20.0–25.7                       |
| Mean daily air relative humidity ( <i>RH</i> )      | %                     | 70–81                            | 70–82                           |
| Cumulative rain                                     | mm                    | 330–1052                         | 280–852                         |
| Cumulative decomposition degree days ( <i>DDD</i> ) |                       | 2498–4154                        | 2321–4255                       |
| Cumulative vapor pressure deficit ( <i>VPD</i> )    | kPa                   | 1761–3981                        | 1761–4070                       |
| Cover crop metrics <sup>§</sup>                     |                       |                                  |                                 |
| Total dry biomass ( <i>RM</i> <sub>0</sub> )        | kg ha <sup>-1</sup>   | 205–10,595                       | 171–8698                        |
| Residue water content ( $\theta_g$ )                | g g <sup>-1</sup>     | 0.6–7.3                          | 0.4–6.0                         |
| N concentrations                                    | %                     | 1.1–5.7                          | 1.1–6.4                         |
| Total N content ( <i>RN</i> <sub>0</sub> )          | kg N ha <sup>-1</sup> | 6.0–165                          | 10.4–240                        |
| Carbohydrate ( <i>CARB</i> )                        | %                     | 24.2–65.0                        | 27.3–64.2                       |
| Holo-cellulose ( <i>CELL</i> )                      | %                     | 31.1–67.8                        | 33.5–66.1                       |
| Lignin ( <i>LIGN</i> )                              | %                     | 1.3–8.3                          | 1.1–8.3                         |

<sup>†</sup>Values provided in the calibration and validation dataset columns were minimum and maximum values for each variable obtained across individual site-years

<sup>‡</sup>Weather variables for individual site-years were summarized for the whole cover crop decomposition period

<sup>§</sup>Measured cover crop metrics (residue quantity, quality, and water content on dry weight basis) at cover crop termination (*t*<sub>0</sub>), i.e., at the start of simulation

a wide range of soil, weather, and management conditions (Fig. S1; Table 1). Sand and clay contents in the experimental sites ranged from 7.7 to 87% and from 4.2 to 38%, respectively. Due to a latitudinal gradient and differences in CC decomposition period (i.e., initiation and end of litter-bag study) among site-years, we observed marked differences in weather variables such as hourly air *RH* and *T*, as well as frequency, intensity, and duration of rainfall. Cumulative rain during the CC decomposition period ranged from 280 to 1052 mm. Cumulative decomposition degree days (*DDD*) calculated based on air *T* at 2-m height, using base *T* of 0 °C (Otte et al. 2019), ranged from 2321 to 4255. Similarly, cumulative vapor pressure deficit (*VPD*) calculated based on hourly air *RH* and *T* at 2-m height ranged from 1761 to 4070 kPa. A greater value for cumulative rain and cumulative *DDD* and a lower value for cumulative *VPD* indicates a more conducive environment for surface residue decomposition. We also observed great variability in CC residue

quantity and quality (e.g., residue N concentrations and residue C chemistry) variables at termination among site-years (Table 1).

Across all site-years, residue mass and N remaining in surface CC residues declined rapidly during the first 1440 h (~60 d) following CC termination. After 60 days, residues may have reached a steady state of decomposition with little or no further loss during the last two sampling times. The exponential decline patterns observed for residue mass loss and N release greatly varied among site-years due to differences in initial residue characteristics (i.e., residue quantity and quality) and environmental (i.e., soil and weather) conditions. For example, the exponential decline patterns were more evident in site-years with low initial CC biomass and residues of higher qualities (i.e., residues with more carbohydrates and low C:N or lignin:N ratios). Large CC biomass samples of inferior quality decomposed gradually and followed a less exponential decline. Even in site-years with similar

**Table 2** Optimal value of the parameters used in the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool after calibration

Same parameter values are used for all residue types

| Parameter  | Calibrated value |
|--|------------------|
| <i>K-coefficients for hourly decay rate constants (<math>k_{POOL}</math>; Eq. 2)</i>                       |                  |
| $K_{CARB}(h^{-1})$   | 0.018            |
| $K_{CELL}(h^{-1})$   | 0.010            |
| $K_{LIGN}(h^{-1})$   | 0.00095          |
| <i><math>k_{POOL}</math> adjustment factors (Eq. 3)</i>  |                  |
| Base temperature for decomposition (°C)  | 0                |
| Critical C:N ratio   | 13               |
| Critical residue mass in direct soil contact ( $RM_{min}$ ; (kg ha <sup>-1</sup> )                         | 1400             |
| Optimal residue mass above which decomposition is no longer impacted ( $RM_{max}$ ; (kg ha <sup>-1</sup> ) | 3000             |

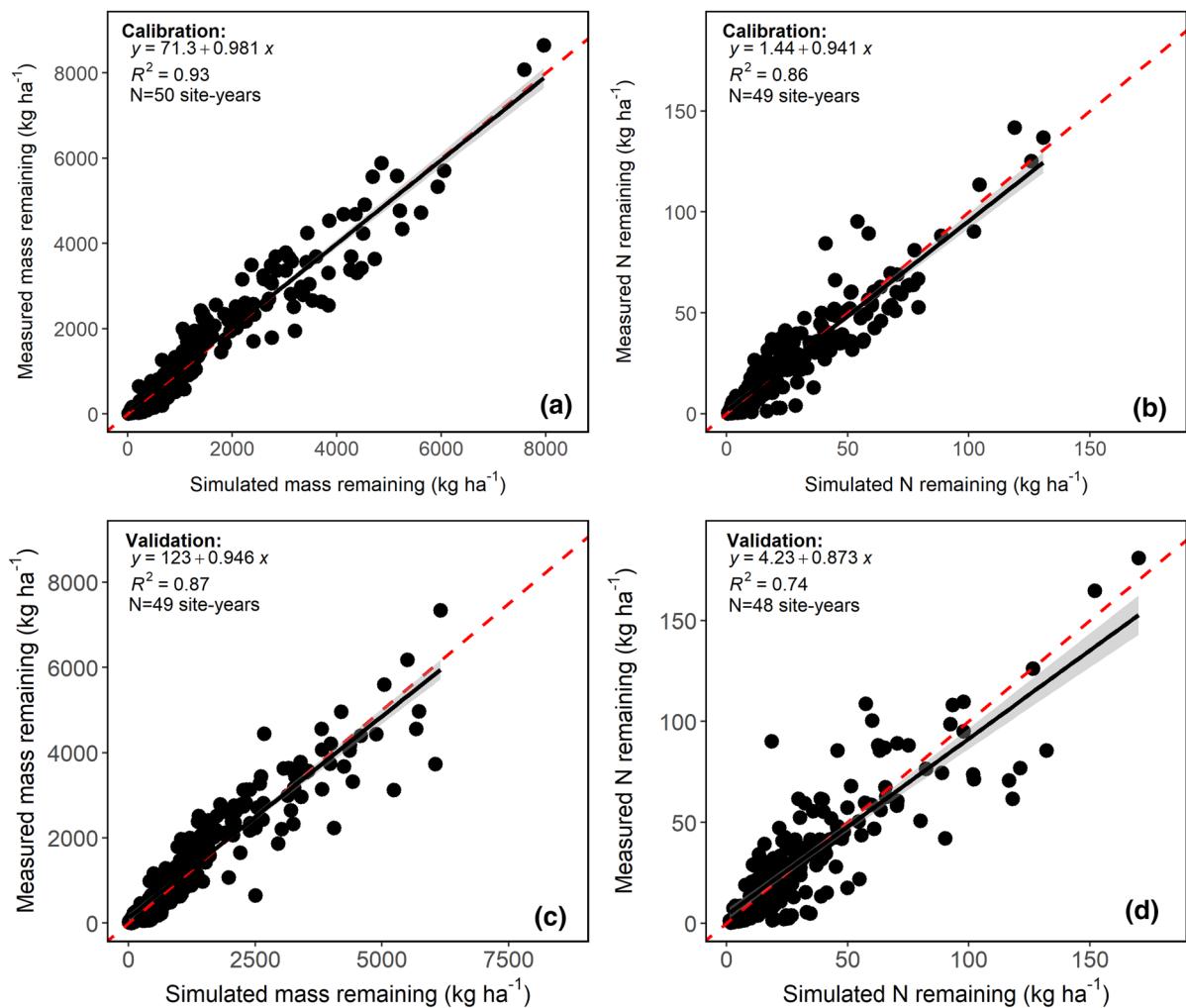
initial residue characteristics, micro-climatic differences caused variations in exponential decay and N release patterns. For example, despite having similar starting values for CC residue quantity and quality, residue mass and N remaining declined quicker due to higher air RH, T, and rainfall in days following CC termination in site-year ID# 74 as compared to that in ID# 75. This existing variability in decomposition and N release patterns among site-years presented an ideal dataset to calibrate and validate the modified CC-NCALC tool across diverse environments.

#### Modified CC-NCALC tool: calibration

The modified CC-NCALC tool was calibrated to accurately simulate CC residue mass and N remaining on the soil surface at different sampling times. First, hourly decay rate constants for each residue C component (i.e.,  $k_{CARB}$ ,  $k_{CELL}$ , and  $k_{LIGN}$ ) were adjusted manually to best fit simulated vs. measured data. For this, we used measured data from site-years with low initial CC biomass ( $RM_o < \sim 2000$  kg ha<sup>-1</sup>) values. When  $RM_o$  is small, all residue particles are most likely in direct contact with underlying soils and hence, residue *ContactFactor* is set to 1, permitting the most rapid decomposition rate. Calibration resulted in the following values of *K* coefficients for all residue types:  $K_{CARB}=0.018\ h^{-1}$ ,  $K_{CELL}=0.010\ h^{-1}$ , and  $K_{LIGN}=0.00095\ h^{-1}$  (Table 2; Fig. 1d). The calibrated value for  $k_{LIGN}$  under non-limiting conditions was the same as estimated by Vigil et al. (1991) and then adapted in other CERES-N sub-model validation studies (Quemada and Cabrera 1995; Woodruff et al. 2018).

During initial simulations using best-fitted hourly decay rate constants, the modified CC-NCALC tool consistently over-predicted decomposition in site-years with greater initial CC biomass. Based on our calibration, the critical value of residue mass in direct soil contact ( $RM_{min}$ ) was 1400 kg ha<sup>-1</sup> for all residue types (Table 2; Fig. 1c). Above 1400 kg ha<sup>-1</sup>, CC residues decomposed at a slower rate. For all residue types, the optimal value of residue mass above which  $k_{POOL}$  does not decrease further ( $RM_{max}$ ) was 3000 kg ha<sup>-1</sup> (Table 2; Fig. 1c). This is probably because CC mulch environmental conditions at the soil-residue interface via. increased thickness of the mulch layer favor increased rates of decomposition and offset the reduced *ContactFactor* within increasing biomass levels above 3000 kg ha<sup>-1</sup>. Decomposition rates decreased as residue mass increased between 1400 and 3000 kg ha<sup>-1</sup>.

Finally, we increased the value of residue rewetting from 0.002 to 0.0026 g water g<sup>-1</sup> residue h<sup>-1</sup> in Eq. (8) in Dann et al. (2021). This is based on the calibration of the surface  $\psi_{residue}$  module using diurnal  $\psi$  data collected on surface residues under the crop canopy. Surface CC residues re-wet faster and gain more moisture under crop canopy than when exposed directly to solar radiation. Moreover, in the surface  $\psi_{residue}$  module, the effect of dew deposition and rain on water content of surface residues varied between cereal rye and crimson clover residues (Dann et al. 2021). Since CC species and mixture composition varied in our dataset, we used functions determined for crimson clover residues only when initial residue N and carbohydrate concentrations were greater than or equal to 2.25 and 50%, respectively. Greater N and soluble carbohydrate concentrations with narrow C:N



**Fig. 2** Regression analysis comparing measured and simulated data on **a, c** cover crop residue mass remaining and **b, d** cover crop residue N remaining on the soil surface at different sampling times across all site-years during calibration and validation phases. Simulated values were obtained using the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool. The red dashed line represents the 1:1 line

phases. Simulated values were obtained using the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool. The red dashed line represents the 1:1 line

( $\leq 18$ ) ratios is a typical characteristic of legume CC residues such as crimson clover. For residues with residue N and carbohydrate concentrations smaller than 2.25% and 50%, respectively, we used functions for cereal rye as developed by Dann et al. (2021).

Overall performance of the modified CC-NCALC tool with the calibrated parameters was satisfactory (Fig. 2a, b). Across all site-years in the calibration dataset, we observed a good fit between measured and simulated data on residue mass (slope = 0.98; intercept =  $71 \text{ kg ha}^{-1}$ ;  $R^2 = 0.93$ ) and N (slope = 0.94; intercept =  $1.44 \text{ kg N ha}^{-1}$ ;

$R^2 = 0.86$ ) remaining in the litter bags at different sampling times (Fig. 2a, b). Similarly, model fit statistics also suggest that simulations were in agreement with measured data for both residue mass ( $\text{RMSE} = 403 \text{ kg ha}^{-1}$ ;  $\text{rRMSE} = 27\%$ ;  $d = 0.98$ ) and N ( $\text{RMSE} = 9.1 \text{ kg N ha}^{-1}$ ;  $\text{rRMSE} = 34\%$ ;  $d = 0.96$ ) remaining during the CC decomposition period (Table 3).

Variations in weather and initial CC residue characteristics among individual site-years in the calibration dataset along with model fit statistics are provided in Fig. 3. Across individual site-years, RMSE for residue

**Table 3** Model fit statistics representing overall performance of the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool during calibration and validation site-years for predicting

cover crop residue mass and N remaining on the soil surface through time in conservation tillage-based corn systems in the mid-Atlantic and Southeastern USA

| Model testing | Site-years | Residue mass remaining                   |                        |                | Residue N remaining           |           |      |
|---------------|------------|--|------------------------|----------------|-------------------------------|-----------|------|
|               |            | RMSE <sup>†</sup> (kg ha <sup>-1</sup> ) | rRMSE <sup>‡</sup> (%) | d <sup>§</sup> | RMSE (kg N ha <sup>-1</sup> ) | rRMSE (%) | d    |
| Calibration   | 50         | 402.5                                    | 27.0                   | 0.98           | 9.1                           | 33.7      | 0.96 |
| Validation    | 49         | 483.0                                    | 33.2                   | 0.97           | 15.1                          | 47.8      | 0.93 |

<sup>†</sup>RMSE, root mean square error

<sup>‡</sup>rRMSE, relative root mean square error

<sup>§</sup>d, Willmott's index of agreement between measured and simulated data

mass and N remaining predictions ranged between 13.5 to 980 kg ha<sup>-1</sup> and 0.7 to 27 kg N ha<sup>-1</sup>, respectively (Fig. 3c). As initial CC biomass increased from 205 to 10,595 kg ha<sup>-1</sup>, RMSE also tended to increase gradually. However, no such trend was observed for other model fit statistics (Fig. 3d, e). The rRMSE was below 50% for both residue mass (rRMSE≤50% in 36 out of 50 site-years; 30%<rRMSE<50% in 12 out of 50 site-years; rRMSE≥50% in 2 out of 50 site-years) and N (rRMSE≤30% in 26 out of 47 site-years; 30%<rRMSE<50% in 19 out of 47 site-years; rRMSE≥50% in 2 out of 47 site-years) remaining predictions for most site-years (Fig. 3d). Similarly, in most cases, the index of agreement (*d*) between simulated and measured values were greater than 0.70 for both residue mass (*d* ≥0.90 in 38 out of 50 site-years; 0.70<*d*<0.90 in 10 out of 50 site-years; *d* ≤0.70 in 2 out of 50 site-years) and N (*d* ≥0.90 in 30 out of 47 site-years; 0.70<*d*<0.90 in 13 out of 47 site-years; *d*≤0.70 in 4 out of 47 site-years) remaining at different sampling times (Fig. 3e). Despite considerable variations in soil, weather, and initial residue characteristics in the calibration dataset, our results suggest that the calibrated version of the modified CC-NCALC tool simulated reasonably well decomposition and N mineralization-immobilization from surface CC residues in conservation tillage-based corn systems (Fig. 3, S1, S2).

#### Modified CC-NCALC tool: validation

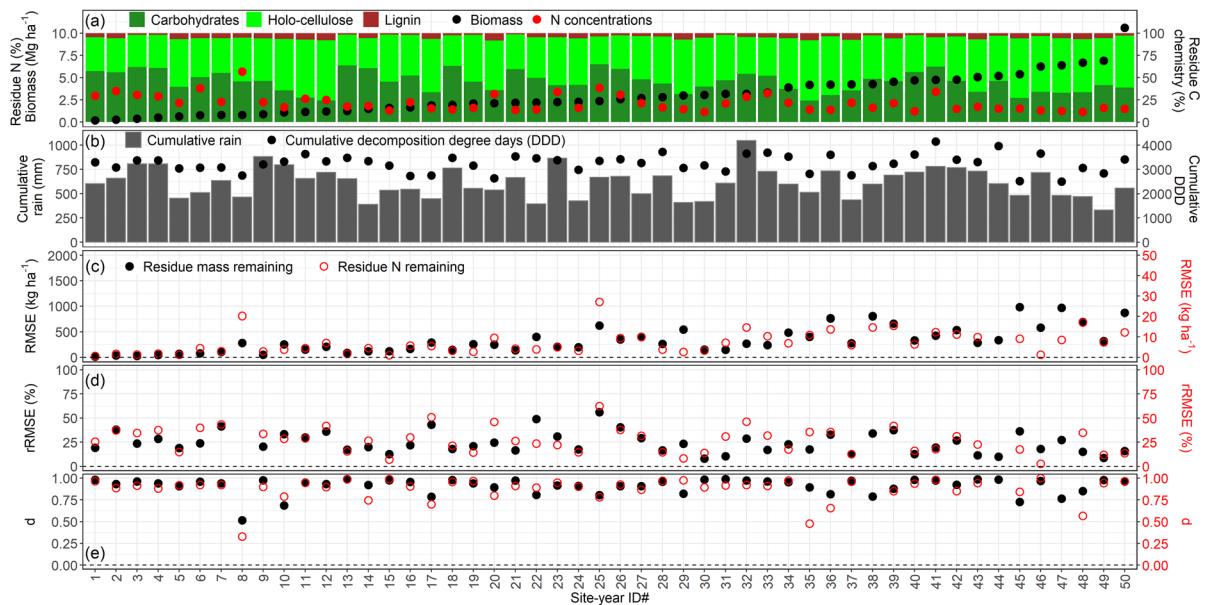
For the validation dataset, overall model simulations were in good agreement with measured data on residue mass (slope=0.95; intercept=123 kg ha<sup>-1</sup>; R<sup>2</sup>=0.87) and N (slope=0.87;

intercept=4.23 kg N ha<sup>-1</sup>; R<sup>2</sup>=0.74) remaining in litter bags at different sampling times (Fig. 2c, d). Similarly, lower values of RMSE and rRMSE and higher values of *d* obtained from comparing simulated and measured data on residue mass (RMSE=483 kg ha<sup>-1</sup>; rRMSE=33%; *d*=0.97) and N (RMSE=15 kg N ha<sup>-1</sup>; rRMSE=48%; *d*=0.93) remaining further indicated reasonably good performance of the calibrated CC-NCALC tool (Table 3).

During validation phase, we further evaluated the performance of the calibrated CC-NCALC tool across individual site-years. For most of the validation site-years, simulated values of residue mass and N remaining fell within the standard deviation of the measured data for most of the sampling times (Figs. 4, 5). The model fit statistics along with variations in weather and initial residue characteristics for individual validation site-years are shown in Fig. 6. For residue mass remaining predictions, RMSE values were below 1000 kg ha<sup>-1</sup> in 48 out of 49 site-years (Fig. 6c). The RMSE values were below 25 kg N ha<sup>-1</sup> for residue N remaining predictions in 44 out of 48 site-years (Fig. 6c). In a similar manner, for most site-years, rRMSE values were below 50% and *d* above 0.70 for both residue mass and N remaining predictions (Fig. 6d, e).

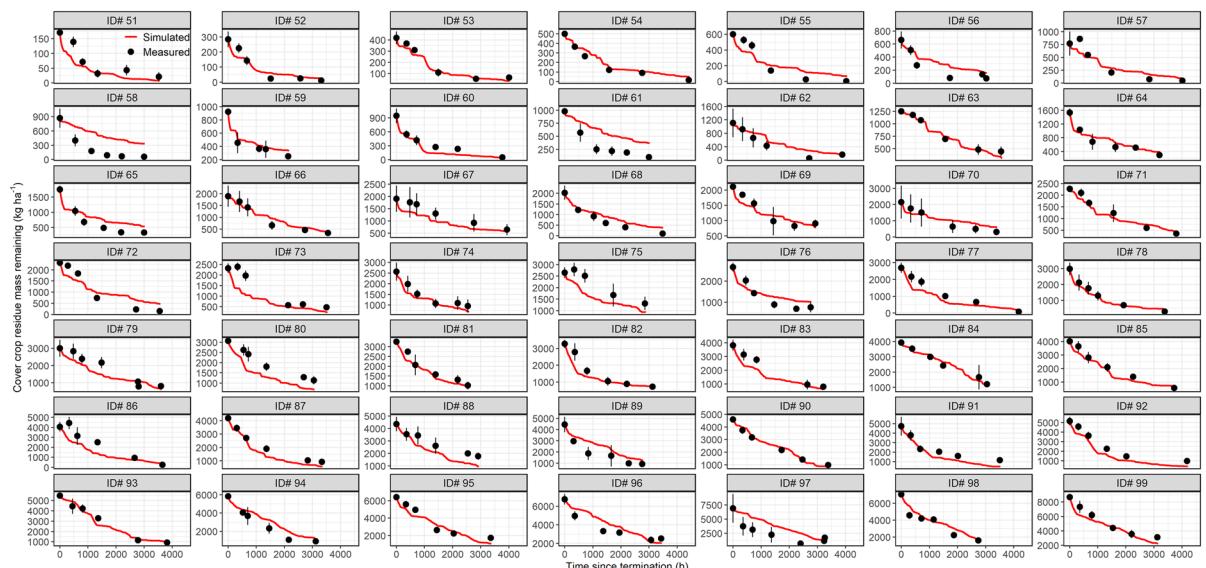
#### Cumulative residue mass loss and N release

The modified CC-NCALC tool also provided an accurate estimate of cumulative mass loss and N release at the end of each single-year CC decomposition period (Fig. 7a, b). In this study, CC decomposition period varied across site-years and ranged from 89 to 184 days following CC termination until corn



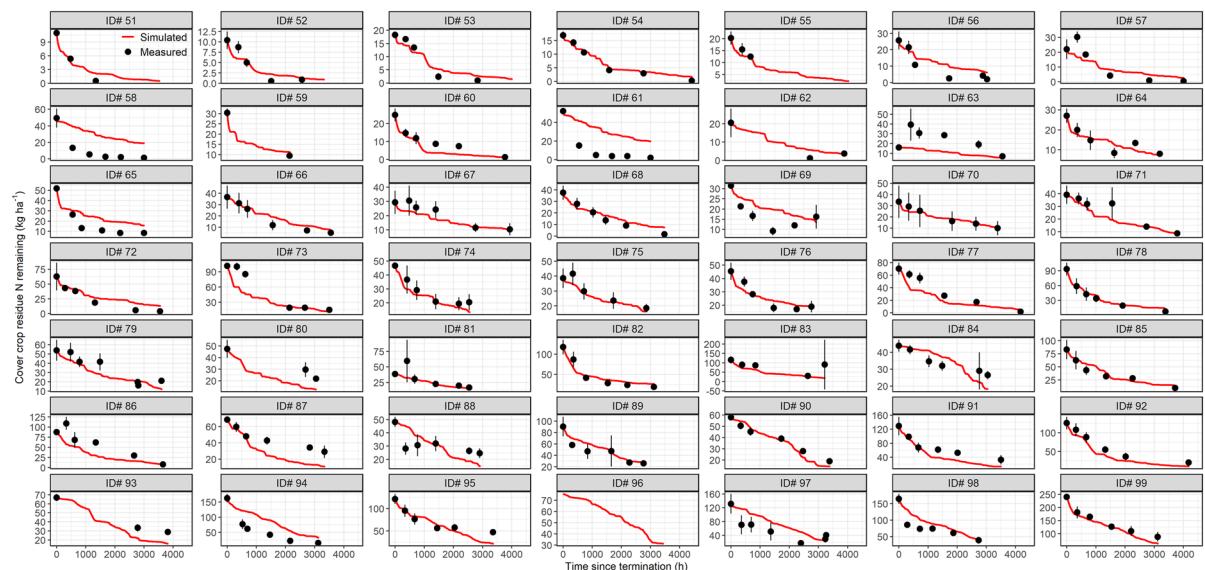
**Fig. 3** Model fit statistics showing the performance of the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool for individual site-years in the calibration dataset: **a** Differences in initial residue characteristics at cover crop termination such as residue dry biomass, residue N concentrations, and residue C chemistry (carbohydrate, holo-cellulose, and lignin fractions); **b** Weather variations during the cover crop decomposition period such as cumulative rain and cumulative

decomposition degree days (DDD); **c** root mean square error (RMSE), **d** relative RMSE (rRMSE), and **e** index of agreement **d** between measured and simulated data on cover crop residue mass (black solid circles) and N (open red circles) remaining on the soil surface at different sampling times. Site-year IDs were arranged in increasing order of cover crop biomass at termination



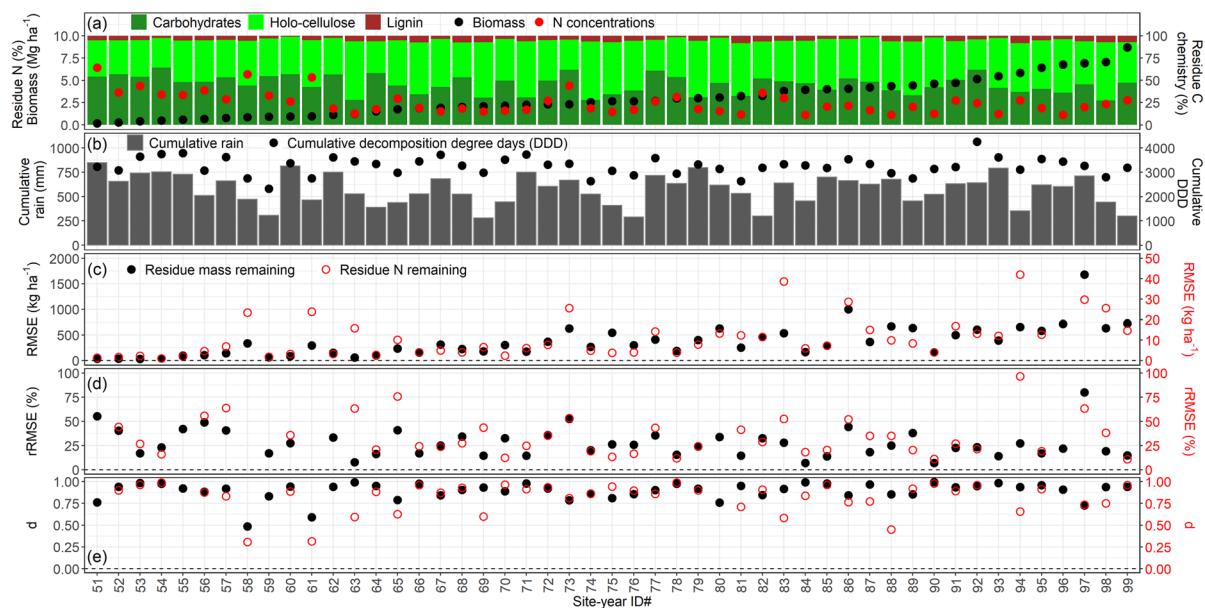
**Fig. 4** Cover crop residue mass remaining ( $\text{kg ha}^{-1}$ ) on the soil surface through time during the decomposition period as predicted by the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool for individual site-years in the validation

dataset. Measured data based on on-farm litter bag decomposition studies are shown as symbols with vertical error bars representing  $\pm$  standard deviations. Note differences in the y-axis values



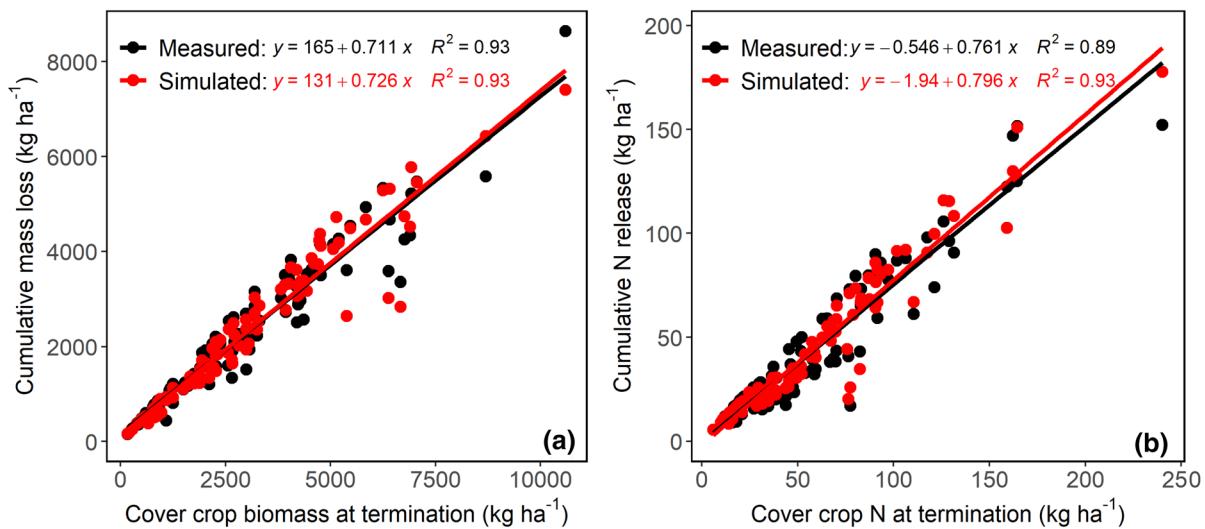
**Fig. 5** Cover crop residue N remaining ( $\text{kg N ha}^{-1}$ ) on the soil surface through time during the decomposition period as predicted by the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool for individual site-years in the validation dataset. Measured data based on on-farm litter bag decomposition stud-

ies are shown as symbols with vertical error bars representing  $\pm$  standard deviations. All measured values were missing for site ID# 96 as samples for this site were lost during sample processing step. Note differences in the y-axis values



**Fig. 6** Model fit statistics showing performance of the modified Cover Crop Nitrogen Calculator (CC-NCALC) tool for individual site-years in the validation dataset: **a** Differences in initial residue characteristics at cover crop termination such as residue dry biomass, residue N concentrations, and residue C chemistry (carbohydrate, holo-cellulose, and lignin fractions); **b** Weather variations during the cover crop decomposition period such as cumulative rain and cumulative decomposi-

tion degree days (DDD); **c** root mean square error (RMSE), **d** relative RMSE (rRMSE), and **e** index of agreement  $d$  between measured and simulated data on cover crop residue mass (black solid circles) and N (open red circles) remaining on the soil surface at different sampling times. Site-year IDs were arranged in increasing order of cover crop biomass at termination



**Fig. 7** Regression analysis showing simulated and observed relationships between **a** cover crop residue biomass at termination versus cumulative residue mass loss and **b** cover crop residue N content at termination versus cumulative residue N

release by the end of a single-year cover crop decomposition period. Cover crop decomposition was tracked from termination until corn harvest, which lasted for 89–184 days across site-years

harvest. Results showed that measured and simulated relationships were in good agreement between cumulative mass loss vs CC biomass at termination and cumulative N release vs CC N content at termination. By the end of the single-year CC decomposition period, approximately 71% of the initial CC biomass at termination was mineralized and lost from surface CC residues as  $\text{CO}_2$  into the atmosphere or added back into soil reserves (Fig. 7a). During the same period, approximately 76% of the initial CC N content at termination was released from surface CC residues (Fig. 7b).

## Discussion

Modified CC-NCALC tool simulates surface residue decomposition and N release in conservation tillage systems

Cover crops are frequently included in conservation tillage-based crop rotations to suppress weeds, conserve soil water, and supply N to subsequent cash crops, among other ecosystem services (Blanco-Canqui et al. 2015; Daryanto et al. 2018; Mirsky et al. 2012). The degree to which CCs provides these services greatly varied both in space and time

due to differences in residue decomposition and N release patterns. Therefore, optimal provisioning of ecosystem services from CCs in cropping systems will require robust models and tools that can provide realistic simulations of surface residue decomposition and N release in CC-based conservation tillage systems.

In general, the decomposition and N release from surface CC residues followed an exponential decay pattern in most site-years (Figs. 4, 5, S2, S3). This is in great accordance with prior CC decomposition studies in conservation tillage systems (Croizer et al. 1994; Jahanzaid et al. 2016; Pantoja et al. 2016; Poffenbarger et al. 2015; Quemada et al. 1997; Ranells and Waggoner 1992; Schomberg and Cabrera 2001; Waggoner 1989; Wilson and Hargrove 1986). In our previous study using the same dataset, we further observed that the exponential decay rate constants decreased with increase in residue biomass and metrics of poor quality (i.e., greater holo-cellulose, high C:N or lignin:N), but increased with increasing carbohydrate fractions (Thapa et al. 2022). Micro-climatic differences among site-years also caused variations in the observed residue decomposition and N release patterns. Weather variables such as higher air RH and frequently occurring rain events keeps surface residues moist for longer duration, thereby

enhancing the decomposition of surface residues in conservation tillage systems (Thapa et al. 2022). We modified the CC-NCALC tool to capture our mechanistic understanding of surface residue decomposition and N release via the integration of surface  $\psi_{residue}$  module within CC-NCALC and the adjustments of  $k_{POOL}$  based on residue environment (*MTRF*), C:N ratio factor (*CNRF*), and fractional soil-residue contact (*ContactFactor*).

Model calibration and validation are also critical components of building robust decision support tools that farmers and agricultural professionals can use to inform their residue and N management decisions. Schomberg and Cabrera (2001) further noted that the applicability of models and tools for management decisions is often restricted to its region of validation. Due to data limitations caused either by incomplete reporting of soil, climate, and management details or disaggregation between primary field researchers and modelers (McClelland et al. 2021), most existing models and tools lack rigorous calibration and validation which greatly restricted their adaptability and applicability in agricultural settings. To overcome such limitations, we calibrate and validate the modified CC-NCALC tool across diverse soils, weather, and management scenarios.

The modified CC-NCALC tool was able to capture the observed variations in surface CC residue decomposition and N release patterns in most site-years during both calibration (Fig. S2, S3) and validation (Fig. 4, 5) phases. Despite considerable variations in residue types and their intrinsic characteristics as well as soils and weather conditions, the simulated results for residue mass as well as N remaining on the soil surface agreed well with the empirical measurements obtained via our on-farm litter bag decomposition studies. The regression and model fit statistics calculated across all site-years (Fig. 2; Table 3) or for each individual site-year (Figs. 3, 6) also indicated good agreement between measured and simulated results. Moreover, the regression and model fit statistics obtained were similar for both calibration and validation site-years and were within the range reported in prior residue decomposition studies (Bowen et al. 1993; Findeling et al. 2007; Melkonian et al. 2017; Mohanty et al. 2011; Quemada et al. 1997; Schomberg and Cabrera 2001). Therefore, we can conclude that the modified CC-NCALC tool provides realistic estimates of surface CC residue persistence and N

release across diverse environments. The modified CC-NCALC tool was also able to capture cumulative residue mass loss and N release in conservation tillage systems and we found good agreement between simulated and measured results (Fig. 7). These results provide greater confidence in the use of the modified CC-NCALC tool as a decision support tool by farmers and land managers to optimize ecosystem services in CC-based conservation tillage systems.

To serve the diverse needs of varied stakeholders (i.e., researchers, farmers, and agricultural professionals), we developed a new user-friendly interface of the modified CC-NCALC tool that is made publicly available for use free of cost (<https://cc-ncalc.org/>). At a minimum, users need to provide their field location, CC termination date, and CC biomass and N concentrations at the time of termination. If other input data that are required to execute the CC-NCALC are unavailable, the tool either will use a default value (e.g., CC residue  $\theta_g$  at termination) or will estimate based on other input variables (e.g., CC residue C chemistry are estimated based on initial residue N concentrations). To further minimize data overload on users, the CC-NCALC tool automatically imports site-specific soil properties from the NRCS' Soil Survey Geographic database and hourly weather data from the in-house weather API. The deployment of the public-facing user-friendly interface with minimum data requirements and fast execution times will likely contribute to the wide-spread adoptability and applicability of the modified CC-NCALC tool for making residue and N management decisions and recommendations among farmers and agricultural professionals.

#### Modified CC-NCALC tool: strengths

Our study also provides key insights into the strengths and limitations of the modified CC-NCALC tool. Unlike residues incorporated into the soil, surface CC residues are heavily under the influence of atmospheric variables (e.g., air RH, T, solar radiation, wind, dew, and rain) and thus, exhibit large fluctuations in the  $\theta_g$  or  $\psi_{residue}$  than underlying soils (Dann et al. 2021; Thapa et al. 2021b). Similar fluctuations in surface residue environmental conditions were found in a series of rainfall simulation experiments under controlled conditions (Coppens et al. 2007; Findeling et al. 2007). Coppens et al. (2007) further observed that the moisture adjustment factor was sensitive to wetting and drying cycles for surface CC

residues; moisture adjustment factor calculated based on surface  $\psi_{residue}$  were significantly lower than those calculated based on surface  $\psi_{soil}$  throughout the drying period. In separate controlled experiments, strong interactive effects of  $\psi_{residue}$  and T on C and N mineralization from surface CC residues have been observed (Quemada and Cabrera 1997; Thapa et al. 2021a). Despite such evidences, existing process-based residue decomposition models adjust  $k_{POOL}$  values based on moisture and T of underlying surface soils. This has led to over-prediction in N mineralization from surface CC residues with existing models. Therefore, a great strength of the modified CC-NCALC tool over existing models and tools is that the  $k_{POOL}$  values are now adjusted based on the residue environment ( $\psi_{residue}$  and T).

Another important modification in the modified CC-NCALC tool is the use of a residue *ContactFactor* to further adjust  $k_{POOL}$  based on fractional mass of surface residues in contact with the soil. Surface residue decomposition rates decreased as biomass increased due to a decrease in proportion of residue mass in contact with underlying soils (Steiner et al. 1999; Stott et al. 1990; Thapa et al. 2022; Thorburn et al. 2001). Only a few process-based residue decomposition models have explicitly considered this aspect. In the PASTIS-mulch model, Findeling et al. (2007) only considered decomposition of the bottom residue layer near soil microorganisms. The upper residue layer remains undecomposed and gradually feeds the actively decomposing bottom layer over time. While the theoretical concept is similar, residue mass effects in the APSIM-Residue model is addressed differently via adjustment of overall decomposition rates of the whole residue layer using the residue *ContactFactor* (See Eq. (7) in Thorburn et al. 2001). Because of its simplicity, we adopted the residue *ContactFactor* proposed by Thorburn et al. (2001) in the modified CC-NCALC tool with slight modifications (See Eq. (3)). The new *ContactFactor* derived in this study provides a more practical approach for adjusting decomposition rates across gradients of surface CC residue masses.

#### Modified CC-NCALC tool: limitations and future research areas

Despite finding good agreement between measured and simulated results in most site-years, the modified CC-NCALC tool under-estimated decomposition and N release from surface CC residues in two out of

three site-years when initial residue N concentrations were greater than 5% (Site-year ID# 58 and ID# 61 in Figs. 4 and 5). In these site-years, a greater proportion of soluble C and N in CC residues, coupled with frequent rainfall events may have resulted in initial leaching and gaseous losses as characterized by measurement points with larger residue N than mass losses. However, the CC-NCALC focuses on microbial-driven decomposition and does not account for initial leaching and gaseous losses of C and N from surface CC residues. Therefore, detailed accounting of initial leaching and gaseous losses would be necessary in the modified CC-NCALC tool, particularly in site-years with high residue N concentrations (i.e., > 5% N).

Another limitation with the modified CC-NCALC tool was a failure to estimate initial N immobilization observed with poor-quality CC residues (e.g., site-year ID# 63 in Fig. 5). This was probably because N immobilization in the modified CC-NCALC tool is estimated by assuming a fixed value of microbial N demand for decomposition (i.e., 0.0213 g N required per g RM decomposed). As described earlier, this value is obtained by multiplying the fraction of C in residues (i.e., 0.426 g g<sup>-1</sup>) by the microbial C use efficiency (i.e., 0.4 g C assimilated g RM decomposed) and then dividing by the microbial biomass C:N (i.e., 8). While C fractions are mostly constant across residue types (Thapa et al. 2022), microbial C use efficiency and microbial biomass C:N varies across residue types and during decomposition depending on environmental (e.g., moisture and temperature), stoichiometric (e.g., residue N availability, residue C:N, and C chemistry), and ecological (e.g., microbial community composition) factors (Manzoni et al. 2010, 2017). Researchers have shown that microbial C use efficiency increases as temperature decreases, residue N availability increases (i.e., residue C:N decreases), and the degree of recalcitrance decreases (Manzoni et al. 2010, 2012, 2017; Moorhead and Sinsabaugh 2006; Nicolardot et al. 2001; Qiao et al. 2019). Similarly, microbial biomass C:N typically lies between 8 and 15 and increases with increasing residue C:N (Manzoni et al. 2010; Nicolardot et al. 2001). Additional work is needed to allow flexible values of microbial C use efficiency and microbial biomass C:N depending on environmental and stoichiometric variables.

In the modified CC-NCALC tool, CC residue is fractionated into CARB, CELL, and LIGN pools all

of which decompose congruently at varying rates. However, N is allocated proportionally among these pools. This means all three pools are assumed to have the same C:N ratio in the CC-NCALC. By allowing for different C:N ratios in each pool in the APSIM SoilN module, Probert et al. (2005) were able to better simulate initial immobilization of N observed for various animal manures and feed materials. This work suggests an additional modification in the CC-NCALC that could probably improve its estimation of N immobilization during residue decomposition. Finally, even if N mineralization from soil organic matter is underpredicted, then N immobilization will be underpredicted due to inaccuracies in the amount of soil inorganic N available for microbial immobilization. Clearly, more work is needed to improve simulation of N immobilization in the modified CC-NCALC tool.

## Summary and conclusions

In this study, we modified the CC-NCALC tool to reflect our mechanistic understanding of the decomposition and N mineralization-immobilization from surface CC residues in conservation tillage systems. We: (1) integrated surface  $\psi_{residue}$  module to provide a realistic simulation of the residue mulch environmental conditions; (2) allowed fresh residue inputs to be specified in terms of its fractionation into three C pools (i.e., CARB, CELL, and LIGN); (3) allowed  $k_{POOL}$  to vary for each pool in such a way to account for lignin control on decomposition; and (4) finally, adjusted  $k_{POOL}$  based on surface residue environment (i.e., MTRF for  $\psi_{residue}$  and T dynamics), N limitations (i.e., CNRF), and fractional soil-residue contact (i.e., ContactFactor). As a result, the modified CC-NCALC was able to capture surface CC residue decomposition and N release patterns across diverse soils, weather, and management conditions. Therefore, the modified CC-NCALC tool is a robust decision support tool that farmers and land managers can use to make evidence-based decisions regarding residue persistence and N management in CC-based conservation tillage systems. Moreover, the user-friendly interface of the modified CC-NCALC tool requires minimum input data from users and has faster execution times. These improvements to the user experience will result in its wide-spread adoptability and

applicability among varied stakeholders. Further improvements to the CC-NCALC decision tool will focus on adequate representation of initial leaching and gaseous losses from low C:N residues, more accurate simulation of initial N immobilization from high C:N residues and N mineralization from soil organic matter, and allowing C:N ratios to also differ for each residue C pools.

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## Declarations

**Conflict of interest** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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