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Review and analysis of strengths and weaknesses of agro-ecosystem models for simulating C and N fluxes

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Title: Review and analysis of strengths and weaknesses of agro-ecosystem models for simulating C and N fluxes

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Abstract: Biogeochemical simulation models are important tools for describing and quantifying the contribution of agricultural systems to C sequestration and GHG source/sink status. The abundance of simulation tools developed over recent decades, however, creates a difficulty because predictions from different models show large variability. Discrepancies between the conclusions of different modelling studies are often ascribed to differences in the physical and biogeochemical processes incorporated in equations of C and N cycles and their interactions. Here we review the literature to determine the state-of-the-art in modelling agricultural (crop and grassland) systems. In order to carry out this study, we selected the range of biogeochemical models used by the CN-MIP consortium of FACCE-JPI (<http://www.faccejpi.com>): APSIM, CERES-EGC, DayCent, DNDC, DSSAT, EPIC, PaSim, RothC and STICS. In our analysis, these models were assessed for the quality and comprehensiveness of underlying processes related to pedo-climatic conditions and management practices, but also with respect to time and space of application, and for their accuracy in multiple contexts. Overall, it emerged that there is a possible impact of ill-defined pedo-climatic conditions in the unsatisfactory performance of the models (45.9%), followed by limitations in the algorithms simulating the effects of management practices (33.8%). The multiplicity of scales in both time and space is a fundamental feature, which explains the remaining weaknesses (i.e. 20.3%). Innovative aspects have been identified for future development of C and N models. They include the explicit representation of soil microbial biomass to drive soil organic matter turnover, the effect of N shortage on SOM decomposition, the improvements related to the production and consumption of gases and an adequate simulations of gas transport in soil. On these bases, the assessment of trends and gaps in the modelling approaches currently employed to

represent biogeochemical cycles in crop and grassland systems appears an essential step for future research.

Response to Reviewers: Revision 2

Reviewer #3: The authors provide a thorough review of models for modeling C and N cycling in agronomic systems. The review is interest and informative, especially with regards to highlighted discrepancies in modeling capacity and accuracy. This research is important for modeling GHG, and impacts of management practices on agricultural output of GHG. Especially useful is the identification of shortcoming and potential sources of error in the models tested. The manuscript should be published after (very) minor revision. Minor suggested changes:

1. Line 58: and an adequate simulation of gas
Response to Reviewer comment No. 1: Modified as suggested.
2. line 58: Given these conditions, the assessment
Response to Reviewer comment No. 2: Modified as suggested.
3. Line 83-84: that C and nitrogen (N) cycling strongly depend on
Response to Reviewer comment No. 3: Modified as suggested.
4. Line 102: even when models are run under the same conditions of
Response to Reviewer comment No. 4: Modified as suggested.
5. Line 150: carbon dioxide (CO₂), and nitrate (NO₃)
Response to Reviewer comment No. 5: Modified as suggested.
6. Line 191: adequate options and parameters values allows to simulate simulation of a wide
Response to Reviewer comment No. 6: Modified as suggested.
7. Line 193: It allows considering consideration of the effect
Response to Reviewer comment No. 7: Modified as suggested.
8. Line 211: Then, in theat level 2
Response to Reviewer comment No. 8: Modified as suggested.
9. Line 218: knowledge on of the
Response to Reviewer comment No. 9: Modified as suggested.
10. line 275: of N in the soil profile
Response to Reviewer comment No. 10: Modified as suggested.
11. line 293-4: Reference evapotranspiration is accounted bycalculated using the Penman-Monteith (56%), or Penman and Priestley-Taylor (44%) equations.
Response to Reviewer comment No. 11: Modified as suggested.
12. Line 311-13: In general from our analysis indicated emerged that the three main processes belonging to the general class of GHG emissions and other fluxes are almost fully simulated by the considered models. Merge single-sentence paragraphs into larger paragraphs throughout results.
Response to Reviewer comment No. 12: Modified in the text: (see L:315:318: "For better assessing how C and N cycles are involved in the simulation of GHG emissions and other fluxes within several models, three

main processes were identified (Table S4, see supplementary material). Overall, our analysis indicates that these three main processes are almost fully simulated by the considered models").

13. Line 314: In the main process called CO2 the The most important C-fluxes from the ecosystems were considered in the main process called "CO2".

Response to Reviewer comment No. 13: Modified as suggested.

14. Line 364: e.g. STICS accounts for burial through tillage

Response to Reviewer comment No. 14: Modified as suggested.

15. Line 393: such as patterns of air temperature, precipitation, solar radiation, also and including

Response to Reviewer comment No. 15: Modified as suggested.

16. Line 427: i.e. under- or over-estimation

Response to Reviewer comment No. 16: Modified as suggested.

17. Line 432: anaerobic conditions, e.g. Bollmann

Response to Reviewer comment No. 17: Modified as suggested.

18. Line 461: The Amount amount of bound enzymes increases with the increasing layer charge of

Response to Reviewer comment No. 18: Modified as suggested.

19. Line 466: affects the amount of soil enzymes

Response to Reviewer comment No. 19: Modified as suggested.

20. Line 467: At leastAnd finally, the increase. Throughout, change "fine texture soil" to "fine textured soil"

Response to Reviewer comment No. 20: Modified as suggested.

21. Line 502: due to different types of

Response to Reviewer comment No. 21: Modified as suggested.

22. Line 529: the models subroutines

Response to Reviewer comment No. 22: Modified as suggested.

23. Line 531: the fact that the model

Response to Reviewer comment No. 23: Modified as suggested.

24. Line 605: underestimation of particulate organic C

Response to Reviewer comment No. 24: Modified as suggested.

25. Line 607: fertilization and tillage, which were probably the most commonly simulated

Response to Reviewer comment No. 25: Modified as suggested.

26. Lines 619-20: related to the ecosystem and climate, which makes it difficult to define the parameter which most strongly

Response to Reviewer comment No. 26: Modified as suggested.

27. Lines 627-8: rice cultivation being too low (i.e. effect of waterlogged soil not included in RothC) being too low

Response to Reviewer comment No. 27: Modified as suggested.

28. Line 643: ones where they have been previously

Response to Reviewer comment No. 28: Modified as suggested.

29. Line 656: with the results of Li et al. (2005),
Response to Reviewer comment No. 29: Modified as suggested.

30. Line 680: agriculture fits
Response to Reviewer comment No. 30: Modified as suggested.

31. Line 693: physics, and the interface between the two that
Response to Reviewer comment No. 31: Modified as suggested.

32. Line 749: to optimize resources
Response to Reviewer comment No. 32: Modified as suggested.

33. Several places: correct spelling of vermiculite
Response to Reviewer comment No. 33: Corrected

34. Line 834: should take into account for ions interactions
Response to Reviewer comment No. 34: Modified as suggested.

35. Lines 858-861: For the N cycle, the main limitations inherent in model structure were found under different pedo-climatic conditions (51.7%), whilst for the scale of application the major weaknesses were due to different pedo-climatic conditions (20.4%). Consider rewrite - it's a bit cumbersome as written.

Response to Reviewer comment No. 35: Modified in the text: (see L:865:867: "For both the N-cycle modelling and scale of application, the main limitations were found in the response to different pedo-climatic conditions (51.1% and 20.2%, respectively).

Reviewer #4: This manuscript is trying to present a comprehensive analysis of the strengths and weaknesses of existing state-of-the-art agro-ecosystems models in terms of simulating C and N fluxes. Such an effort is timely and is expected to contribute to further activities intended to improve agro-ecosystem models to address climate change challenges. I understand that the authors have to review numerous literatures. Here I would like to point out several minor inaccuracies that I hope the authors will fix before acceptance for publication. My specific comments are as follows:

1. Page 1 line 46, instead of citing "www.faccejpi.com", better to cite other literature that focuses on describing the CN-MIP.

Response to Reviewer comment No. 1: We thank the reviewer for the comment. We changed the website address, which now specifically targets to the CN-MIP project. The project being ongoing, peer-review literature has not yet been published from CN-MIP. The current paper is the first main contribution.

2. Page 2 line 60: "appears an essential step for future research". "appears to be ..." is better.

Response to Reviewer comment No. 2: Modified as suggested.

3. page 18 line 575: "... soil capacity to transform crop residue in SOC" is confusing.

Response to Reviewer comment No. 3: The sentence has been rewritten (see: L593:594).

4. Page 6 lines 181-185, the description of EPIC does not reflect the state-of-the-art of its development in C-N cycling. Please consider changes according to the following information.

a) The latest public version of EPIC is 1102. This version is not available on the website at epicapex.tamu.edu, but is available by contacting Jimmy Williams and has already been widely used in the USDA CEAP projects and numerous papers (e.g. Izaurrealde et al. 2006; Zhang et al. 2015).

b) EPIC can simulate more than 100 crops and grasses.

c) The development of EPIC CN algorithms is closely tied to the ongoing soil and water assessment tool (SWAT; Arnold et al. 1998) development efforts as described in Zhang et al. (2013). The agro-ecosystem module within the SWAT model is based on EPIC and provides updates back to EPIC. Therefore, I suggest using EPIC/SWAT as one model, instead of only mentioning EPIC.

d) Recent development of EPIC/SWAT (Yang et al. 2017) enables simulation of "N₂O losses from nitrification" and "Denitrification: N₂/N₂O ratio". So please change this in table 4.

e) relevant references are as follows:

Arnold, J. G., R. Srinivasan, R. S. Muttiah, and J. R. Williams. 1998. Large area hydrologic modeling and assessment part 1: model development. *Journal of the American Water Resources Association* 34:73-89.

Yang, Q., X. Zhang, M. Abraha, S. Del Grosso, G. P. Robertson, and J. Chen. 2017. Enhancing the soil and water assessment tool model for simulating N₂O emissions of three agricultural systems. *Ecosystem Health and Sustainability* 3(2):e01259. doi: 10.1002/ehs2.1259

Zhang, X., Izaurrealde, R.C., Arnold, J.G., Williams, J.R. and Srinivasan, R., 2013. Modifying the Soil and Water Assessment Tool to simulate cropland carbon flux: Model development and initial evaluation. *Science of the Total Environment*, 463, pp.810-822.

Zhang, X., Izaurrealde, R.C., Manowitz, D.H., Sahajpal, R., West, T.O., Thomson, A.M., Xu, M., Zhao, K., LeDuc, S.D. and Williams, J.R., 2015. Regional scale cropland carbon budgets: Evaluating a geospatial agricultural modeling system using inventory data. *Environmental Modelling & Software*, 63, pp.199-216.

Izaurrealde, R.C., Williams, J.R., McGill, W.B., Rosenberg, N.J. and Jakas, M.Q., 2006. Simulating soil C dynamics with EPIC: Model description and testing against long-term data. *Ecological Modelling*, 192(3), pp.362-384.

Response to Reviewer comment No. 4: We thank the reviewer for these comments. We modified the text (see L176-183: "EPIC (Environmental Policy Integrated Climate) (Williams, 1995, Izaurrealde et al., 2012) can simulate about 130 crop and grass species through its plant growth model, which uses unique parameter values for each species. It can predict changes in soil, water, nutrient, pesticide movements, and yields as a consequence of management decisions. It also assesses water quality, N and C cycling, climate change impacts, and the effects of atmospheric CO₂. Moreover, novel algorithms were recently implemented (Izaurrealde et al., 2012) to improve the simulation of C and N transformations, gas (O₂, CO₂, and N₂O) and solute (NO₃⁻, NO₂⁻) movement, and ecosystem C balance and fluxes (Izaurrealde et al., 2012)") and the tables (see Table 4, 5, 6 and 7) according to the information received by the EPIC development team.

For the comment at point C, we consider the use of the notation EPIC/SWAT not appropriate in this case for several reasons. As stated in lines 108-116 of the manuscript, we examined I this study the nine models used within the research project CN-MIP. Only EPIC, and not SWAT, was used within this research project. It is certainly true that EPIC and SWAT

share several algorithms and subroutines. However, the two models cannot be unambiguously associated because EPIC is a field scale model, while SWAT is a watershed model. In particular, EPIC simulates with a higher level of detail the crop growth and some soil processes and dynamics. Because of these differences, the two models produce different results with the same inputs. EPIC and SWAT developing people at Blackland Research Station in Temple, TX (USA), with whom we have interacted prior to revising the manuscript, agree on dealing with EPIC and SWAT as distinct models. This means that the use of EPIC/SWAT is not appropriate. For the comment at point E, SWAT not being part of this exercise, and based on our previous comment, we consider the first three references in list suggested by the reviewer as not applicable to this study. We have included the fourth reference suggested because it supports our analysis, which has also implied to modify the results. The last suggested citation was already included in the previously submitted manuscript.

5. For DOC simulation, I think DayCent can do it. Please double check and revise this information in Table 4.

Response to Reviewer comment No. 5: We thank the reviewer for the comment. The information reported in table 4 has been modified accordingly.

November 29th, 2016

Dear Editor,

We would like to submit the enclosed manuscript entitled “Review and analysis of strengths and weaknesses of agro-ecosystem models for simulating C and N fluxes”, which we wish to be considered for publication in Science of the Total Environment.

This is a review paper analysing strengths and weaknesses of simulation models commonly used to simulate C and N fluxes in crop and grassland systems. The content of the paper mostly reflects the experience of the consortium (bringing together 10 organizations from six countries) and the evaluation conducted in the ongoing project “C and N models intercomparison and improvement to assess management options for GHG mitigation in agro-systems worldwide” (CN-MIP, 2014-2017), established within the Joint Programming Initiative on Agriculture, Food Security and Climate Change (FACCE-JPI, <http://www.facejpi.com>). The study assesses several processes linking soil, vegetation and atmosphere compartments (in interaction with farming practices), and provides an insight on some recent research progresses in the field of biogeochemistry that could inform further model developments

The authors believe the paper fits into the journal’s scope and aim, and would be of interest for journal’s readership. They would thus value and feel privileged to receive feedback from your journal.

The authors declare that they have no conflict of interest. The authors also acknowledge that the content of the manuscript has not been published previously nor is being considered for publication elsewhere.

Sincerely,

The authors

Revision 1

Reviewer #1: This review study performed by Brilli et al. is comprehensive and systematic. In the manuscript, the authors compared nine agricultural models that can simulate C and N cycling, the underlying processes, abilities, and limitations of different models were analyzed and discussed, and also some perspectives on model development are given. The manuscript is written well and informative, and is acceptable by the journal of Science of the Total Environment. However, some minor revisions are needed, especially the format, as listed below.

1. Abstract, the full name of each abbreviation should be given, such as "C", "GHG", "SOM", etc.
Modified as suggested.
2. The section 2.1 is some information on background, so I suggest integrate these two paragraphs into the introduction section. While, the section 3.1 is the method you used to analyze different models, so it would be better to move this part to approaches section.
We agree with these suggestions. Parts of sub-section 2.1. have been integrated into the Introduction section. Sub-section 3.1. has been moved to the Modelling approach section (Section 2), and has become Sub-section 2.2.
3. Line 148, change "Tab." to "Table", and the same for all the text.
Modified as suggested.
4. Line 157, add the full name to each abbreviation when it used first, and then use the abbreviation in the follow text. For example, line 163 "NPP" and "NEE"; line 427, "WFPS" should be given in line 394; line 439 "BD" should be given in line 393; line 469, the abbreviation of "SOM" has been given in line 88. Line 624 "GHG" has been given in line65. Please check the whole text carefully.
Modified as suggested.
5. Line 248, the supplementary tables should be named as Table S1, S2, ... S5.
Modified as suggested.
6. Line 316-317, why use capital letters for "Gross Primary Production" and others?
Modified as suggested (with lower-case letters).
7. Line 325-330, I suggest use "CO₂" rather than "CO₂-GHG", and use "Non CO₂-Gas" instead of "Non CO₂-GHG" because N₂ and NH₃ are not GHG.
Modified as suggested.
8. Line 448, set "2" as subscript.
Modified as suggested.
9. Line 477, not only archaea but also bacteria and fungi can carry out nitrification.
Added to the text.
10. Line 477-487, heterotrophic nitrification has been demonstrated to widely occur in terrestrial ecosystems, including cropland and grassland (Chen et al., 2015). Heterotrophic nitrification is a different process from autotrophic nitrification. Has this process been included in these nine models?

Chen, Z.M., Ding, W.X., Xu, Y.H., Müller, C., Rütting, T., Yu, H.Y., Fan, J.L., Zhang, J.B., Zhu, T.B., 2015. Importance of heterotrophic nitrification and dissimilatory nitrate reduction to ammonium in a cropland soil: Evidences from a ¹⁵N tracing study to literature synthesis. *Soil Biology and Biochemistry* 91, 65-75.

We thank the reviewer for this comment. In our analysis we considered the process of nitrification without discerning if it was from autotrophs or heterotrophs, since none of the models reported in the paper is able to make it.

11. Line 484, moisture is an important factors influencing nitrification rate.

The authors agree. Moisture has also been mentioned in the text

12. Line 508-509, C/N is one of the major factors, so add largely before "depends on". Change "plant residues" to "organic materials".

Modified as suggested (L:502-507 in the revised text).

13. Line 509-513, it has been found that the composition of organic materials rather than a simple indicator of C/N (Bonanomi et al., 2013). Is there any model considering the composition or structure of SOM?

Bonanomi, G., Incerti, G., Giannino, F., Mingo, A., Lanzotti, V., Mazzoleni, S., 2013. Litter quality assessed by solid state ¹³C NMR spectroscopy predicts decay rate better than C/N and lignin/N ratios. *Soil Biology and Biochemistry* 56, 40-48.

We thank the reviewer for this comment. Biogeochemical processes are hard to be reproduced and their representation is often simpler than reality. As far as nitrification, we did not consider the composition of organic materials since the nine models used are mainly based on C/N ratios without distinct differences between organic components. However, this could be another point which could be treated by future modelling works.

14. Line 579-582, this sentence is confusing. Do you mean "compared with conventional tillage, no/reduced tillage may lead to ..."? Generally, we compared conservation tillage with conventional tillage.

The authors agree. The sentence has been rewritten accordingly.

15. Section 5, this section mainly focuses on SOM decomposition, how about model development in N transformation and management which are also major aspects in this review?

We thank the reviewer for the suggestion. We acknowledge in the text the importance of N transformation and management, as well as plant-soil interactions (several references have been added. See L:690-692) without developing them, which would have excessively expanded the text. As specified in the text, in this section we made a choice to focus soil biology and soil physics for the reasons explained in L:693-702

16. Line 673-678, some other important areas also generally not have been considered in the current models, such as the microbial traits, including the abundance, community structure and function, the plant-soil interaction and the feedback of ecosystem process to climate change. Particularly, the ignored microbial characteristic is an important cause of the discrepancies of model results.

We thank the reviewer for the suggestion. We have added a short paragraph concerning the inclusion of microbial traits in models at the end of the section relative to soil microbial biomass representation in models (L:729-736 in the revised text). As above, we acknowledge that other suggested areas are important without developing them, which would have made the text too heavy.

17. Table 7 is too large and there are too many references, move Table 7 and the involved references to supplementary material.

The authors believe Table 7 should be in the main text as it provides accurate information, which is essential to the rationale of the paper.

18. The references need to be carefully formatted. The issue number is presented in some reference but not all. Delete the issue number. List all the author names of each reference. The initials of the titles should be in low case except the first word (such as line 959-961, 1341-1343, etc.). Carefully check all the superscripts and subscripts (such as line 903, 906, 1033, 1037, 1041, 1136, 1273, 1364, 1496, 1499, etc.).

The format of references was corrected.

Reviewer #2:

1. Page 4, Line 112: The word "... improvement ..." should be changed to "... improving ..."
Modified as suggested.

2. Page 4, line 126. (Graux et al., 2013). In the "References" section the "et al" should be replaced with names of other contributors.

Done.

3. Page 4, Lines 127-18: In other places such as: (Palosuo et al., 2011, Rotter et al., 2012, Asseng et al., 2013, Sándor et al., 2016) references are not fully cited in the "References" section. Apparently, these authors have used this format throughout this manuscript. This approach makes it somewhat more time consuming to keep track of works of other contributors when searching databases available on the Internet.

The reference section has been improved by adding the names of all co-authors to multi-author papers in the list.

4. Page 5, line 134: "... understanding grounded in state-of-the art knowledge." "When the phrase (state of the art) is used as a noun it is not hyphenated. It is hyphenated when it is used as an adjective. Adjective Example: I like your state-of-the-art technology. Noun Example: The technology is state of the art."

Modified as suggested.

5. Page 5, line 147: "... (Tab. 1)..." Is this abbreviation for the word "Table" permitted? The same format follows later in this manuscript. Even in the captions of table the word "Table" is abbreviated to "Tab."

The word "Tab." has been changed to "Table" in the whole text and caption.

6. Page 5, line 156: "... agriculture activity..." should read, "agricultural activity..."

Modified as suggested.

7. Page 6, line 163: "... model allows to simulate also..." Revise this please...

Modified in the text (i.e. Also, the model can simulate...).

8. Page 6, line 173: "... integrates..." should be changed to, "... integrate..."

Modified as suggested.

9. Page 5, line 181: "... model which..." should be changed to, "... model, which..."
Modified as suggested.
10. Page 5, line 189: "viii) RothC..." should be changed to, "viii) RothC..."
The formatting does not allow this change.
11. Page 6, line 194: "... model which..." should be changed to, "... model, which..."
Modified as suggested.
12. Page 7, line 197: "It allows to consider the..." should be changed to, "It allows considering the..."
Modified as suggested.
13. Page 7, line 215. Reference has been made to Table 2 but in Table 2, the parameter (*NA) has been defined as "Not information available." The proper word is "No," i.e.: "No information is available." This applies to other tables. By the way, "NA" should be defined clearly within the text of the manuscript and/or in the caption for all tables.
Modified as suggested.
14. In Table 3, column 2: The number in the parentheses should be defined.
We thank the reviewer for this comment. Numbers in brackets have been detailed in the figure caption of the text.
15. Page 7, line 25: "... (Tab. 2a-e in supplementary material)." I did not find this information. Please clarify.
We referred to the five tables in supplementary material. Sentence has been rewritten as follows: (Tables S1-5 in supplementary material).
16. Page 8, line 245: "... longer term..." could be changed to "... longer-term..."
Modified as suggested.
17. Page 8, line 247. I could not find Table 3a.
"Table 3a" has been modified to "Table S1". It can be found in supplementary material.
18. Page 9, line 268. I could not find Table 3b.
"Table 3b" has been modified to "Table S2". It can be found in supplementary material.
19. Page 9, line 273: "The water transport calculation scheme in soil is mainly described by the capacity (or tipping bucket) approach (78%)." This needs to be rewritten. Perhaps: The soil water balance is primarily described by estimation of soil water availability through adding daily rainfall and subtracting transpiration, evaporation and runoff from an estimated maximum soil water holding capacity. The curious readers perhaps find the works by Paul et al. (2003) and Weiskittel et al. (2010)...
We thank the reviewer for this comment. We gave now a better description of the soil water balance (L:269-274 in the revised text).
20. Page 9, line 276: "... or/and..." should be changed to "... and/or..."
Modified as suggested.
21. Page 9, line 283. I could not find (Tab. 3c).
"Table 3c" has been modified to "Table S3". It can be found in supplementary material.

22. Page 10, line 309. Could not find Table 3d.
"Table 3d" has been modified to "Table S4". It can be found in supplementary material.
23. Page 11, line 358. Could not find Table 3e.
"Table 3e" has been modified to "Table S5". It can be found in supplementary material.
24. Page 13, lines 401 to 410: The "scale of application" should better defined. Authors' definition is not clear.
We added in the text (L:396-400 in the revised text) *"The scale of application refers to the influence on the model performances of the data types used. They may go from high-frequency measurements specific to the study site, which have been collected experimentally within carefully designed plans, to low-frequency data which have been administratively aggregated at a coarse spatial resolution (e.g. regional or national summaries)"*.
25. Page 13, line 417: "... features..." could be changed to properties.
Modified as suggested
26. Page 14, line 447. Make sure N₂O is correctly typed.
Done
27. Page 14, line 456: It is true that in soils rich in expanding pedogenic 2:1 phyllosilicates some organic molecules penetrate between the layers are as such fixed and are less susceptible to decomposition through soil enzyme activities. Additionally, however, soil enzyme activities are reduced by association of enzymes' active sites with such phyllosilicates resulting in reduced decomposition of organic matter. Lack of oxygen in clayey soils also negatively affects amount of soil enzymes through reduction in the number of enzyme-producing microorganisms. Note that a soil can have a clayey texture but different types of clay have different effect on SOC decomposition. In other words, soil enzyme activities are reduced more significantly in a soil that is montmorillonitic than a soil that is kaolinitic. The increase in temperature expected to increase the rate of microbial and biochemical reactions in the pedosphere but only at the upper part of the A horizon if soil is highly montmorillonitic. For reference, look at work by Tabatabai, Bayan and Eivazi, among others.
We thank the reviewer for the comment. We have added a paragraph concerning the response of enzyme activities in different soil types. (L:459-471 in the revised text): *"In addition, a relevant fraction of microbial extracellular enzymes is adsorbed by external and internal surfaces of clay size particles of soil phyllosilicate minerals (Burns et al., 2013). Amount of bound enzymes increases with increasing layer charge of phyllosilicates (montmorillonite > illite > kaolinite) (Bayan and Eivazi, 1999). Sorption causes conformational changes of enzymes' active sites, and in turn reduces or even suppresses the activity of enzymes (Bayan and Eivazi, 1999, Burns et al., 2013). Moreover, anaerobic conditions, that are expected to occur mostly in finer texture soils, also negatively affects amount of soil enzymes through reduction in the number of enzyme-producing microorganisms (Inglett et al., 2005). At least, the increase of clay content affects soil aggregation, indirectly affecting SOC through the creation of macro-aggregates that can physically protect organic matter molecules from further microbial mineralization (Rice, 2002, Plante et al., 2006). Thus, an overall reduction in SOM turnover in fine texture soils is expected due to reduced substrate availability and overall microbial activity."*
28. Page 14, lines 461 and 462: Rewrite starting with, "... , thus..."

The sentence has been rewritten: (L:472-474 in the revised text) *“However, the effect of texture on SOC decomposition is controversial. For instance, for 10 sites in Canada (¹³C-labelled study) Gregorich et al. (2016) found that temperature (neither soil texture nor other soil properties) was the only driver of decomposition”.*

29. Page 15, line 496 and 497: "... whilst soils with high organic matter content (high dissolved organic C) and anaerobic conditions..." Here, it appears that these authors equate the high organic matter content to high level of dissolved organic C in the soil solution. This is not necessarily correct. When it comes to decomposition of soil organic matter, the role of soil enzymes cannot be underestimated.
To avoid any ambiguities, we delated the sentence within brackets (i.e. high dissolved organic C).
30. Caption for Table 17: "... has been considered." Should read, "... have been considered."
Modified as suggested.
31. Page 19, line 609: "... infuences" should be changed to "influences"
Done.
32. Page 19, line 614: "... disturbances which..." change to, "... disturbances, which..."
Modified as suggested.
33. Page 20, line 646: change "... 1 day ..." to, "... 1-day...")
Modified as suggested.
34. Page 20, line 648: Change "... soil which..." to, "... soil, which..."
Modified as suggested.
35. Page 22, lines 721 to 735: The argument regarding CUE and NUE must involve soil enzyme activities. Without reference to enzymes involved in mineralization of N and C in the SOM, the discussion becomes highly speculative.
We agree with the reviewer. We have added a short paragraph in the revised text (L:747-757) about the effect of soil enzyme activities on CUE and NUE.
36. Page 23, line 761: "... SOM in soil..." change to, "... SOM..."
Modified as suggested.
37. Page 23, line 766 and page 25, line 836: Please check O2 to make sure it is not O3.
Modified as suggested.
38. Page 24, line 782: "... soil ammonium concentration are accurately..." Change to, "... soil ammonium concentration be accurately...".
Modified as suggested.
39. Page 24, lines 780 to 794. The research on NH₄⁺ fixation has been done. If the soil is vermiculitic (includes vermiculite or Al-interlayered vermiculite) NH₄⁺, having an ionic radius similar to K⁺ will be fixed in the interlayer spaces of vermiculite. Upon drying of such pedogenic clay size vermiculite, the fixation become more permanent as the vermiculate structure collapses to that of muscovite. Authors should search the literature to find proper references... A good place to start might be to look at the book: Methods of Soil

Analysis: Physical and Mineralogical Methods. ISBN-13: 978-0891180883 - ISBN-10: 0891180885

We have added a short paragraph in the revised text (L:814-837) explaining the theory of ion (ammonium) fixation by 2:1 clay minerals. However we did not address all aspects related to fixation and release, directing interested readers to the reviews by Nõmmik and Vahtras (1982) and Nieder et al. (2011).

40. Page 25, lines 825 to 827: "Although the above reported weaknesses were already known due to a wide number of published studies, in the present analysis we have tried to relate them to their causes in the view of using them as an effective basis for improving current modelling approaches.". I find some of the explanations to be limited in scope. Please see comments above.

We agree with the reviewer. Based on both reviewers' comments we provided better explanation in several parts of the (revised) text about soil physical and biological processes (see responses to above comments). These explanations would hopefully result in an improvement of the text. Highlighting the complexity of physical, chemical and biological processes, we emphasize how they are difficult to be reproduced within process-based models. The added text mostly indicate as these processes should be described in more detail into models in order to increase the reliability of outputs.

Revision 2

Reviewer #3: The authors provide a thorough review of models for modeling C and N cycling in agronomic systems. The review is interest and informative, especially with regards to highlighted discrepancies in modeling capacity and accuracy. This research is important for modeling GHG, and impacts of management practices on agricultural output of GHG. Especially useful is the identification of shortcoming and potential sources of error in the models tested. The manuscript should be published after (very) minor revision. Minor suggested changes:

1. Line 58: and an adequate simulation of gas
Modified as suggested.
2. line 58: Given these conditions, the assessment
Modified as suggested.
3. Line 83-84: that C and nitrogen (N) cycling strongly depend on
Modified as suggested.
4. Line 102: even when models are run under the same conditions of
Modified as suggested.
5. Line 150: carbon dioxide (CO₂), and nitrate (NO₃)
Modified as suggested.
6. Line 191: adequate options and parameters values allows to simulate simulation of a wide
Modified as suggested.
7. Line 193: It allows considering consideration of the effect
Modified as suggested.
8. Line 211: Then, in that level 2
Modified as suggested.
9. Line 218: knowledge on of the
Modified as suggested.
10. line 275: of N in the soil profile
Modified as suggested.
11. line 293-4: Reference evapotranspiration is accounted bycalculated using the Penman-Monteith (56%), or Penman and Priestley-Taylor (44%) equations.
Modified as suggested.
12. Line 311-13: In general from our analysis indicated emerged that the three main processes belonging to the general class of GHG emissions and other fluxes are almost fully simulated by the considered models. Merge single-sentence paragraphs into larger paragraphs throughout results.
Modified in the text: (see L:315:318: “For better assessing how C and N cycles are involved in the simulation of GHG emissions and other fluxes within several models, three main processes were identified (Table S4, see supplementary material). Overall, our analysis

indicates that these three main processes are almost fully simulated by the considered models”).

13. Line 314: In the main process called CO₂ the The most important C-fluxes from the ecosystems were considered in the main process called "CO₂".
Modified as suggested.
14. Line 364: e.g. STICS accounts for burial through tillage
Modified as suggested.
15. Line 393: such as patterns of air temperature, precipitation, solar radiation, also and including
Modified as suggested.
16. Line 427: i.e. under- or over-estimation
Modified as suggested.
17. Line 432: anaerobic conditions, e.g. Bollmann
Modified as suggested.
18. Line 461: The Amount amount of bound enzymes increases with the increasing layer charge of
Modified as suggested.
19. Line 466: affects the amount of soil enzymes
Modified as suggested.
20. Line 467: At leastAnd finally, the increase. Throughout, change "fine texture soil" to "fine textured soil"
Modified as suggested.
21. Line 502: due to different types of
Modified as suggested.
22. Line 529: the models subroutines
Modified as suggested.
23. Line 531: the fact that the model
Modified as suggested.
24. Line 605: underestimation of particulate organic C
Modified as suggested.
25. Line 607: fertilization and tillage, which were probably the most commonly simulated
Modified as suggested.
26. Lines 619-20: related to the ecosystem and climate, which makes it difficult to define the parameter which most strongly
Modified as suggested.

27. Lines 627-8: rice cultivation being too low (i.e. effect of waterlogged soil not included in RothC) being too low
Modified as suggested.
28. Line 643: ones where they have been previously
Modified as suggested.
29. Line 656: with the results of Li et al. (2005),
Modified as suggested.
30. Line 680: agriculture fits
Modified as suggested.
31. Line 693: physics, and the interface between the two that
Modified as suggested.
32. Line 749: to optimize resources
Modified as suggested.
33. Several places: correct spelling of vermiculite
Corrected
34. Line 834: should take into account for ions interactions
Modified as suggested.
35. Lines 858-861: For the N cycle, the main limitations inherent in model structure were found under different pedo-climatic conditions (51.7%), whilst for the scale of application the major weaknesses were due to different pedo-climatic conditions (20.4%). Consider rewrite - it's a bit cumbersome as written.
Modified in the text: (see L:865:867: "For both the N-cycle modelling and scale of application, the main limitations were found in the response to different pedo-climatic conditions (51.1% and 20.2%, respectively).

Reviewer #4: This manuscript is trying to present a comprehensive analysis of the strengths and weaknesses of existing state-of-the-art agro-ecosystems models in terms of simulating C and N fluxes. Such an effort is timely and is expected to contribute to further activities intended to improve agro-ecosystem models to address climate change challenges. I understand that the authors have to review numerous literatures. Here I would like to point out several minor inaccuracies that I hope the authors will fix before acceptance for publication. My specific comments are as follows:

1. Page 1 line 46, instead of citing "www.facejpi.com", better to cite other literature that focuses on describing the CN-MIP.

We thank the reviewer for the comment. We changed the website address, which now specifically targets to the CN-MIP project. The project being ongoing, peer-review literature has not yet been published from CN-MIP. The current paper is the first main contribution.

2. Page 2 line 60: "appears an essential step for future research". "appears to be ..." is better. Modified as suggested.
3. page 18 line 575: "... soil capacity to transform crop residue in SOC" is confusing. The sentence has been rewritten (see: L593:594).
4. Page 6 lines 181-185, the description of EPIC does not reflect the state-of-the-art of its development in C-N cycling. Please consider changes according to the following information.
 - a) The latest public version of EPIC is 1102. This version is not available on the website at epicapex.tamu.edu, but is available by contacting Jimmy Williams and has already been widely used in the USDA CEAP projects and numerous papers (e.g. Izaurrealde et al. 2006; Zhang et al. 2015).
 - b) EPIC can simulate more than 100 crops and grasses.
 - c) The development of EPIC CN algorithms is closely tied to the ongoing soil and water assessment tool (SWAT; Arnold et al. 1998) development efforts as described in Zhang et al. (2013). The agro-ecosystem module within the SWAT model is based on EPIC and provides updates back to EPIC. Therefore, I suggest using EPIC/SWAT as one model, instead of only mentioning EPIC.
 - d) Recent development of EPIC/SWAT (Yang et al. 2017) enables simulation of "N₂O losses from nitrification" and "Denitrification: N₂/N₂O ratio". So please change this in table 4.
 - e) relevant references are as follows:

Arnold, J. G., R. Srinivasan, R. S. Muttiah, and J. R. Williams. 1998. Large area hydrologic modeling and assessment part 1: model development. *Journal of the American Water Resources Association* 34:73-89.

Yang, Q., X. Zhang, M. Abraha, S. Del Grosso, G. P. Robertson, and J. Chen. 2017. Enhancing the soil and water assessment tool model for simulating N₂O emissions of three agricultural systems. *Ecosystem Health and Sustainability* 3(2):e01259. doi: 10.1002/ehs2.1259

Zhang, X., Izaurrealde, R.C., Arnold, J.G., Williams, J.R. and Srinivasan, R., 2013. Modifying the Soil and Water Assessment Tool to simulate cropland carbon flux:

Model development and initial evaluation. *Science of the Total Environment*, 463, pp.810-822.

Zhang, X., Izaurralde, R.C., Manowitz, D.H., Sahajpal, R., West, T.O., Thomson, A.M., Xu, M., Zhao, K., LeDuc, S.D. and Williams, J.R., 2015. Regional scale cropland carbon budgets: Evaluating a geospatial agricultural modeling system using inventory data. *Environmental Modelling & Software*, 63, pp.199-216.

Izaurralde, R.C., Williams, J.R., McGill, W.B., Rosenberg, N.J. and Jakas, M.Q., 2006. Simulating soil C dynamics with EPIC: Model description and testing against long-term data. *Ecological Modelling*, 192(3), pp.362-384.

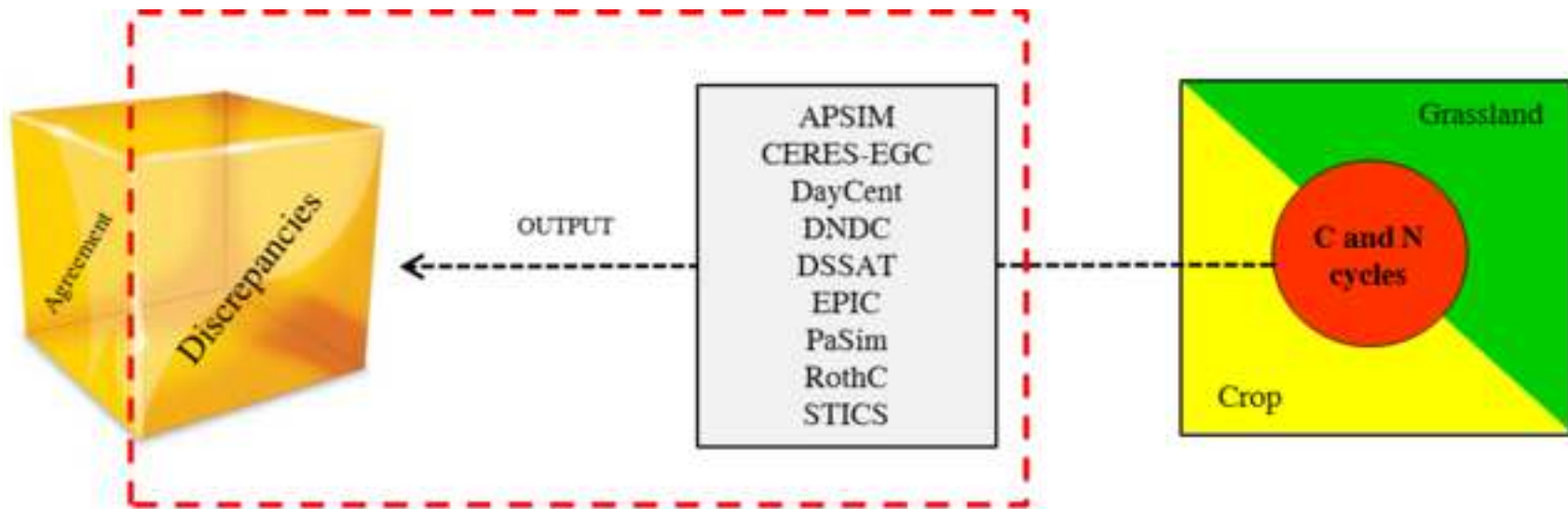
We thank the reviewer for these comments. We modified the text (see L176-183: "EPIC (Environmental Policy Integrated Climate) (Williams, 1995, Izaurralde et al., 2012) can simulate about 130 crop and grass species through its plant growth model, which uses unique parameter values for each species. It can predict changes in soil, water, nutrient, pesticide movements, and yields as a consequence of management decisions. It also assesses water quality, N and C cycling, climate change impacts, and the effects of atmospheric CO₂. Moreover, novel algorithms were recently implemented (Izaurralde et al., 2012) to improve the simulation of C and N transformations, gas (O₂, CO₂, and N₂O) and solute (NO₃⁻, NO₂⁻) movement, and ecosystem C balance and fluxes (Izaurralde et al., 2012)") and the tables (see Table 4, 5, 6 and 7) according to the information received by the EPIC development team.

For the comment at point C, we consider the use of the notation EPIC/SWAT not appropriate in this case for several reasons. As stated in lines 108-116 of the manuscript, we examined in this study the nine models used within the research project CN-MIP. Only EPIC, and not SWAT, was used within this research project. It is certainly true that EPIC and SWAT share several algorithms and subroutines. However, the two models cannot be unambiguously associated because EPIC is a field scale model, while SWAT is a watershed model. In particular, EPIC simulates with a higher level of detail the crop growth and some soil processes and dynamics. Because of these differences, the two models produce different results with the same inputs. EPIC and SWAT developing people at Blackland Research Station in Temple, TX (USA), with whom we have interacted prior to revising the manuscript, agree on dealing with EPIC and SWAT as distinct models. This means that the use of EPIC/SWAT is not appropriate.

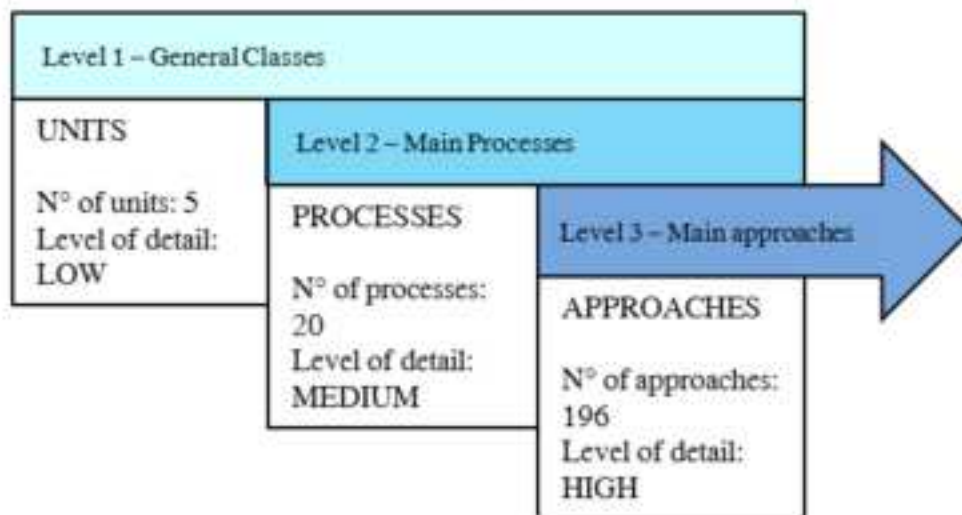
For the comment at point E, SWAT not being part of this exercise, and based on our previous comment, we consider the first three references in list suggested by the reviewer as not applicable to this study. We have included the fourth reference suggested because it supports our analysis, which has also implied to modify the results. The last suggested citation was already included in the previously submitted manuscript.

5. For DOC simulation, I think DayCent can do it. Please double check and revise this information in Table 4.

We thank the reviewer for the comment. The information reported in table 4 has been modified accordingly.



Top-down approach
(132 modelling studies)



Model weaknesses

- Limitations in simulating the effects of pedo-climatic conditions
- Limitations in the algorithms simulating the effects of management practices
- Multiplicity of scales in both time and space

Highlights

- We assess simulated C and N cycles in agricultural systems based on published modelling studies
- Biogeochemical models have limits in simulating pedo-climatic conditions and management effects
- We propose explicit modelling of soil microbial biomass to drive SOC turnover
- Improved approaches of gas transport in soil are required for future modelling work

35

36 **Abstract**

37 Biogeochemical simulation models are important tools for describing and quantifying the
38 contribution of agricultural systems to **carbon** sequestration and **greenhouse gas** source/sink
39 status. The abundance of simulation tools developed over recent decades, however, creates a
40 difficulty because predictions from different models show large variability. Discrepancies
41 between the conclusions of different modelling studies are often ascribed to differences in the
42 physical and biogeochemical processes incorporated in equations of **carbon** and **nitrogen**
43 cycles and their interactions. Here we review the literature to determine the state-of-the-art in
44 modelling agricultural (crop and grassland) systems. In order to carry out this study, we
45 selected the range of biogeochemical models used by the CN-MIP consortium of FACCE-JPI
46 (<https://www6.inra.fr/cnmip/Project>): APSIM, CERES-EGC, DayCent, DNDC, DSSAT,
47 EPIC, PaSim, RothC and STICS. In our analysis, these models were assessed for the quality
48 and comprehensiveness of underlying processes related to pedo-climatic conditions and
49 management practices, but also with respect to time and space of application, and for their
50 accuracy in multiple contexts. Overall, it emerged that there is a possible impact of ill-defined
51 pedo-climatic conditions in the unsatisfactory performance of the models (**45.9%**), followed
52 by limitations in the algorithms simulating the effects of management practices (**33.8%**). The
53 multiplicity of scales in both time and space is a fundamental feature, which explains the
54 remaining weaknesses (*i.e.* **20.3%**). Innovative aspects have been identified for future
55 development of **carbon** and **nitrogen** models. They include the explicit representation of soil
56 microbial biomass to drive soil organic matter turnover, the effect of **nitrogen** shortage on **soil**
57 **organic matter** decomposition, the improvements related to the production and consumption
58 of gases and an adequate **simulation** of gas transport in soil. **Given these conditions**, the
59 assessment of trends and gaps in the modelling approaches currently employed to represent
60 biogeochemical cycles in crop and grassland systems appears **to be** an essential step for future
61 research.

62

63 *Keywords: Biogeochemical models, C cycle, N cycle, management, pedo-climate*

64

65 1. Introduction

66 The sensitivity of soil carbon (C) stocks and greenhouse gas (GHG) emissions to
67 climate and management practices demands a comprehensive methodology for effective
68 policy analyses (Li et al., 1994). Enhancing soil C sequestration and reducing GHG emissions
69 from agricultural soils are key objectives for reducing the climate impact of food production
70 and they strongly depend on agricultural practices such as crop residue return, soil tillage
71 modalities, and enhanced nitrogen (N) fertilization management. Whether C return to soils
72 appear as a main controlling factor, in some cases (e.g. dry climates) reduced tillage may also
73 be an effective measure for enhancing C sequestration (e.g. Chatskikh et al., 2008; Powlson et
74 al., 2012). To avoid pollution swapping, assessments of the potential to reduce climate impact
75 should also include other impacts such as nitrate (NO_3^-) leaching into groundwater, ammonia
76 volatilization and soil erosion, which can also be reduced, for example, by increasing the use
77 of grazed pastures in dairy farms (Rotz et al., 2009, Peyraud, 2011). In addition, it is
78 important to consider the interactions on the hundred-year timescale of soil C equilibration
79 (Lardy et al., 2011) and the relatively more rapid changes induced by agricultural practices
80 (Angers et al., 1995). It is likely that most agricultural soils are not in equilibrium with respect
81 to C storage and have the greatest potential for short-term C losses or gains, while they may
82 also be sensitive to the effects of long-term, climate-driven processes (Wutzler and
83 Reichstein, 2007). It is also important to recall that C and nitrogen (N) cycling strongly
84 **depend** on interactions among plant growth processes, soil water dynamics and soil N
85 dynamics that are highly non-linear and thus difficult to predict with simple approaches.

86 Process-based ecosystem models take the approach of simulating underlying
87 biogeochemical processes, such as plant photosynthesis and respiration, using mathematical
88 equations that determine the allocation of C from atmospheric CO_2 into biomass down to the
89 soil organic matter (**SOM**). A relatively complete suite of biogeochemical processes (e.g.
90 plant growth, organic matter decomposition, fermentation, ammonia volatilisation,
91 nitrification and denitrification) is generally embedded in these models, enabling computation
92 of transport and transformations in plant–soil ecosystems. Sub-models are designed to interact
93 with each other to describe cycles of water, C and N for target ecosystems, thus any change in
94 the environmental factors collectively affect a group of biogeochemical reactions. Extensively
95 tested biogeochemical models (with the coupled C-N cycling) are effective tools for
96 examining the magnitude and spatial-temporal patterns of C and N fluxes, and play an
97 important role in designing specific policies appropriate to the soils, climate, and agricultural
98 conditions of a location or region. **In recent decades, these tools have also been used for**

99 assessing the expected impacts of future climate, as represented by several climate change
100 scenarios (Graux et al., 2013). However, results of state-of-the-art terrestrial biogeochemical
101 models, describing the contribution of agricultural systems to C sequestration and GHG
102 source/sink status, may diverge significantly even when models are run under the same
103 conditions of climate, soil and management (Palosuo et al., 2011, Rotter et al., 2012, Asseng
104 et al., 2013, Sándor et al., 2016; Sandor et al., 2017). Such differences between model results
105 are often attributed to physical and biogeochemical processes being inadequately resolved
106 and, for these models, the improvement of algorithms and structure is recommended beyond
107 parameter optimization (Tian et al., 2011, Lu and Tian, 2013).

108 It is the goal of this paper to examine the strengths and weaknesses of nine crop and
109 grassland models that incorporate C and N fluxes into biogeochemical frameworks and fully
110 assess C and GHG dynamics in agricultural soils. These models are commonly applied
111 worldwide and are used to simulate biogeochemical and related outputs by the project “C and
112 N models intercomparison and improvement to assess management options for GHG
113 mitigation in agro-systems worldwide” (CN-MIP, 2014-2017), established within the Joint
114 Programming Initiative on Agriculture, Food Security and Climate Change (FACCE-JPI,
115 <http://www.facejpi.com>), which brings together 10 organizations from six countries. With
116 this analysis we are not arguing against the quality of models. While highlighting weaknesses
117 and limits of current modelling approaches as documented in several published studies, we
118 intend to offer a general overview as a basis for new ways of improving current modelling
119 approaches.

120 The following rationale has been used in the organization of this article. We first present
121 the conceptual basis of the models analysed and the approach used for gaining insight into
122 their compositional sub-systems. Section 3 presents results of the approach used. Section 4
123 reports on the documented performance of biogeochemical models against data, and discuss
124 their relative strengths and weaknesses. Section 5 presents an outlook on recent research
125 developments and future approaches. In Section 6, remarks are made concerning the bearing
126 of the findings on a wider interpretation of biogeochemical modelling.

127

128 **2. Modelling approaches**

129 *2.1. The CN-MIP models*

130 The nine models considered for the CN-MIP exercise are process-based models mainly
131 developed for crop or grassland ecosystems. They attempt to reproduce the most relevant
132 ecological and physiological process through a theoretical understanding grounded in state of

133 the art knowledge. In this way, they reproduce specific agro-ecological dynamics under
134 prescribed conditions of climate, soil and management, thanks to the concepts and
135 relationships that interlink entities of the real world. Most models represent plant phenology
136 and yield-formation processes, together with functional processes at the basis of SOM (Soil
137 Organic Matter) turnover, gas exchange at the soil-plant-atmosphere interface and soil water
138 dynamics.

139 The nine models analysed for this intercomparison are: *APSIM*, *CERES-EGC*, *DayCent*,
140 *DNDC*, *DSSAT*, *EPIC*, *PaSim*, *RothC* and *STICS* (Table 1). Below, a brief description of each
141 model is provided.

142 i) *APSIM* (The Agricultural Production Systems sIMulator) (Keating et al., 2003;
143 Holzworth et al., 2014) simulates several systems through the interaction among plants,
144 animals, soil, climate and management. The model allows the analysis of the whole-farm
145 system, including crop and pasture sequences and rotations, and livestock.

146 ii) *CERES-EGC* (Crop Environment REsource Synthesis - Environnement et Grandes
147 Cultures) (Gabrielle et al., 1995) simulates the biogeochemical cycles of water, C and N in
148 agro-ecosystems. The model predicts crop production and the environmental impacts related
149 to the agricultural activity (e.g. nitrous oxide (N₂O), nitrogen oxide (NO), ammonia (NH₃),
150 carbon dioxide (CO₂), and nitrate (NO₃)) based on management for a wide range of arable
151 crops (e.g. wheat, barley, maize, sorghum, sunflower, pea, sugar-beet, oilseed rape and
152 miscanthus). Crop-specific modules include approaches for plant growth and development,
153 coupled to a generic soil sub-model.

154 iii) *DayCent* (Parton et al., 1994) is a biogeochemical model able to simulate crop growth,
155 soil C dynamics, N leaching, gaseous emissions (e.g. N₂O, NO, nitrogen (N₂), NH₃, methane
156 (CH₄) and CO₂) and C fluxes - e.g. net primary production (NPP), net ecosystem exchange
157 (NEE) - in crop fields, grassland, forest, and savanna ecosystems. Also, the model can
158 simulate several management practices (i.e. fertilization, tillage, pruning, cutting, grazing,
159 etc.) as well as specific external disturbances (i.e. fires).

160 iv) *DNDC* (DeNitrification-DeComposition) (Li et al., 1992a) simulates C and N
161 biogeochemistry in agro-ecosystems. The model predicts crop growth, soil regimes (i.e.
162 temperature and moisture), soil C dynamics, N leaching, and trace gases emissions (e.g. N₂O,
163 NO, N₂, NH₃, CH₄ and CO₂). The model was expanded in 2012 to include biophysical
164 processes in whole-farm systems (Li et al., 2012).

165 v) *DSSAT* (Decision Support System For Agrotechnology Transfer) (IBSNAT,
166 1993, Tsuji, 1998, Uehara, 1998 and Jones et al., 1998), was originally developed to facilitate

167 the application of crop models in a systems approach to agronomic research. DSSAT ver. 4.6
168 (i.e. cropping system model, CSM) and its crop simulation models **integrate** the effects of soil,
169 crop phenotype, weather and management options. DSSAT includes improved application
170 programs for seasonal, spatial, sequence and crop rotation analyses that assess the economic
171 risks and environmental impacts associated with irrigation, fertilizer and nutrient
172 management, climate variability, climate change, soil carbon sequestration, and precision
173 management. The model can predict crop yield, resource dynamics such as for water, N and
174 C, environmental impact (i.e. N leaching), evapotranspiration and **soil organic matter (SOM)**
175 accumulation.

176 vi) *EPIC* (Environmental Policy Integrated Climate) (Williams, 1995, Izaurralde et al.,
177 2012) can simulate about 130 crop and grass species through its plant growth model, which
178 uses unique parameter values for each species. It can predict changes in soil, water, nutrient,
179 pesticide movements, and yields as a consequence of management decisions. It also assesses
180 water quality, N and C cycling, climate change impacts, and the effects of atmospheric CO₂.
181 Moreover, novel algorithms were recently implemented (Izaurralde et al., 2012) to improve
182 the simulation of C and N transformations, gas (O₂, CO₂, and N₂O) and solute (NO₃⁻, NO₂⁻)
183 movement, and ecosystem C balance and fluxes (Izaurralde et al., 2012).

184 vii) *PaSim* (Pasture Simulation model) (Riedo et al., 1998) is a process-based, grassland-
185 specific ecosystem model that simulates grassland and pasture productivity and GHG
186 emissions to the atmosphere. The model consists of sub-models for grass, animals,
187 microclimate, soil biology, soil physics and management.

188 viii) *RothC* (Rothamsted Carbon model) (Coleman and Jenkinson, 1999) is a
189 specific tool for the assessment of organic C turnover in non-waterlogged topsoil. The model
190 allows for the effects of soil type, temperature, moisture content and plant cover on the
191 turnover process.

192 ix) *STICS* (Simulateur multIdisciplinaire pour les Cultures Standard) (Brisson et al., 1998)
193 is a soil-crop model, which is built on a generic framework for plant description. Within this
194 framework, the selection of adequate options and parameters values allows **the simulation of** a
195 wide range of plants, from annual crops to perennial grasses or trees. The model simulates
196 plant growth as well as water, C and N fluxes. It allows **consideration of** the effect of a large
197 range of management options on agronomic (biomass or grain productivity and quality) and
198 environmental (C and N storage, nitrate leaching, N₂O emissions) outputs.

199 Most of the models included in this review are in active development and use, and this
200 activity can result in a temporal fluidity of model descriptions. The information provided in

201 this section is based on the authors' knowledge of the state of the models at the beginning of
202 the project CN-MIP as well as on published material.

203

204 **2.2.** *Model analysis*

205 For reducing the uncertainty in estimating the magnitude and spatial-temporal patterns
206 of C and N fluxes from several agro-systems (i.e. crops, grassland and livestock), and for
207 improving the understanding of how these tools work, we analysed the most important
208 processes and approaches implemented into the models. This analysis was based on a top-
209 down approach focused at gaining insight into compositional sub-systems. On this basis, we
210 indicated three levels of information containing specific processes/approaches that were sub-
211 divided according to different levels of detail.

212 The starting point (level 1) was the detection of discrete units considered in agricultural
213 modelling, which are essential to characterize agricultural systems. In this level, characterized
214 by the lowest level of detail required for the analysis, we differentiated five general classes
215 that should be implemented within all biophysical/biogeochemical process-based models for
216 crops and grasslands. These classes concern ecological and physiological processes,
217 management options, soil structure, and weather inputs (**Table 2**).

218 Then, **at** the level 2 (intermediate level of detail) specific processes were identified
219 within each general class (level 2). In this level 20 "main processes" were identified, which
220 we retained as basic to describe the most important biophysical/biogeochemical dynamics
221 (**Table 3**) of each general class indicated in the previous level.

222 Finally, in the level 3 (highest level of detail) almost 200 modelling approaches (i.e.
223 methods, options or components), identifying specific dynamics or mechanisms contained
224 within the previous main processes (supplementary material) were reported (level 3). These
225 approaches were extrapolated taking into account the current existing knowledge of the
226 different methods, options and components able to describe the most important
227 biophysical/biogeochemical dynamics (**Tables S1-5** in supplementary material).

228 There are a number of advantages to such a "top-down" approach. An advantage is the
229 insight that can be gained from examining the level of detail that each model provides. This in
230 turn helps in identifying areas in the model structures to establish their reliability and
231 relevance for intended purposes. Such an approach also helps in tracing possible links with
232 the basic processes of each model (identification of the strengths and weaknesses) either in
233 the case of mismatch between model outputs and measurements, or in the case of
234 disagreement among model results in similar conditions.

235 Results reported below were based on the highest level of detail (level 3 – see
236 supplementary material).

237

238 **3. Results**

239 *3.1. Meteorological variables*

240 Meteorological inputs strongly influence model outputs since they affect plant growth,
241 plant development stages, and soil turnover/balances, including flux exchanges at the soil-
242 plant-atmosphere interface. The number and type of climatic variables required by each model
243 informs us about the relationship between model outputs and climate drivers. In principle, for
244 the modelling of surface reactions and diffusion of volatile products (e.g. N₂O emissions, soil
245 water content dynamics), the higher the resolution in the climate information (e.g. hourly to
246 sub-hourly weather inputs), the more accurate the model response is for short-term processes
247 but the higher the probability that missing data may be present in the weather series used. For
248 **longer-term** processes such as soil organic carbon (SOC) decomposition, higher temporal
249 resolution data may not improve the accuracy of the model response.

250 From our analysis (**Table S1**, see supplementary material) we observed that the nine
251 models involved in CN-MIP mostly use climate inputs at daily resolution (89%), whereas
252 PaSim uses the hourly time scale (but with an option also available for daily inputs), and
253 RothC uses a monthly time-step.

254 The most commonly used meteorological variables are precipitation, air temperature
255 and wind speed. Concerning air temperature, the daily maximum and minimum air
256 temperatures are used by almost all models (89%).

257 Relative humidity (daily mean) and global solar radiation are also used by 67% and
258 56% of the models, respectively. The atmospheric concentration of CO₂ is an optional input
259 for many models (78%), with the exception of CERES-EGC and RothC.

260 Finally, only a few models use specific meteorological variables such as cloudiness,
261 sunshine duration, dew-point temperature and actual vapour pressure.

262

263 *3.2. Soil*

264 Similarly to climate inputs, soil characteristics also have a great influence on model
265 outputs. These characteristics strongly influence crop growth and fluxes related to the gaseous
266 biogeochemical cycles as water, C and N. Some soil inputs are assumed as constant values
267 (i.e. parameters), not changing during the simulation. Different soil properties (e.g. texture,
268 pH, bulk density, etc.) can affect plant growth and the environmental conditions for the

269 microbial activity driving the formation and decomposition of SOM and mediating
270 biochemical processes.

271 From our analysis (Table S2, see supplementary material), it emerged that soil processes
272 are mostly calculated based on the differentiation of the soil profile into a sequence of distinct
273 layers, with generation of outputs for each of these subdivisions. In PaSim model, the whole
274 soil profile is the basis for the modelling of C dynamics. The soil temperature is calculated
275 from energy balance (44%) or based on a response function of air temperature (56%).

276 The soil water balance is mainly simulated by using the ‘tipping bucket’ approach
277 (78%), in which the soil water availability is accounted for by adding rainfall and subtracting
278 evapotranspiration and runoff (Weiskittel et al., 2010) from an estimated maximum soil water
279 holding capacity (which depends on texture and the soil organic matter content). This
280 approach is also defined "cascading", since it assumes that water can move only downward
281 through the soil profile, filling up the layers until field capacity is reached.

282 For the transport and transformation of N in the soil profile, most models estimate pools
283 and fluxes of NO₃-N (78%) and/or NH₄-N (89%).

284

285 3.3. Plant ecophysiology and partitioning

286 Crop and grassland models differ in the algorithms reflecting plant ecophysiology
287 (growth and development) and partitioning (above and below-ground biomass and yield),
288 which can lead to differences in simulated yield and total biomass, in turn affecting estimated
289 C and N fluxes.

290 In our analysis (Table S3, see supplementary material), almost half of the models
291 consider the mechanism of C allocation as a function of development stage (56%), whilst
292 almost all the models take into account C assimilation (89%). The latter is mainly driven by
293 RUE-type processes (Radiation Use Efficiency) and/or P-R = gross photosynthesis –
294 respiration-type processes (56%).

295 Phenology is simulated by almost all models (89%) through the use of growing degree
296 days (GDD) (89%), whilst photoperiod and vernalization are represented by 56% of the
297 models.

298 Leaf area is accounted for by considering the leaf area index (LAI) (89%), whilst the
299 simulation of the number of leaves and evolution of the specific leaf area are almost ignored.

300 Reference evapotranspiration is accounted for using Penman-Monteith (56%), Penman
301 and Priestley–Taylor (44%).

302 Root distribution is simulated by 78% of the models, mainly through a linear approach
303 (56%).

304 For the most part, models consider a dynamic partitioning of assimilates among plant
305 organs (78%), based on the age of organs (78%). Within-plant partitioning occurs across
306 roots, grains, stems and sheaths, and leaf blades, for 89, 78, 78 and 67% of the models,
307 respectively.

308 Yield formation is mainly based on partitioning during reproductive stages (67%) and
309 harvest index-type (44%). The yields mostly simulated are forage (89%), roots and grains
310 (78%), tubers (67%) and fibre (56%).

311 The factors limiting plant growth most strongly among the nine models were water
312 deficit and nitrogen deficiency (88%).

313

314 *3.4. GHG emissions and other fluxes*

315 For better assessing how C and N cycles are involved in the simulation of GHG
316 emissions and other fluxes within several models, three main processes were detected (Table
317 S4, see supplementary material). Overall, our analysis indicates that these three main
318 processes are almost fully simulated by the considered models.

319 The most important C-fluxes from the ecosystems were considered in the main process
320 called "CO₂". More specifically, they include the gross primary production (GPP), NPP, NEE,
321 the net biome production (NBP) and several types of respiration processes, e.g. ecosystem
322 respiration (RECO), heterotrophic respiration from both soil and grazing animals, and
323 autotrophic respiration.

324 NPP and NEE are the most commonly simulated C-fluxes (67%), followed by GPP
325 (56%) and RECO (44%), whilst just a few models simulate the NBP. Despite only 44% of the
326 models taking into account RECO, most of them only consider soil respiration (89%). Plant
327 respiration is considered by 56% of the models, whilst only 33% of the models take into
328 account respiration from grazing animals.

329 Among all of the models analysed only DNDC is able to simulate all the CO₂ fluxes
330 considered. More than 70% of CO₂-GHG can be simulated also by APSIM, DayCent and
331 PaSim. The CO₂ simulated by the highest number of models (i.e. six models) are NPP, NEE
332 and soil respiration.

333 The main non-CO₂ fluxes (for simplicity called non CO₂-gas) include CH₄, N₂O, several
334 N emissions (i.e. NH₃, NO_x, N₂) and O₃.

335 N₂O emissions are most commonly simulated (78%), followed by NH₃ (56%). By
336 contrast, only a few models generate CH₄ and N₂ emission outputs (44%) and NO_x (33%).
337 None of the models provide ozone (O₃) emissions output.

338 N₂O emissions provided by the models are mostly generated by denitrification and
339 nitrification (78%), mainly based (i.e. >70% of the models) on a soil N pools (e.g. nitrate
340 pool, NH₄ pool) with soil water and temperature acting as main drivers of change on mineral
341 N pools.

342 Among all models analysed DayCent and DNDC were able to simulate all non CO₂-gas
343 considered in our analysis. However, more than 70% of non CO₂-gas can be simulated also by
344 APSIM, PaSim and CERES-EGC. The non CO₂-GHG simulated by the highest number of
345 models (i.e. seven models) was N₂O. The models able to simulate the highest number of
346 variables (i.e. CH₄, N₂O and N₂) were APSIM, DayCent, DNDC and PaSim.

347 Ten specific N processes were considered in the models: nitrification, denitrification,
348 volatilization, leaching, symbiotic fixation, assimilation, mineralization, immobilization, plant
349 uptake, and clay fixation. All these processes were widely simulated (i.e. >70%) by the
350 models considered in our analyses, with the only exception of clay fixation, that is considered
351 only by DNDC model.

352 Among the models analysed, only RothC does not take into account any N process. All
353 the remaining models are able to simulate each of the N processes considered in our analysis,
354 with the only exceptions being APSIM, which does not consider NH₃ volatilization, and
355 PaSim and STICS, which only take account of assimilation indirectly (C:N-driven).

356

357 **3.5.** *Management*

358 All models are able to simulate the impact of the most common farming practices (i.e.
359 harvesting, mowing, fertilization, tillage, irrigation, etc.) on the processes described so far. By
360 contrast, specific options for grasslands, such as plant use and nutrient returns from grazing
361 animals (as well as animal performances such as weight growth and milk production) are
362 simulated by a lower number of models (Table S5, see supplementary material).

363 Harvesting, cutting, tillage, irrigation and crop rotation are widely simulated (>70% of
364 models). Moreover, all models simulate fertilization and residue management. Concerning
365 fertilization, however, only application of mineral N and organic amendments are widely
366 simulated, while only a few models simulate other types of fertilizer such as phosphorus,
367 potassium, sulphur and calcium. Similarly, the management of crop residues is based mainly
368 on their burning or leaving on the ground surface, whilst only 33% of the models also

369 consider burial (e.g. STICS accounts for burial through tillage). Among other agricultural
370 practices, about half of the models consider pruning and water management (i.e. rice), but
371 only a few consider pesticide application.

372 The practices considered in the analysis are generally set by users. Some models also
373 offer options to trigger management events (i.e. fertilization and irrigation) based on changing
374 conditions during the simulation.

375 Simulation of grazing, animal performances and nutrient returns were taken into
376 account as specific options for grasslands.

377 Concerning grazing, models are for the most part based on user-determined settings
378 (start and end dates, animal density); some of them also include options related to evolving
379 conditions (APSIM, EPIC and PaSim), selective grazing (APSIM and PaSim) and trampling
380 effect (APSIM).

381 Animal performance simulation is considered by 55% of the models through
382 simple/static methods (APSIM and EPIC) or detailed/dynamic methods (PaSim), and based
383 on feeding standards or fill units (APSIM, DNDC and RothC).

384 Finally, nutrient return was considered by 66% of the models, based on uniform
385 distribution of returns across the whole field.

386 CERES-EGC, DSSAT and STICS do not include very specific agricultural options for
387 grasslands. APSIM is the most detailed model for grasslands.

388

389 **4. C and N cycles: performance, strengths and weaknesses**

390 In this section, we provide an overview of the C and N approaches used by the CN-MIP
391 models (see Table 4 and supplementary), and their performance as documented for a broad
392 gradient of geographic and climatic conditions, as well as a variety of soil types and
393 management practices, to gain insight into their main strengths and weaknesses. To do that,
394 we have summarised the results of 130 published modelling studies (Table 5).

395 In the analysis of the effects on C and N cycles of pedo-climatic conditions, we
396 considered variations of soil features such as temperature and moisture, texture, bulk density
397 (BD), pH, SOC, C and N dynamics and water-filled pore space (WFPS), and climate
398 conditions such as patterns of air temperature, precipitation, solar radiation, and including
399 frequency and intensity of extreme events such as floods and drought. Management practices
400 include changes in agricultural practices such as tillage, fertilization, irrigation, crop variety
401 on soil and vegetation and, in turn, on C and N cycles. The scale of application refers to the
402 influence on the model performances of the data types used. They may go from high-

403 frequency measurements specific to the study site, which have been collected experimentally
404 within carefully designed plans, to low-frequency data which have been administratively
405 aggregated at a coarse spatial resolution (e.g. regional or national summaries).

406 Several types of weaknesses emerged in 95 modelling studies (Table 6), where
407 criticalities in assessing the impact of pedo-climatic conditions (45.9%) and management
408 practices (33.8%) on environmental variables are reflected in unsatisfactory model
409 performances. These latter were mostly related to limitations of model structure with respect
410 to difficulties of the algorithms in simulating the effects of different management practices on
411 C and N cycling. By contrast, only a few weaknesses were due to the scale of application,
412 strictly related to the high variability in time and space of C and N cycles (16.2% and 4.1%
413 for pedo-climatic conditions and management practices, respectively). For the C cycle, major
414 limitations of model structure were related to management practices (43.6%), whilst for the
415 scale of application, the major weaknesses were due to different pedo-climatic conditions
416 (11.5%). For the N cycle, however, limitations inherent in model structure were predominant
417 under different pedo-climatic conditions (51.1%), whilst for the scale of application, major
418 weaknesses were due to different pedo-climatic conditions (20.2%).

419

420 4.1. Model structures and pedo-climatic conditions

421 Soil properties and climate conditions emerged as important factors for ensuring the
422 effective representation of outputs (Table 7). While climate issues were mainly related to
423 precipitation only, pedological factors concerned both the effect of changes of physical
424 (texture, bulk density and soil hydrologic properties) and chemical (C and N processes) soil
425 properties on C and N cycles.

426 Concerning soil physical characteristics, a primary role in modelling issues was played
427 by the soil water properties. Errors in the simulation of soil water content (SWC) were the
428 main cause of general discrepancies concerning C and N emissions in many studies (Table 7).
429 Discrepancies in C and N outputs were also observed under specific soil water conditions
430 such as the impact of soil freezing and thawing (Li et al., 2010) or soil shrinking and swelling
431 (Babu et al., 2006). Again, an inappropriate setting of initial state variables determined
432 discrepancies in N emissions (i.e. under- or over-estimation of N₂O emissions peaks,
433 Gabrielle et al., 2006). Considerable overestimations of N₂O emissions were found to be
434 closely related to overestimation of WFPS. WFPS is indeed one of the most important soil
435 variables influencing C and N cycles. For instance, microbially-mediated soil respiration and
436 N cycling processes tend to be higher or lower with increasing soil water content (e.g.

437 increased nitrification under aerobic conditions, increased denitrification under anaerobic
438 conditions, e.g. Bollmann. As WFPS reaches high values, soil respiration tends to decline and
439 denitrification occurs, resulting in N losses via N₂O and N₂ emissions. This condition was
440 observed especially for DayCent (Stehfest and Muller, 2004, Abdalla et al., 2010, Xing et al.,
441 2011, Ryals et al., 2014, 2015) and DNDC (Saggar et al., 2004, Abdalla et al., 2010). Fast
442 drainage is a particular issue for both the DayCent and DNDC models which drain water in
443 excess of field capacity immediately. This condition makes these models unable to accurately
444 predict N emissions at sites that consistently show soil moisture above FC (e.g. Uzoma et al.,
445 2015).

446 Soil bulk density (BD) was also a source of modelling error in simulating C and N
447 cycles. For CERES-EGC, Gabrielle et al. (2006) found a discrepancy in N₂O emission peaks
448 due to inappropriate parametrization of soil water retention properties and bulk density from
449 test site to regional scales. Drouet et al. (2011) confirmed that BD was one of the most
450 influential factors for N₂O emissions in CERES-EGC. The effect of BD increase was also
451 reported for DayCent by De Gryze et al. (2010) and Abdalla et al. (2009), respectively, which
452 observed an underestimation of N₂O emissions in a conservation tillage treatment due to the
453 increase in BD, and an associated decrease in pore space over time as DayCent maintains a
454 steady BD and simulation compaction, while the conservation tilled field site resulted in
455 increased BD and reduced N₂O emissions (Pisante et al., 2015). In fact, most of the selected
456 models, with the exception of EPIC, DNDC and STICS, do not simulate soil compaction or
457 loosening, as BD remains constant over time.

458 Texture was also found to be an influential soil physical characteristic. Congreves et al.
459 (2016) found an underestimation in NH₃ emissions with the DNDC model, which is unable to
460 simulate a heterogeneous soil profile. Similarly, Gagnon et al. (2016) confirmed that DNDC
461 does not effectively discriminate across soil textures to simulate soil CO₂ respiration. Clay
462 concentration affects SOC accumulation in different ways. According to some studies
463 (Nichols, 1984, Burke et al., 1989), SOC increases with increasing clay content due to the
464 bonds between the surface of clay particles and organic matter that retard the decomposition
465 process. In addition, a relevant fraction of microbial extracellular enzymes is adsorbed by
466 external and internal surfaces of clay size particles of soil phyllosilicate minerals (Burns et al.,
467 2013). The amount of bound enzymes increases with the increasing layer charge of
468 phyllosilicates (montmorillonite > illite > kaolinite) (Bayan and Eivazi, 1999). Sorption
469 causes conformational changes of enzymes' active sites, and in turn reduces or even
470 suppresses the activity of enzymes (Bayan and Eivazi, 1999, Burns et al., 2013). Moreover,

471 anaerobic conditions, that are expected to occur mostly in finer texture soils, also negatively
472 affect the amount of soil enzymes through reduction in the number of enzyme-producing
473 microorganisms (Inglett et al., 2005). Finally, the increase of clay content affects soil
474 aggregation, indirectly affecting SOC through the creation of macro-aggregates that can
475 physically protect organic matter molecules from further microbial mineralization (Rice,
476 2002, Plante et al., 2006). Thus, an overall reduction in SOM turnover in fine textured soils is
477 expected due to reduced substrate availability and overall microbial activity.

478 However, the effect of texture on SOC decomposition is controversial. For instance, for
479 10 sites in Canada (¹³C-labelled study) Gregorich et al. (2016) found that temperature (neither
480 soil texture nor other soil properties) was the only driver of decomposition. Furthermore,
481 texture parametrization is another possible source of error. For instance, Gijsman et al. (2002)
482 indicated that inaccuracies in soil texture data used as inputs may have affected soil retention
483 characteristics, thus resulting in discrepancies in SOC and soil mineral N dynamics.

484 Soil chemical processes are generally similar between the models and all models
485 considered showed difficulty in reproducing the observed C and N cycles. The processes
486 influencing SOM in the models include nitrification, denitrification, immobilization and
487 mineralization.

488 Discrepancies between modelled and observed data were often related to an
489 inappropriate SOC content parametrization (Pathak et al., 2005, Calanca et al., 2007,
490 Causarano et al., 2007, Smith et al., 2012, Gagnon et al., 2016). However, a considerable
491 source of error was also due to overestimation of SOC content (Abdalla et al., 2010, Gijsman
492 et al., 2002) or to the rate of soil C decomposition (Snow et al., 1999, De Gryze et al., 2010,
493 Li et al., 2015).

494 Nitrification is a two-stage process, performed by different groups of Archaea, bacteria
495 and fungi, consisting in the oxidation of ammonia or ammonium to nitrite (step 1) followed
496 by the oxidation of the nitrite to nitrate (step 2). For DayCent, Li et al. (2005) and Del Grosso
497 et al. (2008) found that overestimation in the nitrification rate was one of the main sources of
498 error for N emissions estimation. This was also found by Drouet et al. (2011), showing that
499 discrepancies in N₂O emissions simulated by CERES-EGC were due to the high sensitivity of
500 the model to the maximum rate of nitrification. The nitrification rate, however, is usually
501 associated with a number of environmental factors including the substrate and oxygen (O₂)
502 concentration, moisture, temperature and pH. For instance, this was observed by Li et al.
503 (2005), who pointed out that poor simulation of NH₄⁺ was caused by the inaccurate regulation
504 of the effect of temperature on nitrification in DayCent.

505 Denitrification is a process where the reduction of soil nitrate to N-containing gases
506 takes place. The major discrepancies between modelled and observed N emissions were due
507 to an underestimation of the denitrification rate (Thorburn et al., 2010, Xing et al. 2011, Fitton
508 et al., 2014a, b). The underestimation of the denitrification rate can be due to different **types**
509 of errors. For instance, for APSIM, Thorburn et al. (2010) found the source of error in the
510 model parametrization, with the default value of denitrification coefficient much lower than
511 the optimized value. By contrast, Xing et al. (2011) indicated the response of denitrification
512 rate to soil temperature and moisture (or WFPS) as the main source leading to the
513 underestimation of denitrification. Generally, denitrification rates have been reported to be
514 directly proportional to temperature (Seitzinger, 1988), whilst soils with high organic matter
515 content (high dissolved organic C) and anaerobic conditions (i.e. waterlogged or poorly-
516 drained soils) can more easily favour high denitrification rates.

517 Another important source of modelling error resulted from the inaccurate estimation of
518 the immobilization-mineralization processes. **N immobilization or mineralization depends on**
519 **the C:N ratio of the organic materials. The C:N ratio generally tends to decrease as the**
520 **organic matter becomes more decomposed. Inaccurate C:N parametrization can easily lead to**
521 **errors in C and N cycle related outputs. For instance, Li et al. (2015) observed for the DSSAT**
522 **model that differences between the modelled and measured soil C:N ratios led to SOC**
523 **overestimation.** In the EPIC model, He et al. (2006) observed that general discrepancies in C
524 and N dynamics (i.e. lower net N mineralization rate, humification, etc.) were likely due to N
525 mineralization algorithms which may have underpredicted net N mineralization (NMN)
526 observable under field conditions. Smith et al. (2008) and Fitton et al. (2014a, b) found that
527 the underestimation in mineralization rate led to underestimation of N₂O emissions. In the
528 same way, Del Grosso et al. (2010) indicated that overestimation of N₂O emissions was due to
529 N mineralization rates that were too high and too responsive to climate drivers.

530 Finally, climate conditions influence the C and N outputs in several studies analysed.
531 Some issues were related to how the climate data have been used. For instance, in APSIM,
532 Thorburn et al. (2010) found discrepancies in N emissions (i.e. underestimation of
533 denitrification and N₂O peaks) due to the application of spatially averaged rainfall data
534 instead of the use of specific test-site rainfall data. In other cases, the main issues were due to
535 the sensitivity of the model subroutines. For instance, Wattenbach et al. (2010) observed
536 overestimation in NEE peaks in southern European regions due to issues in coupling water
537 and C-fluxes. These issues were probably caused by the fact **that** the model was originally
538 developed to represent conditions typical of Northern regions. Again, Lawton et al. (2006)

539 reported overestimation of NEE because of the oversensitivity of PaSim to initial
540 conditions/winter conditions. Most of the issues related to general discrepancies in simulated
541 C and N cycles, however, were related to precipitation only (Stehfest and Muller, 2004,
542 Jarecki et al., 2008, De Gyrze et al., 2010, Ludwig et al., 2011, Lehuger et al., 2014).
543 Precipitation and the resulting soil water dynamics strongly influence N cycling in terrestrial
544 ecosystems since it affects both physical transport and N biological transformations by soil
545 microorganisms (Brooks et al., 1999, Corre et al., 2002, Aranibar et al., 2004).

546

547 **4.2.** *Model structure and management*

548 Management has a great impact on C and N cycles. In biophysical and biogeochemical
549 models, the correct representation of practices such as fertilization, irrigation and tillage in
550 crop systems, and cutting and grazing in grassland systems, is needed to ensure the greatest
551 suitability of outputs.

552 In the models, fertilization, which influences soil C and N transformations (e.g.
553 acidification following fertilization) and trace gas emissions, was often not well represented
554 (Table 7). For DayCent, Fitton et al. (2014a, b) indicated an underestimation of N₂O
555 emissions due to the low sensitivity of the model at low N application rates. In DNDC,
556 Congreves et al. (2016) found that NH₃ emissions were underestimated due to a simple
557 modelled cascade water flow, which may have limited the ability of the model to simulate
558 slurry infiltration rates. Also, Causarano et al. (2007) observed general discrepancies in C-
559 dynamics (i.e. overestimation of microbial biomass C and total organic C, underestimation of
560 particulate organic C), due to inadequate representation of the effects of tillage and manure in
561 the EPIC model. Another issue related to fertilization was the inability of many models to
562 replicate the effect of specific types of fertilizer. For instance, using DayCent Stehfest and
563 Muller (2004) found overestimation of N₂O emissions under urine application, where N was
564 concentrated in small hotspots. For the same model, Ryals et al. (2014 and 2015)
565 underestimated CO₂ emissions since no soil water benefits were provided by adding compost.
566 This condition was likely due to the lack of increased modelled decomposition because the
567 model was not able to increase soil water contents when compost was added. Gu et al. (2014)
568 overestimated N₂O emissions, soil nitrate and ammonia concentrations due to the inability of
569 DNDC to include canopy interception and foliar N uptake when spraying liquid fertilizer.

570 Finally, residue management was one of the main weaknesses related to N management
571 (Cavero et al., 1996, Sleutel et al., 2006, Rampazzo Todorovic et al., 2010, Wang et al.,
572 2013). The amount of N applied with residues depends on the quantity of residues and their N

573 concentration. These two factors affect the mineralization-immobilization turnover, whilst
574 their net balance varies with environmental conditions (mainly soil moisture and temperature)
575 and the characteristics of the **organic matter** (i.e. C:N and the decomposition rate). Since
576 residues directly influence soil C and N processes, residue management in the models resulted
577 in consistent modelling weaknesses. For instance, Justes et al. (2009) underestimated the N
578 mineralization in STICS due to inappropriate parametrization of the model (i.e. default values
579 of the decomposition module were used). In a similar way, Liu et al. (2009) overestimated the
580 SOC content when stubble (wheat and lupine) was applied due to the use of the conventional
581 setting of the stubble retention factor in RothC. Using DayCent and DNDC, Smith et al.
582 (2012) underestimated SOC due to a slight overestimation of residue removal impact.
583 However, the authors indicated that this could have been partly due to the inherent variability
584 in SOC measurements. Smith et al. (2012) also found that DNDC tended to underestimate the
585 rate of SOC change as affected by residue removal at some sites. Using DSSAT, Hartkamp et
586 al. (2004) overestimated SOC in the crop rotations with N fertilization. This overestimation
587 was due to inaccurate initial SOC (i.e. overestimated SOC values) which was related to an
588 overestimation of the biomass incorporated into the soil. Similarly, Wang et al. (2005)
589 underestimated the SOC content using the EPIC model due to a structural error in
590 underestimating the return of corn residues. He et al. (2006) found general discrepancies in C
591 and N dynamics **because the EPIC model underestimated the capacity of the soil to transform**
592 **crop residues into SOM.**

593 Tillage is one of the agricultural practices most commonly simulated by the models and
594 an issue in most modelling applications. The use of tillage or reduced tillage can greatly affect
595 soil properties, and since the models do not adjust some soil properties overtime (such as bulk
596 density) which results in inaccuracies in simulations. Compared with conventional tillage,
597 no/reduced tillage may lead to increasing rather than decreasing emissions (e.g. due to higher
598 density and WFPS, more SOM near the soil surface thus higher denitrification potential,
599 tendency to acidification and thus lower reduction of N₂O to N₂, etc.). Identifying
600 mechanisms which help understand simulate emissions with no tillage is thus a key issue. In
601 our analysis management effects (i.e. tillage) which influences topsoil erosion emerged as a
602 point of weakness. This is because many models do not take into account adequately C-losses
603 due to erosion. For instance, Nieto et al. (2010, 2013) overestimated SOC content using
604 RothC, whilst Billen et al. (2009) observed general discrepancies in SOC content with EPIC.

605 Another point of weakness in simulated tillage was the inadequate representation of
606 changes in soil properties over time. For instance, Luo et al. (2011), using APSIM,

607 underestimated SOC decomposition. In this case, whilst tillage may have led to acceleration
608 in soil C oxidation due to changes in soil environmental parameters (i.e. water retention,
609 porosity, aeration, etc.), APSIM failed to simulate changes in these soil properties over time,
610 which is a common issue amongst most models. Similarly, Causarano et al. (2007) found
611 general discrepancies in C dynamics (i.e. overestimation of microbial biomass C and total
612 organic C, underestimation of particulate organic C) due to an inadequate reproduction of the
613 effects of tillage and manure on soil properties.

614 In addition to fertilization and tillage, which were probably the most commonly
615 simulated agronomic practices, model weaknesses were found in relation to other practices.
616 For instance irrigation, especially accompanied by fertilization, was observed to affect
617 simulated C and N cycles. Jackson et al. (1994) and Caverro et al. (1999) underestimated N
618 fluxes under irrigated experiments using EPIC. The main source of error was related to an
619 overestimation of the soil N losses *via* leaching or denitrification during the irrigated crop
620 period. Grassland management was also seen to be a possible point of weakness for the
621 models. For instance, Lawton et al. (2006), Vuichard et al. (2007) and Ma et al. (2015)
622 observed general discrepancies in C-fluxes (i.e. net ecosystem exchange and ecosystem
623 respiration) under different grazing intensities using a grassland-specific model (PaSim). As
624 suggested by Vuichard et al. (2007), a continuous defoliation by grazing is indeed difficult to
625 account for as a permanent disturbance in the model. The grazing effect, however, is
626 associated with other parameters related to ecosystem and climate conditions, which makes it
627 difficult to pinpoint the parameter which most strongly influences the uncertainty of the
628 model output (Gottschalk et al., 2007).

629 Finally, model weaknesses also result from management options that are not included.
630 This type of weakness has emerged in several studies carried out using the RothC model. For
631 instance Skjemstad et al. (2004) found general discrepancies in C dynamics due to ecosystem
632 disturbances, which were not included in RothC (i.e. clearing and burning of pulled
633 vegetation). Shirato and Yokazawa (2005) underestimated SOC content due to the
634 decomposition rate of SOM under rice cultivation being too low (i.e. effect of waterlogged
635 soil not included in RothC), and Farina et al. (2013) reported some discrepancies in C-fluxes
636 when the model simulated rotations that included a fallow period.

637

638 4.3. Time-scale

639 Biophysical and biogeochemical models enable the estimation of C and N emissions at
640 various temporal and spatial scales. Compared to the emission factor approaches often used

641 by organizations and individuals to calculate GHG emissions for a range of activities, these
642 tools include the influences of agricultural practices, land-use change and soil properties, and
643 estimate the influences of weather on emissions over time.

644 The ability of these models to accurately reproduce detailed dynamics of C and N
645 emissions depends on the degrees of complexity of the model itself. Current process models,
646 with high complexity, are able to calculate in detail both C and N emissions due to their
647 consideration of all soil-plant-atmosphere interactions. These tools are able to provide
648 reasonable estimates of trace gas emissions from soils, usually for a specific site and at
649 seasonal or annual time scales. By contrast, however, they are less successful at finer time
650 resolution (e.g. daily) and on different sites from the ones where **they** have been previously
651 calibrated. In our analysis several studies showed weaknesses due to the time-spatial scale
652 associated with both pedo-climatic conditions and management.

653 Concerning time-scale weaknesses, Xing et al. (2011) underestimated N₂O emissions at
654 the daily time step using APSIM, while the use of the hourly time step may have likely
655 improved the estimate of predicted total daily emissions. This is because, in the APSIM
656 model, as in most models, N₂O emissions were released immediately to the atmosphere
657 without delay upon change in environmental conditions whereas the observations indicated
658 that there was a 1-10 hour lag between peaks of soil moisture and gaseous emissions.
659 Similarly, Lehuger et al. (2011) using CERES-EGC indicated an overestimation in N₂O
660 emissions, probably due to a possible time lag between the production of gaseous N₂O in the
661 soil and its emission to the atmosphere. Also, several studies carried out using DayCent
662 (Parton et al., 2001, Del Grosso et al., 2005, 2010) observed some discrepancies in simulated
663 N emissions due to time-lag. This was found to agree with **the results of** Li et al. (2005),
664 which indicated that DayCent often has a **1-day** lag before emissions occur. In all these cases,
665 the use of hourly time step may result in better predictions especially in conjunction with the
666 addition of a description of gas diffusion into soil, which could result in a delay between N₂O
667 production and emission.

668 Concerning spatial-scale weaknesses, Gabrielle et al. (2006) found discrepancies in N₂O
669 emission peaks using CERES-EGC. This was probably due to soil property parametrization
670 (i.e. soil water retention properties and bulk density) which may have led to differences in N
671 outputs from test sites to the regional scale. Using EPIC, general discrepancies in C-fluxes
672 (i.e. overestimation of microbial biomass C and total organic C, underestimation of particulate
673 organic C) were likely caused by spatial differences in C fraction due to differing soil
674 landscapes (Calanca et al., 2007). Schnebelen et al. (2004) overestimated soil N absorption

675 with the STICS model. This was probably due to propagation of errors for continuous
676 simulations compared to single-year simulations. More specifically, the underestimation of
677 some parameters in the previous year may have led to errors in the following years.

678

679 **5. New developments/future perspectives**

680 In the above analysis, an indication was given of models' predictive strength, while also
681 hinting at possible limitations in the underlying hypotheses from the literature in the cases
682 where discrepancies between model and observation occurred. Despite this extensive analysis,
683 knowledge of basic mechanisms driving C and N cycles in agricultural systems is still far
684 from complete and key questions remain, including: what exactly triggers the cascade of
685 events that finally lead to biological responses? How to differentiate between causes and
686 consequences? How does the knowledge derived from system observations relate to
687 mechanistic events? How does the current knowledge on C and N cycling in agriculture fit
688 with available mechanistic representations? Discrepancies between model outputs and
689 observations can be ascribed to a wide diversity of causes, without any real tendency to
690 associate them with one or another cause. The analysis reported in this work suggested
691 however three (quite large) areas of interest for possible improvements of C and N models: i)
692 soil biology, comprising SOM heterogeneity, decomposition kinetics, and N immobilization;
693 ii) soil physics, including the representation of soil physical properties and the simulation of
694 its effects on reaction rates; and iii) soil management, which indirectly affect soil processes by
695 modifying soil physical, chemical and biological properties.

696 Based on the main issues found in our analysis, despite recognizing the importance of
697 soil management (Andales et al., 2000), N transformations (Heinen, 2006, Congreves et al.,
698 2016), and plant-soil interactions (Kuzyakov, 2002, Roose and Schnepf, 2008, Kuzyakov and
699 Xu, 2013), here we focus on some innovative aspects related to soil biology and soil physics,
700 and the interface between the two that requires attention (Blagodatsky and Smith, 2012). This
701 choice is justified in that development of robust predictive frameworks is critical to managing
702 soil biology and its essential functions and services (Thrall et al., 2011). They can help
703 disentangling the causal links between soil biology and structure, physical-chemical factors
704 and ecological processes (e.g. nutrient cycling, soil C sequestration) that contribute to plant
705 community development and function. In addition, how soil communities respond to and
706 impact on plant succession (e.g. via regulatory networks that respond to the availability of
707 fixed N) may be important for predicting the role of plant–soil feedbacks in determining the

708 dynamics of soil microbial communities and the impact of anthropogenic disturbance on soil
709 diversity and function.

710 Soil microbial biomass (SMB) is generally only implicitly modelled by representing it
711 as a C pool not affecting substrate decomposition directly (Manzoni and Porporato, 2009).
712 Approaches of this type mostly implement solutions that are biologically meaningful (e.g.
713 representing realistically SOM turnover) and computationally tractable within a simulation
714 (i.e. with reduced overall complexity of the full model and a limited number of free
715 parameters to be tuned), which make them suitable for analyses in long-term studies
716 (Manzoni and Porporato, 2009, Sierra et al., 2015a). In recent years, researchers have
717 advocated a representation of SOM turnover driven by SMB to gain insight into decomposing
718 SOM-SMB interactions (Schimel and Weintraub, 2003, Lawrence et al., 2009, Blagodatsky et
719 al., 2010, Schmidt et al., 2011). For C and N substrates, concentration constraints driven by
720 microbial allocation patterns could thus be represented in novel biogeochemical models based
721 on microbial physiology (Allison et al., 2014). In this way, models based on microbial
722 biomass-driven SOM decomposition are promising to provide a realistic simulation of SOM
723 turnover in relation to changes in environmental conditions compared to existing models that
724 do not explicitly simulate SMB (Lawrence et al., 2009, Allison et al., 2010, Conant et al.,
725 2011, Sierra et al., 2015b). It is quite common to use classical enzymatic kinetics like
726 Michaelis-Menten or Monod-type kinetics to implement substrate-SMB co-limitation
727 (Blagodatsky and Richter, 1998, Hadas et al., 1998, Wutzler and Reichstein, 2013, Cavalli et
728 al., 2016), even if simpler decomposition kinetics have also been proposed (Manzoni and
729 Porporato, 2007, Withmore, 2007, Wutzler and Reichstein, 2008). Conversely, more general
730 model formulations are described in Neill and Gignoux (2006) and Neill and Guenet (2010) to
731 simulate microbial growth in soil accounting for both positive and negative priming effects.
732 The priming effect is defined as any change (positive or negative) of native SOM
733 decomposition rate following the addition of exogenous organic matter or nutrients, compared
734 to no addition (Fontaine et al., 2007, Kuzyakov et al., 2000, Kuzyakov, 2010, Chen et al.,
735 2014, Perveen et al., 2014).

736 Even in models with explicit SMB, microbial community is usually simulated with one
737 or few pools, each representing microorganisms belonging to a different functional group
738 (Moorhead and Sinsabaugh, 2006). However, further model developments could be achieved
739 if diversity in soil microbial traits is included in the model, allowing microorganisms with
740 optimal strategies to outperform other microorganisms with less favorable traits in a given
741 environment (Allison et al., 2012, 2014). In such models, genomic and metagenomics data

742 can be integrated with other sources of information to define distributions of microbial traits
743 that are used to characterize the microbial community (Vereecken et al., 2016).

744 Another important aspect regarding SOM turnover is the effect of N shortage on SOM
745 decomposition. Soil microorganisms are characterised by a narrow range of variation in their
746 C to N ratio (Cleveland and Liptzin, 2007, Xu et al., 2013); thus, they can be approximately
747 considered homeostatic (i.e. they do not change markedly their C to N ratio according to
748 substrate C to N ratio). Mechanisms of adaptation to stoichiometric imbalances between
749 substrates and SMB were reviewed in detail by Mooshammer et al. (2014a). One postulated
750 mechanism of adaptation regards the variation of microbial C use efficiency (CUE, defined as
751 the ratio between newly-formed biomass C and decomposed C) and of N use efficiency
752 (NUE, defined similarly to CUE) to accommodate for excess or deficit of C or N (Manzoni et
753 al., 2012, Sinsabaugh et al., 2013, Mooshammer et al., 2014b, Jeyer et al., 2016).

754 Soil organic matter decomposition is operated mostly by the activity of extracellular
755 enzymes (Burns et al., 2013), and any cost associated with the production of enzymes
756 decreases CUE (Manzoni et al., 2012). Microorganisms evolved to optimize resource
757 allocation for the synthesis of exoenzymes in response to environmental and physiological
758 factors (Allison et al., 2011). According to Sinsabaugh and Follstad Shah (2012) and
759 Sinsabaugh et al. (2016) CUE and NUE are both related to the activities of C and N acquiring
760 exoenzymes (measured as potential activities of β -1,4-glucosidase, and β -1,4-N-
761 acetylglucosaminidase and leucine aminopeptidase, respectively). Thus, variations in CUE
762 and NUE arise because SMB regulates exoenzyme production (in terms of amounts and type
763 of synthesized enzymes) to attenuate the differences between their growth requirements and
764 available resources (Sinsabaugh et al., 2016).

765 Another mechanism of CUE regulation by SMB when SOM decomposition is N-limited
766 is overflow metabolism (Russel and Cook, 1995): excess C is excreted as extracellular C
767 compounds (like polysaccharides) (Hadas et al., 1998, Cavalli et al., 2016), or lost as CO₂
768 (Schimel and Weintraub, 2003, Neill and Gignoux, 2006). Conversely, when N is in excess
769 relative to C (decomposition is limited by C availability), net N mineralisation occurs. Models
770 usually implement N deficit effects on SOM decomposition with the N inhibition hypothesis
771 (Manzoni and Porporato, 2009), that is, SOM turnover is reduced according to N availability,
772 and thus CUE does not change. Alternatively, other models (Izaurrealde et al., 2006,
773 Withmore, 2007) allow SMB to vary its C to N ratio according to stoichiometric imbalances,
774 and thus they consider SMB as non-homeostatic.

775 Decomposition of SOM in soil occurs at microsites showing varying N availability
776 (Schimel and Bennett, 2004). This is caused by heterogeneity of both SOM and of soil
777 physical properties (Schmidt et al., 2011). Thus, N is supposed to flow from micro-sites
778 showing net N mineralisation to others showing net N immobilisation (Schimel and Bennett,
779 2004). Mathematically, the heterogeneity of SOM decomposition in a first approximation can
780 be simulated considering that not all organic N in substrates is available to SMB, according to
781 the parallel hypothesis (Manzoni and Porporato, 2007). The use of a simple lumped SOM
782 model, based on the parallel approach, was shown to provide almost similar results to the
783 same model structure that explicitly took into account the heterogeneity of soil
784 decomposition, and in which all organic N in substrates was available to decomposers,
785 according to a direct assimilation pathway (Manzoni et al., 2008).

786 The heterogeneity of SOM is simulated with models that comprise several pools of
787 different decomposability (Nicolardot et al., 2001, Manzoni and Porporato, 2009, Sierra et al.,
788 2011, Sierra and Müller, 2015). In many models, decomposition constants of model pools
789 incorporate intrinsic chemical recalcitrance of SOM, and availability of SOM to decomposers
790 (Nicolardot et al., 2001, Sierra and Müller, 2015). However, it was recently emphasised that
791 chemically-labile (or high-quality, and thus potentially easily-degradable) molecules can
792 persist in soil for a long time due to constraints on their microbial decomposition not related
793 to intrinsic chemical characteristics (Kleber, 2010, Marschner et al., 2008): biology of
794 decomposers, abiotic reactions and desorption, environmental variables and physicochemical
795 stabilisation processes (Ekschmitt et al., 2005, Kemmit et al., 2008, Kleber et al., 2011,
796 Schmidt et al., 2011, Dungait et al., 2012). Regarding SOM physical and chemical
797 stabilisation, models that explicitly represent protected and unprotected SOM pools of similar
798 chemical characteristics (Kuka et al., 2007) allow separating intrinsic recalcitrance (substrate
799 quality) from availability, and thus enable simulating long-term stabilisation of chemically
800 easily-decomposable high-quality SOM (Dungait et al., 2012). In addition, more sophisticated
801 and realistic approaches to simulate soil physicochemical heterogeneity, and thus variability
802 of SOM decomposition, were implemented in SOM models that represent soil as 3D structure
803 in which decomposition takes place (Garnier et al., 2008, Masse et al., 2007, Monga et al.,
804 2009, 2014).

805 Improving soil biology aspects related to the production and consumption of gases (O_2 ,
806 CO_2 , CH_4 , N_2O , and N_2) will improve the simulation of soil gas concentrations. However, this
807 is not sufficient to achieve proper simulations of GHG emissions, as accounting for gas
808 transport through the soil profile is also important. As pointed out by Blagodatsky and Smith

809 (2012), it is necessary to find the right balance in complexity between biological and soil
810 physical simulations. For example, the higher soil tortuosity the higher the N_2/N_2O ratio,
811 because N_2O has more possibilities to be reduced when the escape pathway from the N_2O
812 production sites to the atmosphere (and thus its diffusion time) is longer. Adequate simulation
813 of gas transport in soil can be achieved using mechanistic models based on water, heat, and
814 gas transport equations, and gas-liquid phase exchange. A further connection among soil
815 biology and soil physics research will be to simulate SOM turnover and gas production,
816 consumption, and transport in a 3D soil structure using the concepts presented above, so as to
817 achieve a more realistic representation of environmental effects (soil temperature and
818 moisture), especially in the context of climate change.

819 One final observation is that all of the model improvements presented above require
820 adequate simulation of initial conditions of inorganic N availability. Thus, it is mandatory that
821 all processes affecting soil ammonium concentration be accurately simulated. **Among these,**
822 **ammonium fixation in non-exchangeable form by clay minerals in fine-textured soils can play**
823 **a central role in determining the availability of N for microorganisms. Research on cation**
824 **exchange in soil demonstrated that monovalent cations with low hydration energy and ionic**
825 **radius that fits the ditrigonal cavities of the basal oxygen planes of 2:1 clay minerals are**
826 **selectively sorbed at frayed edges of illite (partially weathered micas) and vermiculite, and at**
827 **interlayer positions of vermiculite (Sawhney, 1972). Sorption of NH_4^+ (like K^+ , Rb^+ , and Cs^+)**
828 **in such exchange sites causes interlayer dehydration and layer collapse (Nieder et al., 2011).**
829 **Such ions are strongly held against replacement by other cations and are termed fixed.** After
830 its application to soil with fertilisers, a relevant fraction of ammonium can be very rapidly
831 (hours or days) fixed by clay minerals (Nõmmik, 1957) and is very slowly released during the
832 following weeks or months (Steffens and Sparks, 1997). This fraction of applied N is thus not
833 immediately available for nitrification, microbial immobilisation, and plant uptake. **For a**
834 **comprehensive survey of the factors influencing ammonium fixation / release readers can**
835 **refer to reviews by Nõmmik & Vahtras (1982) and Nieder et al. (2011).**

836 Despite its importance, ammonium fixation / release is not commonly simulated by
837 crop/grassland system and SOM models. The rapid fixation can be simulated with well-
838 known isotherms, which represent the static adsorption of an ion onto a surface (Cameron and
839 Kowalenko, 1976, Cavalli et al., 2015) as a function of ion concentration. **However,**
840 **ammonium exchange reactions in soil are affected by the presence of other cations (such as**
841 **K^+ and Ca^{2+}), and thus models should take into account for ion interactions (Bradbury and**
842 **Baeyens, 2000; Evangelou and Lumbanraja, 2002). Research is needed to estimate model**

843 parameters depending on soil characteristics (such as type of clay, potassium concentration,
844 and soil water content) and to simulate ammonium release over time.

845

846 **6. Summary and concluding remarks**

847 At present, process-based biogeochemical models represent a valuable tool for
848 examining the magnitude and spatial-temporal patterns of C and N fluxes in terrestrial
849 biosphere dynamics. Our analysis shows that there is still great divergence between models in
850 the simulation of C sequestration and GHG source/sink status, in relation to a different
851 interpretation of physical and biogeochemical processes.

852 Representative works have been summarized to provide a general overview of the state-
853 of-the-art of models, and to allow process-based models (the nine identified in this study) to
854 be compared and selected for the simulation of C and N cycles in crop and grassland systems.
855 We classified models into categories according to three levels of knowledge: five general
856 classes (level 1), 20 main processes (level 2), and 196 methods/options/components (level 3),
857 and then we assessed the tools in terms of the comprehensiveness of processes related to
858 pedo-climatic and management options, and their accuracy in a variety of contexts.

859 This review highlighted strengths and weaknesses of the models analysed. Essentially,
860 they involve limitations in simulating the effects of pedo-climatic conditions (45.9%) and
861 different management practices (33.8%). Other weaknesses (i.e. 20.3%) were due to the scale
862 of application in time and space.

863 The major limitations of model structure related to C-cycles were observed under
864 management practices (43.6%), whilst for the scale of application the major weaknesses were
865 due to different pedo-climatic conditions (11.5%). **For both the N-cycle modelling and scale
866 of application, the main limitations were found in the response to different pedo-climatic
867 conditions (51.1% and 20.2%, respectively).**

868 All the models considered here showed positive and negative features and none may
869 necessarily be ideal in any particular circumstance. If the model chosen is not able to
870 reproduce the output required, two or more of these models may be combined to derive upper
871 and lower values for all simulated outputs. Moreover, a decision about which model or
872 models to use should be seen as dynamic, not static. As conditions change, or if one model
873 proves unsuccessful, they can be adapted or replaced with other, more suitable, models.

874 Although the above reported weaknesses were already known due to a wide number of
875 published studies, in the present analysis we have tried to relate them to their causes in the
876 view of using them as an effective basis for improving current modelling approaches.

877 Although different avenues could be considered to improve models (e.g. Coucheney et al.,
878 2015), mainly depending on the purpose of modelling, to overcome the reported limitations
879 and account for the effect of multiple disturbances (i.e. pedo-climatic conditions, management
880 practices, scale of analysis) affecting basic processes, as well as to simplify the decision of
881 which model to choose to understand mechanistically specific study-contexts and to make
882 detailed predictions in a large diversity of situations, some innovative aspects should be
883 considered in the modelling work. Among these, we target the representation of SOM
884 turnover driven by SMB, the effect of N shortage on SOM decomposition, improvement
885 related to the production and consumption of gases (O₂, CO₂, CH₄, N₂O, and N₂), adequate
886 simulations of gas transport in soil, the use of a 3D soil structure in order to achieve a more
887 realistic representation of environmental effects (soil temperature and moisture), especially in
888 the context of climate change.

889 Model improvement thus implies extending the existing body of knowledge on
890 ecological and biogeochemical concepts, to allow them to be incorporated using novel
891 approaches, thus improving the representation of the dynamics of the ecosystems, and the
892 related advantages for stakeholders.

893

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906

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1883

35

36 **Abstract**

37 Biogeochemical simulation models are important tools for describing and quantifying the
38 contribution of agricultural systems to C sequestration and GHG source/sink status. The
39 abundance of simulation tools developed over recent decades, however, creates a difficulty
40 because predictions from different models show large variability. Discrepancies between the
41 conclusions of different modelling studies are often ascribed to differences in the physical and
42 biogeochemical processes incorporated in equations of C and N cycles and their interactions.
43 Here we review the literature to determine the state-of-the-art in modelling agricultural (crop
44 and grassland) systems. In order to carry out this study, we selected the range of
45 biogeochemical models used by the CN-MIP consortium of FACCE-JPI
46 (<http://www.facejpi.com>): APSIM, CERES-EGC, DayCent, DNDC, DSSAT, EPIC, PaSim,
47 RothC and STICS. In our analysis, these models were assessed for the quality and
48 comprehensiveness of underlying processes related to pedo-climatic conditions and
49 management practices, but also with respect to time and space of application, and for their
50 accuracy in multiple contexts. Overall, it emerged that there is a possible impact of ill-defined
51 pedo-climatic conditions in the unsatisfactory performance of the models (46.2%), followed
52 by limitations in the algorithms simulating the effects of management practices (33.1%). The
53 multiplicity of scales in both time and space is a fundamental feature, which explains the
54 remaining weaknesses (i.e. 20.7%). Innovative aspects have been identified for future
55 development of C and N models. They include the explicit representation of soil microbial
56 biomass to drive soil organic matter turnover, the effect of N shortage on SOM
57 decomposition, the improvements related to the production and consumption of gases and an
58 adequate simulations of gas transport in soil. On these bases, the assessment of trends and
59 gaps in the modelling approaches currently employed to represent biogeochemical cycles in
60 crop and grassland systems appears an essential step for future research.

61

62 *Keywords: Biogeochemical models, C cycle, N cycle, management, pedo-climate*

63

64 **1. Introduction**

65 The sensitivity of soil carbon (C) stocks and greenhouse gas (GHG) emissions to
66 climate and management practices demands a comprehensive methodology for effective
67 policy analyses (Li et al., 1994). Enhancing soil C sequestration and reducing GHG emissions
68 from agricultural soils are key objectives for reducing the climate impact of food production
69 and they strongly depend on agricultural practices such as crop residue return, soil tillage
70 modalities, and enhanced nitrogen (N) fertilization management. Whether C return to soils
71 appear as a main controlling factor, in some cases (e.g. dry climates) reduced tillage may also
72 be an effective measure for enhancing C sequestration (e.g. Chatskikh et al., 2008; Powlson et
73 al., 2012). To avoid pollution swapping, assessments of the potential to reduce climate impact
74 should also include other impacts such as nitrate (NO_3^-) leaching into groundwater, ammonia
75 volatilization and soil erosion, which can also be reduced, for example, by increasing the use
76 of grazed pastures in dairy farms (Rotz et al., 2009, Peyraud, 2011). In addition, it is
77 important to consider the interactions on the hundred-year timescale of soil C equilibration
78 (Lardy et al., 2011) and the relatively more rapid changes induced by agricultural practices
79 (Angers et al., 1995). It is likely that most agricultural soils are not in equilibrium with respect
80 to C storage and have the greatest potential for short-term C losses or gains, while they may
81 also be sensitive to the effects of long-term, climate-driven processes (Wutzler and
82 Reichstein, 2007). It is also important to recall that C and nitrogen (N) cycling strongly
83 depends on interactions among plant growth processes, soil water dynamics and soil N
84 dynamics that are highly non-linear and thus difficult to predict with simple approaches.

85 Process-based ecosystem models take the approach of simulating underlying
86 biogeochemical processes, such as plant photosynthesis and respiration, using mathematical
87 equations that determine the allocation of C from atmospheric CO_2 into biomass down to the
88 soil organic matter (SOM). A relatively complete suite of biogeochemical processes (e.g.
89 plant growth, organic matter decomposition, fermentation, ammonia volatilisation,
90 nitrification and denitrification) is generally embedded in these models, enabling computation
91 of transport and transformations in plant–soil ecosystems. Sub-models are designed to interact
92 with each other to describe cycles of water, C and N for target ecosystems, thus any change in
93 the environmental factors collectively affect a group of biogeochemical reactions. Extensively
94 tested biogeochemical models (with the coupled C-N cycling) are effective tools for
95 examining the magnitude and spatial-temporal patterns of C and N fluxes, and play an
96 important role in designing specific policies appropriate to the soils, climate, and agricultural
97 conditions of a location or region. However, results of state-of the-art terrestrial

98 biogeochemical models, describing the contribution of agricultural systems to C sequestration
99 and GHG source/sink status, may diverge significantly. Such differences between model
100 results are often attributed to physical and biogeochemical processes being inadequately
101 resolved and, for these models, the improvement of algorithms and structure is recommended
102 beyond parameter optimization (Tian et al., 2011, Lu and Tian, 2013).

103 It is the goal of this paper to examine the strengths and weaknesses of nine crop and
104 grassland models that incorporate C and N fluxes into biogeochemical frameworks and fully
105 assess C and GHG dynamics in agricultural soils. These models are commonly applied
106 worldwide and are used to simulate biogeochemical and related outputs by the project “C and
107 N models intercomparison and improvement to assess management options for GHG
108 mitigation in agro-systems worldwide” (CN-MIP, 2014-2017), established within the Joint
109 Programming Initiative on Agriculture, Food Security and Climate Change (FACCE-JPI,
110 <http://www.facejpi.com>), which brings together 10 organizations from six countries. With
111 this analysis we are not arguing against the quality of models. While highlighting weaknesses
112 and limits of current modelling approaches as documented in several published studies, we
113 intend to offer a general overview as a basis for new ways of improvement current modelling
114 approaches.

115 The following rationale has been used in the organization of this article. We first present
116 the conceptual basis and the equations of the modelling approaches examined (Section 2).
117 Section 3 reports on the documented performance of biogeochemical models against data, and
118 discuss their relative strengths and weaknesses. Section 4 presents an outlook on recent
119 research developments and future approaches. In Section 5, remarks are made concerning the
120 bearing of the findings on a wider interpretation of biogeochemical modelling.

121

122 **2. Modelling approaches**

123 *2.1. Basic model assumptions*

124 Biophysical and biogeochemical models are widely applied for studying crop and
125 grassland productivity and GHG emissions in agricultural systems worldwide. In recent
126 decades, these tools have also been used for assessing the expected impacts of future climate,
127 as represented by several climate change scenarios (Graux et al., 2013). According to several
128 studies, however (Palosuo et al., 2011, Rotter et al., 2012, Asseng et al., 2013, Sándor et al.,
129 2016), key model limitations have been identified, and different models have been found to
130 provide different results when run in the same conditions of climate, soil and management.

131 More specifically, a typical process can be described by using different approaches, thus
132 resulting in different final outputs.

133 All the models selected within CN-MIP are process-based models. They attempt to
134 reproduce the most relevant ecological and physiological process through a theoretical
135 understanding grounded in state-of-the art knowledge. In this way, they reproduce specific
136 agro-ecological dynamics under prescribed conditions of climate, soil and management,
137 thanks to the concepts and relationships that interlink entities of the real world. Most models
138 represent plant phenology and yield-formation processes, together with functional processes
139 at the basis of SOM (Soil Organic Matter) turnover, gas exchange at the soil-plant-atmosphere
140 interface and soil water dynamics.

141

142 2.2. *The CN-MIP models*

143 The nine models considered for the CN-MIP exercise were mainly developed for crop
144 or grassland ecosystems. These models were chosen since they are able to simulate GHG
145 emissions under several management options. We were able to assess their ability to represent
146 the GHG emission mitigation by modelling a variety of land management practices. The nine
147 models analysed for this intercomparison are: *APSIM*, *CERES-EGC*, *DayCent*, *DNDC*,
148 *DSSAT*, *EPIC*, *PaSim*, *RothC* and *STICS* (Tab. 1). Below, a brief description of each model is
149 provided.

150 i) *APSIM* (The Agricultural Production Systems sIMulator) (Keating et al., 2003)
151 simulates several systems through the interaction among plants, animals, soil, climate and
152 management. The model allows the analysis of the whole-farm system, including crop and
153 pasture sequences and rotations, and livestock.

154 ii) *CERES-EGC* (Crop Environment REsource Synthesis - Environnement et Grandes
155 Cultures) (Gabrielle et al., 1995) simulates the biogeochemical cycles of water, C and N in
156 agro-ecosystems. The model predicts crop production and the environmental impacts related
157 to the agriculture activity (e.g. N₂O, NO, NH₃, CO₂, NO₃) based on management for a wide
158 range of arable crops (e.g. wheat, barley, maize, sorghum, sunflower, pea, sugar-beet, oilseed
159 rape and miscanthus). Crop-specific modules include approaches for plant growth and
160 development, coupled to a generic soil sub-model.

161 iii) *DayCent* (Parton et al., 1994) is a biogeochemical model able to simulate crop growth,
162 soil C dynamics, N leaching, gaseous emissions (e.g. N₂O, NO, N₂, NH₃, CH₄ and CO₂) and
163 C fluxes (e.g. NPP, NEE) in crop fields, grasslands, forests, and savanna ecosystems. The

164 model allows to simulate also several management practices (i.e. fertilization, tillage, pruning,
165 cutting, grazing, etc.) as well as specific external disturbances (i.e. fires).

166 iv) *DNDC* (DeNitrification-DeComposition) (Li et al., 1992a) simulates C and N
167 biogeochemistry in agro-ecosystems. The model predicts crop growth, soil regimes (i.e.
168 temperature and moisture), soil C dynamics, N leaching, and trace gases emissions (e.g. N₂O,
169 NO, N₂, NH₃, CH₄ and CO₂). The model was expanded in 2012 to include biophysical
170 processes in whole-farm systems (Li et al., 2012).

171 v) *DSSAT* (Decision Support System For Agrotechnology Transfer) (IBSNAT,
172 1993, Tsuji, 1998, Uehara, 1998 and Jones et al., 1998), was originally developed to facilitate
173 the application of crop models in a systems approach to agronomic research. *DSSAT* ver. 4.6
174 (i.e. cropping system model, CSM) and its crop simulation models integrates the effects of
175 soil, crop phenotype, weather and management options. *DSSAT* includes improved
176 application programs for seasonal, spatial, sequence and crop rotation analyses that assess the
177 economic risks and environmental impacts associated with irrigation, fertilizer and nutrient
178 management, climate variability, climate change, soil carbon sequestration, and precision
179 management. The model can predict crop yield, resource dynamics such as for water, N and
180 C, environmental impact (i.e. N leaching), evapotranspiration and SOM accumulation.

181 vi) *EPIC* (Environmental Policy Integrated Climate) (Williams, 1995) can simulate about
182 80 crops through its crop growth model which uses unique parameter values for each crop. It
183 can predict changes in soil, water, nutrient, pesticide movements, and crop yields due to
184 effects of management decisions. Moreover, it can also assess water quality, N and C cycling,
185 climate change impacts, and the effects of atmospheric CO₂.

186 vii) *PaSim* (Pasture Simulation model) (Riedo et al., 1998) is a process-based, grassland-
187 specific ecosystem model that simulates grassland and pasture productivity and GHG
188 emissions to the atmosphere. The model consists of sub-models for grass, animals,
189 microclimate, soil biology, soil physics and management.

190 viii) *RothC* (Rothamsted Carbon model) (Coleman and Jenkinson, 1999) is a
191 specific tool for the assessment of organic C turnover in non-waterlogged topsoil. The model
192 allows for the effects of soil type, temperature, moisture content and plant cover on the
193 turnover process.

194 ix) *STICS* (Simulateur multIdisciplinaire pour les Cultures Standard) (Brisson et al., 1998)
195 is a soil-crop model which is built on a generic framework for plant description. Within this
196 framework, the selection of adequate options and parameters values allows to simulate a wide
197 range of plants, from annual crops to perennial grasses or trees. The model simulates plant

198 growth as well as water, C and N fluxes. It allows to consider the effect of a large range of
199 management options on agronomic (biomass or grain productivity and quality) and
200 environmental (C and N storage, nitrate leaching, N₂O emissions) outputs.

201

202 **3. Results**

203 *3.1. Model analysis*

204 For reducing the uncertainty in estimating the magnitude and spatial-temporal patterns
205 of C and N fluxes from several agro-systems (i.e. crops, grassland and livestock), and for
206 improving the understanding of how these tools work, we analysed the most important
207 processes and approaches implemented into the models. This analysis was based on a top-
208 down approach focused at gaining insight into compositional sub-systems. On this basis, we
209 indicated three levels of information containing specific processes/approaches that were sub-
210 divided according to different levels of detail.

211 The starting point (level 1) was the detection of discrete units considered in agricultural
212 modelling, which are essential to characterize agricultural systems. In this level, characterized
213 by the lowest level of detail required for the analysis, we differentiated five general classes
214 that should be implemented within all biophysical/biogeochemical process-based models for
215 crops and grasslands. These classes concern ecological and physiological processes,
216 management options, soil structure, and weather inputs (Tab. 2).

217 Then, in the level 2 (intermediate level of detail) specific processes were identified
218 within each general class (level 2). In this level 20 "main processes" were identified, which
219 we retained as basic to describe the most important biophysical/biogeochemical dynamics
220 (Tab. 3) of each general class indicated in the previous level.

221 Finally, in the level 3 (highest level of detail) almost 200 modelling approaches (i.e.
222 methods, options or components), identifying specific dynamics or mechanisms contained
223 within the previous main processes (supplementary material) were reported (level 3). These
224 approaches were extrapolated taking into account the current existing knowledge on the
225 different methods, options and components able to describe the most important
226 biophysical/biogeochemical dynamics (Tab. 3a-e in supplementary material).

227 There are a number of advantages to such a "top-down" approach. An advantage is the
228 insight that can be gained from examining the level of detail that each model provides. This in
229 turn helps in identifying areas in the model structures to establish their reliability and
230 relevance for intended purposes. Such an approach also helps in tracing possible links with
231 the basic processes of each model (identification of the strengths and weaknesses) either in

232 the case of mismatch between model outputs and measurements, or in the case of
233 disagreement among model results in similar conditions.

234 Results reported below were based on the highest level of detail (level 3 – see
235 supplementary material).

236

237 3.1.1. *Meteorological variables*

238 Meteorological inputs strongly influence model outputs since they affect plant growth,
239 plant development stages, and soil turnover/balances, including flux exchanges at the soil-
240 plant-atmosphere interface. The number and type of climatic variables required by each model
241 informs us about the relationship between model outputs and climate drivers. In principle, for
242 the modelling of surface reactions and diffusion of volatile products (e.g. N₂O emissions, soil
243 water content dynamics), the higher the resolution in the climate information (e.g. hourly to
244 sub-hourly weather inputs), the more accurate the model response is for short-term processes
245 but the higher the probability that missing data may be present in the weather series used. For
246 longer term processes such as soil organic carbon (SOC) decomposition, higher temporal
247 resolution data may not improve the accuracy of the model response.

248 From our analysis (Tab. 3a, see supplementary material) we observed that the nine
249 models involved in CN-MIP mostly use climate inputs at daily resolution (89%), whereas
250 PaSim uses the hourly time scale (but with an option also available for daily inputs), and
251 RothC uses a monthly time-step.

252 The most commonly used meteorological variables are precipitation, air temperature
253 and wind speed. Concerning air temperature, the daily maximum and minimum air
254 temperatures are used by almost all models (89%).

255 Relative humidity (daily mean) and global solar radiation are also used by 67% and
256 56% of the models, respectively. The atmospheric concentration of CO₂ is an optional input
257 for many models (78%), with the exception of CERES-EGC and RothC.

258 Finally, only a few models use specific meteorological variables such as cloudiness,
259 sunshine duration, dew-point temperature and actual vapour pressure.

260

261 3.1.2. *Soil*

262 Similarly to climate inputs, soil characteristics also have a great influence on model
263 outputs. These characteristics strongly influence crop growth and fluxes related to the gaseous
264 biogeochemical cycles as water, C and N. Some soil inputs are assumed as constant values
265 (i.e. parameters), not changing during the simulation. Different soil properties (e.g. texture,

266 pH, bulk density, etc.) can affect plant growth and the environmental conditions for the
267 microbial activity driving the formation and decomposition of SOM and mediating
268 biochemical processes.

269 From our analysis (Tab. 3b, see supplementary material), it emerged that soil processes
270 are mostly calculated based on the differentiation of the soil profile into a sequence of distinct
271 layers, with generation of outputs for each of these subdivisions. In PaSim model, the whole
272 soil profile is the basis for the modelling of C dynamics. The soil temperature is calculated
273 from energy balance (44%) or based on a response function of air temperature (56%).

274 The water transport calculation scheme in soil is mainly described by the capacity (or
275 tipping bucket) approach (78%).

276 For the transport and transformation of N in soil profile, most models estimate pools
277 and fluxes of NO₃-N (78%) or/and NH₄-N (89%).

278

279 3.1.3. *Plant ecophysiology and partitioning*

280 Crop and grassland models differ in the algorithms reflecting plant ecophysiology
281 (growth and development) and partitioning (above and below-ground biomass and yield),
282 which can lead to differences in simulated yield and total biomass, in turn affecting estimated
283 C and N fluxes.

284 In our analysis (Tab. 3c, see supplementary material), almost half of the models
285 consider the mechanism of C allocation as a function of development stage (56%), whilst
286 almost all the models take into account C assimilation (89%). The latter is mainly driven by
287 RUE-type processes (Radiation Use Efficiency) and/or P-R = gross photosynthesis –
288 respiration-type processes (56%).

289 Phenology is simulated by almost all models (89%) through the use of growing degree
290 days (GDD) (89%), whilst photoperiod and vernalization are represented by 56% of the
291 models.

292 Leaf area is accounted for by considering the leaf area index (LAI) (89%), whilst the
293 simulation of the number of leaves and evolution of the specific leaf area are almost ignored.

294 Reference evapotranspiration is accounted by Penman-Monteith (56%), Penman and
295 Priestley–Taylor (44%).

296 Root distribution is simulated by 78% of the models, mainly through a linear approach
297 (56%).

298 For the most part, models consider a dynamic partitioning of assimilates among plant
299 organs (78%), based on the age of organs (78%). Within-plant partitioning occurs across

300 roots, grains, stems and sheaths, and leaf blades, for 89, 78, 78 and 67% of the models,
301 respectively.

302 Yield formation is mainly based on partitioning during reproductive stages (67%) and
303 harvest index-type (44%). The yields mostly simulated are forage (89%), roots and grains
304 (78%), tubers (67%) and fibre (56%).

305 The factors limiting plant growth most strongly among the nine models were water
306 deficit and nitrogen deficiency (88%).

307

308 3.1.4. *GHG emissions and other fluxes*

309 For better assessing how C and N cycles were involved in terms of GHG emissions and
310 processes within several models, three main processes were detected (Tab. 3d, see
311 supplementary material).

312 In general from our analysis emerged that the three main processes belonging to the
313 general class of GHG emissions and other fluxes are almost fully simulated by the considered
314 models.

315 In the main process called CO₂-GHG the most important C-fluxes from the ecosystems
316 were considered. More specifically, they include the Gross Primary Production (GPP), the Net
317 Primary Production (NPP), the Net Ecosystem Exchange (NEE), the Net Biome Production
318 (NBP) and several types of respiration processes (i.e. Ecosystem respiration or RECO),
319 heterotrophic respiration from both soil and grazing animals, and autotrophic respiration.

320 NPP and NEE are the most commonly simulated C-fluxes (67%), followed by GPP
321 (56%) and RECO (44%), whilst just a few models simulate the NBP. Despite only 44% of the
322 models taking into account RECO, most of them only consider soil respiration (89%). Plant
323 respiration is considered by 56% of the models, whilst only 33% of the models take into
324 account respiration from grazing animals.

325 Among all of the models analysed only DNDC is able to simulate all the CO₂-GHG
326 fluxes considered. More than 70% of CO₂-GHG can be simulated also by APSIM, DayCent
327 and PaSim. The CO₂-GHG simulated by the highest number of models (i.e. six models) are
328 NPP, NEE and soil respiration.

329 The main non-CO₂ fluxes (for simplicity called Non CO₂-GHG) include CH₄, N₂O,
330 several N emissions (i.e. NH₃, NO_x, N₂) and O₃.

331 N₂O emissions are most commonly simulated (78%), followed by NH₃ (56%). By
332 contrast, only a few models generate CH₄ and N₂ emission outputs (44%) and NO_x (33%).
333 None of the models provide O₃ emissions output.

334 N₂O emissions provided by the models are mostly generated by denitrification and
335 nitrification (78%), mainly based (i.e. >70% of the models) on a soil N pools (e.g. nitrate
336 pool, NH₄ pool) with soil water and temperature acting as main drivers of change on mineral
337 N pools.

338 Among all models analysed DayCent and DNDC were able to simulate all non CO₂-
339 GHG considered in our analysis. However, more than 70% of non CO₂-GHG can be
340 simulated also by APSIM, PaSim and CERES-EGC. The non CO₂-GHG simulated by the
341 highest number of models (i.e. seven models) was N₂O. The models able to simulate the
342 highest number of variables (i.e. CH₄, N₂O and N₂) were APSIM, DayCent, DNDC and
343 PaSim.

344 Ten specific N processes were considered in the models: nitrification, denitrification,
345 volatilization, leaching, symbiotic fixation, assimilation, mineralization, immobilization, plant
346 uptake, and clay fixation. All these processes were widely simulated (i.e. >70 %) by the
347 models considered in our analyses, with the only exception of clay fixation, that is considered
348 only by DNDC model.

349 Among the models analysed, only RothC does not take into account any N process. All
350 the remaining models are able to simulate each of the N processes considered in our analysis,
351 with the only exceptions being APSIM, which does not consider NH₃ volatilization, and
352 PaSim and STICS, which only take account of assimilation indirectly (C:N-driven).

353

354 3.1.5. *Management*

355 All models are able to simulate the impact of the most common farming practices (i.e.
356 harvesting, mowing, fertilization, tillage, irrigation, etc.) on the processes described so far. By
357 contrast, specific options for grasslands, such as plant use and nutrient returns from grazing
358 animals (as well as animal performances such as weight growth and milk production) are
359 simulated by a lower number of models (Tab. 3e, see supplementary material).

360 Harvesting, cutting, tillage, irrigation and crop rotation are widely simulated (>70% of
361 models). Moreover, all models simulate fertilization and residue management. Concerning
362 fertilization, however, only application of mineral N and organic amendments are widely
363 simulated, while only a few models simulate other types of fertilizer such as phosphorus,
364 potassium, sulphur and calcium. Similarly, the management of crop residues is based mainly
365 on their burning or leaving on the ground surface, whilst only 33% of the models also
366 consider burial (e.g. STICS accounts burial through tillage). Among other agricultural

367 practices, about half of the models consider pruning and water management (i.e. rice), but
368 only a few consider pesticide application.

369 The practices considered in the analysis are generally set by users. Some models also
370 offer options to trigger management events (i.e. fertilization and irrigation) based on changing
371 conditions during the simulation.

372 Simulation of grazing, animal performances and nutrient returns were taken into
373 account as specific options for grasslands.

374 Concerning grazing, models are for the most part based on user-determined settings
375 (start and end dates, animal density); some of them also include options related to evolving
376 conditions (APSIM, EPIC and PaSim), selective grazing (APSIM and PaSim) and trampling
377 effect (APSIM).

378 Animal performance simulation is considered by 55% of the models through
379 simple/static methods (APSIM and EPIC) or detailed/dynamic methods (PaSim), and based
380 on feeding standards or fill units (APSIM, DNDC and RothC).

381 Finally, nutrient return was considered by 66% of the models, based on uniform
382 distribution of returns across the whole field.

383 CERES-EGC, DSSAT and STICS do not include very specific agricultural options for
384 grasslands. APSIM is the most detailed model for grasslands.

385

386 **4. C and N cycles: performance, strengths and weaknesses**

387 In this section, we provide an overview of the C and N approaches used by the CN-MIP
388 models (see Tab. 4 and supplementary), and their performance as documented for a broad
389 gradient of geographic and climatic conditions, as well as a variety of soil types and
390 management practices, to gain insight into their main strengths and weaknesses. To do that,
391 we have summarised the results of 130 published modelling studies (Tab. 5).

392 In the analysis of the effects on C and N cycles of pedo-climatic conditions, we
393 considered variations of soil features such as temperature and moisture, texture, bulk density,
394 pH, SOC, C and N dynamics and water-filled pore space, and climate conditions such as
395 patterns of air temperature, precipitation, solar radiation, also including frequency and
396 intensity of extreme events such as floods and drought. Management practices include
397 changes in agricultural practices such as tillage, fertilization, irrigation, crop variety on soil
398 and vegetation and, in turn, on C and N cycles.

399 Several types of weaknesses emerged in 94 modelling studies (Tab. 6), where
400 criticalities in assessing the impact of pedo-climatic conditions (46.2%) and management

401 practices (33.1%) on environmental variables are reflected in unsatisfactory model
402 performances. These latter were mostly related to limitations of model structure with respect
403 to difficulties of the algorithms in simulating the effects of different management practices on
404 C and N cycling. By contrast, only a few weaknesses were due to the scale of application,
405 strictly related to the high variability in time and space of C and N cycles (16.5% and 4.2%
406 for pedo-climatic conditions and management practices, respectively). For the C cycle, major
407 limitations of model structure were related to management practices (43.4%), whilst for the
408 scale of application, the major weaknesses were due to different pedo-climatic conditions
409 (11.8%). For the N cycle, however, limitations inherent in model structure were predominant
410 under different pedo-climatic conditions (51.7%), whilst for the scale of application, major
411 weaknesses were due to different pedo-climatic conditions (20.4%).

412

413 4.1. *Model structures and pedo-climatic conditions*

414 Soil properties and climate conditions emerged as important factors for ensuring the
415 effective representation of outputs (Tab. 7). While climate issues were mainly related to
416 precipitation only, pedological factors concerned both the effect of changes of physical
417 (texture, bulk density and soil hydrologic properties) and chemical (C and N processes) soil
418 features on C and N cycles.

419 Concerning soil physical characteristics, a primary role in modelling issues was played
420 by the soil water properties. Errors in the simulation of soil water content (SWC) were the
421 main cause of general discrepancies concerning C and N emissions in many studies (Tab. 7).
422 Discrepancies in C and N outputs were also observed under specific soil water conditions
423 such as the impact of soil freezing and thawing (Li et al., 2010) or soil shrinking and swelling
424 (Babu et al., 2006). Again, an inappropriate setting of initial state variables determined
425 discrepancies in N emissions (i.e. under- overestimation of N₂O emissions peaks, Gabrielle et
426 al., 2006). Considerable overestimations of N₂O emissions were found to be closely related to
427 overestimation of water-filled pore space (WFPS). WFPS is indeed one of the most important
428 soil variables influencing C and N cycles. For instance, microbially-mediated soil respiration
429 and N cycling processes tend to be higher or lower with increasing soil water content (e.g.
430 increased nitrification under aerobic conditions, increased denitrification under anaerobic
431 conditions, e.g. Bollmann, 1988). As WFPS reaches high values, soil respiration tends to
432 decline and denitrification occurs, resulting in N losses via N₂O and N₂ emissions. This
433 condition was observed especially for DayCent (Stehfest and Muller, 2004, Abdalla et al.,
434 2010, Xing et al., 2011, Ryals et al., 2014, 2015) and DNDC (Saggar et al., 2004, Abdalla et

435 al., 2010). Fast drainage is a particular issue for both the DayCent and DNDC models which
436 drain water in excess of field capacity immediately. This condition makes these models
437 unable to accurately predict N emissions at sites that consistently show soil moisture above
438 FC (e.g. Uzoma et al., 2015).

439 Soil bulk density (BD) was also a source of modelling error in simulating C and N
440 cycles. For CERES-EGC, Gabrielle et al. (2006) found a discrepancy in N₂O emission peaks
441 due to inappropriate parametrization of soil water retention properties and bulk density from
442 test site to regional scales. Drouet et al. (2011) confirmed that BD was one of the most
443 influential factors for N₂O emissions in CERES-EGC. The effect of BD increase was also
444 reported for DayCent by De Gryze et al. (2010) and Abdalla et al. (2009), respectively, which
445 observed an underestimation of N₂O emissions in a conservation tillage treatment due to the
446 increase in BD, and an associated decrease in pore space over time as DayCent maintains a
447 steady BD and simulation compaction, while the conservation tilled field site resulted in
448 increased BD and reduced N₂O emissions (Pisante et al, 2015). In fact, most of the selected
449 models, with the exception of EPIC, DNDC and STICS, do not simulate soil compaction or
450 loosening, as BD remains constant over time.

451 Texture was also found to be an influential soil physical characteristic. Congreves et al.
452 (2016) found an underestimation in NH₃ emissions with the DNDC model, which is unable to
453 simulate a heterogeneous soil profile. Similarly, Gagnon et al. (2016) confirmed that DNDC
454 does not effectively discriminate across soil textures to simulate soil CO₂ respiration. Clay
455 concentration affects SOC accumulation in different ways. According to some studies
456 (Nichols, 1984, Burke et al., 1989), SOC increases with increasing clay content due to the
457 bonds between the surface of clay particles and organic matter that retard the decomposition
458 process. Also, the increase of clay content affects soil aggregation, indirectly affecting SOC
459 through the creation of macro-aggregates that can physically protect organic matter molecules
460 from further microbial mineralization (Rice, 2002, Plante et al., 2006). However, a recent
461 study (Gregorich et al., 2016) indicated that only temperature (not soil texture or other soil
462 properties) was a driver of decomposition for 10 sites in Canada (¹³C-labelled study), thus
463 suggesting as the effect of texture on SOC decomposition is controversial. Furthermore,
464 texture parametrization is another possible source of error. For instance, Gijsman et al. (2002)
465 indicated that inaccuracies in soil texture data used as inputs may have affected soil retention
466 characteristics, thus resulting in discrepancies in SOC and soil mineral N dynamics.

467 Soil chemical processes are generally similar between the models and all models
468 considered showed difficulty in reproducing the observed C and N cycles. The processes

469 influencing soil organic matter (SOM) in the models include nitrification, denitrification,
470 immobilization and mineralization.

471 Discrepancies between modelled and observed data were often related to an
472 inappropriate SOC content parametrization (Pathak et al., 2005, Calanca et al., 2007,
473 Causarano et al., 2007, Smith et al., 2012, Gagnon et al., 2016). However, a considerable
474 source of error was also due to overestimation of SOC content (Abdalla et al., 2010, Gijsman
475 et al., 2002) or to the rate of soil C decomposition (Snow et al., 1999, De Gryze et al., 2010,
476 Li et al., 2015).

477 Nitrification is a two-stage process, performed by different groups of Archaea,
478 consisting in the oxidation of ammonia or ammonium to nitrite (step 1) followed by the
479 oxidation of the nitrite to nitrate (step 2). For DayCent, Li et al. (2005) and Del Grosso et al.
480 (2008) found that overestimation in the nitrification rate was one of the main sources of error
481 for N emissions estimation. This was also found by Drouet et al. (2011), showing that
482 discrepancies in N₂O emissions simulated by CERES-EGC were due to the high sensitivity of
483 the model to the maximum rate of nitrification. The nitrification rate, however, is usually
484 associated with a number of environmental factors including the substrate and oxygen
485 concentration, temperature and pH. For instance, this was observed by Li et al. (2005), who
486 pointed out that poor simulation of NH₄⁺ was caused by the inaccurate regulation of the effect
487 of temperature on nitrification in DayCent.

488 Denitrification is a process where the reduction of soil nitrate to N-containing gases
489 takes place. The major discrepancies between modelled and observed N emissions were due
490 to an underestimation of the denitrification rate (Thorburn et al., 2010, Xing et al. 2011, Fitton
491 et al., 2014a, b). The underestimation of the denitrification rate can be due to different type of
492 errors. For instance, for APSIM, Thorburn et al. (2010) found the source of error in the model
493 parametrization, with the default value of denitrification coefficient much lower than the
494 optimized value. By contrast, Xing et al. (2011) indicated the response of denitrification rate
495 to soil temperature and moisture (or WFPS) as the main source leading to the underestimation
496 of denitrification. Generally, denitrification rates have been reported to be directly
497 proportional to temperature (Seitzinger, 1988), whilst soils with high organic matter content
498 (high dissolved organic C) and anaerobic conditions (i.e. waterlogged or poorly-drained soils)
499 can more easily favour high denitrification rates.

500 Another important source of modelling error resulted from the inaccurate estimation of
501 the immobilization-mineralization processes. In the EPIC model, He et al. (2006) observed
502 that general discrepancies in C and N dynamics (i.e. lower net N mineralization rate,

503 humification, etc.) were likely due to N mineralization algorithms which may have
504 underpredicted net N mineralization (NMN) observable under field conditions. Smith et al.
505 (2008) and Fitton et al. (2014a, 2014b) found that the underestimation in mineralization rate
506 led to underestimation of N₂O emissions. In the same way, Del Grosso et al. (2010) indicated
507 that overestimation of N₂O emissions was due to N mineralization rates that were too high
508 and too responsive to climate drivers. Nitrogen immobilization or mineralization depends on
509 the C/N ratio of the plant residues. The C/N ratio generally tends to decrease as the organic
510 matter becomes more decomposed. Erroneous C/N parametrization can easily lead to errors in
511 C and N cycle related outputs. For instance, Li et al. (2015) observed for the DSSAT model
512 that differences between the modelled and measured soil C/N ratio led to SOC
513 overestimation.

514 Finally, climate conditions influence the C and N outputs in several studies analysed.
515 Some issues were related to how the climate data have been used. For instance, in APSIM,
516 Thorburn et al. (2010) found discrepancies in N emissions (i.e. underestimation of
517 denitrification and N₂O peaks) due to the application of spatially averaged rainfall data
518 instead of the use of specific test-site rainfall data. In other cases, the main issues were due to
519 the sensitivity of the models subroutines. For instance, Wattenbach et al. (2010) observed
520 overestimation in NEE peaks in southern European regions due to issues in coupling water
521 and C-fluxes. These issues were probably caused by the fact the model was developed for
522 Northern regions. Again, Lawton et al. (2006) reported overestimation of NEE because of the
523 oversensitivity of PaSim to initial conditions/winter conditions. Most of the issues related to
524 general discrepancies in simulated C and N cycles, however, were related to precipitation only
525 (Stehfest and Muller, 2004, Jarecki et al., 2008, De Gyrze et al., 2010, Ludwig et al., 2011,
526 Lehuger et al., 2014). Precipitation and the resulting soil water dynamics strongly influence N
527 cycling in terrestrial ecosystems since it affects both physical transport and N biological
528 transformations by soil microorganisms (Brooks et al., 1999, Corre et al., 2002, Aranibar et
529 al., 2004).

530

531 4.2. *Model structure and management*

532 Management has a great impact on C and N cycles. In biophysical and biogeochemical
533 models, the correct representation of practices such as fertilization, irrigation and tillage in
534 crop systems, and cutting and grazing in grassland systems, is needed to ensure the greatest
535 suitability of outputs.

536 In the models, fertilization, which influences soil C and N transformations (e.g.
537 acidification following fertilization) and trace gas emissions, was often not well represented
538 (Tab. 7). For DayCent, Fitton et al. (2014a, b) indicated an underestimation of N₂O emissions
539 due to the low sensitivity of the model at low N application rates. In DNDC, Congreves et al.
540 (2016) found that NH₃ emissions were underestimated due to a simple modelled cascade
541 water flow, which may have limited the ability of the model to simulate slurry infiltration
542 rates. Also, Causarano et al. (2007) observed general discrepancies in C-dynamics (i.e.
543 overestimation of microbial biomass C and total organic C, underestimation of particulate
544 organic C), due to inadequate representation of the effects of tillage and manure in the EPIC
545 model. Another issue related to fertilization was the inability of many models to replicate the
546 effect of specific types of fertilizer. For instance, using DayCent Stehfest and Muller (2004)
547 found overestimation of N₂O emissions under urine application, where N was concentrated in
548 small hotspots. For the same model, Ryals et al. (2014 and 2015) underestimated CO₂
549 emissions since no soil water benefits were provided by adding compost. This condition was
550 likely due to the lack of increased modelled decomposition because the model was not able to
551 increase soil water contents when compost was added. Gu et al. (2014) overestimated N₂O
552 emissions, soil nitrate and ammonia concentrations due to the inability of DNDC to include
553 canopy interception and foliar N uptake when spraying liquid fertilizer.

554 Finally, residue management was one of the main weaknesses related to N management
555 (Cavero et al., 1996, Sleutel et al., 2006, Rampazzo Todorovic et al., 2010, Wang et al.,
556 2013). The amount of N applied with residues depends on the quantity of residues and their N
557 concentration. These two factors affect the mineralization-immobilization turnover, whilst
558 their net balance varies with environmental conditions (mainly soil moisture and temperature)
559 and the characteristics of the OM (i.e. C:N and the decomposition rate). Since residues
560 directly influence soil C and N processes, residue management in the models resulted in
561 consistent modelling weaknesses. For instance, Justes et al. (2009) underestimated the N
562 mineralization in STICS due to inappropriate parametrization of the model (i.e. default values
563 of the decomposition module were used). In a similar way, Liu et al. (2009) overestimated the
564 SOC content when stubble (wheat and lupine) was applied due to the use of the conventional
565 setting of the stubble retention factor in RothC. Using DayCent and DNDC, Smith et al.
566 (2012) underestimated SOC due to a slight overestimation of residue removal impact.
567 However, the authors indicated that this could have been partly due to the inherent variability
568 in SOC measurements. Smith et al. (2012) also found that DNDC tended to underestimate the
569 rate of SOC change as affected by residue removal at some sites. Using DSSAT, Hartkamp et

570 al. (2004) overestimated SOC in the crop rotations with N fertilization. This overestimation
571 was due to inaccurate initial SOC (i.e. overestimated SOC values) which was related to an
572 overestimation of the biomass incorporated into the soil. Similarly, Wang et al. (2005)
573 underestimated the SOC content using the EPIC model due to a structural error in
574 underestimating the return of corn residues. He et al. (2006) found general discrepancies in C
575 and N dynamics due to underestimation of the soil capacity to transform crop residue in SOC.

576 Tillage is one of the agricultural practices most commonly simulated by the models and
577 an issue in most modelling applications. The use of tillage or reduced tillage can greatly affect
578 soil properties, and since the models don't adjust some soil properties overtime (such as bulk
579 density) which results in inaccuracies in simulations. Also, the use of tillage or no/reduced
580 tillage may lead to increasing rather than decreasing emissions (e.g. due to higher density and
581 WFPS, more SOM near the soil surface thus higher denitrification potential, tendency to
582 acidification and thus lower reduction of N₂O to N₂, etc.). Identifying mechanisms which help
583 understand simulate emissions with no tillage is thus a key issue. In our analysis management
584 effects (i.e. tillage) which influences topsoil erosion emerged as a point of weakness. This is
585 because many models do not take into account adequately C-losses due to erosion. For
586 instance, Nieto et al. (2010, 2013) overestimated SOC content using RothC, whilst Billen et
587 al. (2009) observed general discrepancies in SOC content with EPIC.

588 Another point of weakness in simulated tillage was the inadequate representation of
589 changes in soil properties over time. For instance, Luo et al. (2011), using APSIM,
590 underestimated SOC decomposition. In this case, whilst tillage may have led to acceleration
591 in soil C oxidation due to changes in soil environmental parameters (i.e. water retention,
592 porosity, aeration, etc.), APSIM failed to simulate changes in these soil properties over time,
593 which is a common issue amongst most models. Similarly, Causarano et al. (2007) found
594 general discrepancies in C dynamics (i.e. overestimation of microbial biomass C and total
595 organic C, underestimation particulate organic C) due to an inadequate reproduction of the
596 effects of tillage and manure on soil properties.

597 In addition to fertilization and tillage, probably the most common simulated agronomic
598 practices, model weaknesses were found in relation to other practices. For instance irrigation,
599 especially accompanied by fertilization, was observed to affect simulated C and N cycles.
600 Jackson et al. (1994) and Caverro et al. (1999) underestimated N fluxes under irrigated
601 experiments using EPIC. The main source of error was related to an overestimation of the soil
602 N losses *via* leaching or denitrification during the irrigated crop period. Grassland
603 management was also seen to be a possible point of weakness for the models. For instance,

604 Lawton et al. (2006), Vuichard et al. (2007a) and Ma et al. (2015) observed general
605 discrepancies in C-fluxes (i.e. net ecosystem exchange and ecosystem respiration) under
606 different grazing intensities using a grassland-specific model (PaSim). As suggested by
607 Vuichard et al. (2007a), a continuous defoliation by grazing is indeed difficult to account for
608 as a permanent disturbance in the model. The grazing effect, however, links with many other
609 parameters related to the ecosystem and climate which makes it difficult to define the
610 parameter which most strongly influences the uncertainty of the model output (Gottschalk et
611 al., 2007).

612 Finally, model weaknesses also result from management options that are not included.
613 This type of weakness has emerged in several studies carried out using the RothC model. For
614 instance Skjemstad et al. (2004) found general discrepancies in C dynamics due to ecosystem
615 disturbances which were not included in RothC (i.e. clearing and burning of pulled
616 vegetation). Shirato and Yokazawa (2005) underestimated SOC content due to the
617 decomposition rate of SOM under rice cultivation (i.e. effect of waterlogged soil not included
618 in RothC) being too low, and Farina et al. (2013) reported some discrepancies in C-fluxes
619 when the model simulated rotations that included a fallow period.

620

621 4.3. *Time-scale*

622 Biophysical and biogeochemical models enable the estimation of C and N emissions at
623 various temporal and spatial scales. Compared to the emission factor approaches often used
624 by organizations and individuals to calculate greenhouse gas (GHG) emissions for a range of
625 activities, these tools include the influences of agricultural practices, land-use change, soil
626 properties and estimate the influences of weather on emissions over time.

627 The ability of these models to accurately reproduce detailed dynamics of C and N
628 emissions depends on the degrees of complexity of the model itself. Current process models,
629 with high complexity, are able to calculate in detail both C and N emissions due to their
630 consideration of all soil-plant-atmosphere interactions. These tools are able to provide
631 reasonable estimates of trace gas emissions from soils, usually for a specific site and at
632 seasonal or annual time scales. By contrast, however, they are less successful at finer time
633 resolution (e.g. daily) and on different sites from the ones where have been previously
634 calibrated. In our analysis several studies showed weaknesses due to the time-spatial scale
635 associated with both pedo-climatic conditions and management.

636 Concerning time-scale weaknesses, Xing et al. (2011) underestimated N₂O emissions at
637 the daily time step using APSIM, while the use of the hourly time step may have likely

638 improved the estimate of predicted total daily emissions. This is because, in the APSIM
639 model, as in most models, N₂O emissions were released immediately to the atmosphere
640 without delay upon change in environmental conditions whereas the observations indicated
641 that there was a 1-10 hour lag between peaks of soil moisture and gaseous emissions.
642 Similarly, Lehuger et al. (2011) using CERES-EGC indicated an overestimation in N₂O
643 emissions, probably due to a possible time lag between the production of gaseous N₂O in the
644 soil and its emission to the atmosphere. Also, several studies carried out using DayCent
645 (Parton et al., 2001, Del Grosso et al., 2005, 2010) observed some discrepancies in simulated
646 N emissions due to time-lag. This was found to agree with Li et al. (2005), which indicated
647 that DayCent often has a 1 day lag before emissions occur. In all these cases, the use of hourly
648 time step may result in better predictions especially in conjunction with the addition of a
649 description of gas diffusion into soil which could result in a delay between N₂O production
650 and emission.

651 Concerning spatial-scale weaknesses, Gabrielle et al. (2006) found discrepancies in N₂O
652 emission peaks using CERES-EGC. This was probably due to soil property parametrization
653 (i.e. soil water retention properties and bulk density) which may have led to differences in N
654 outputs from test sites to the regional scale. Using EPIC, general discrepancies in C-fluxes
655 (i.e. overestimation of microbial biomass C and total organic C, underestimation of particulate
656 organic C) were likely caused by spatial differences in C fraction due to differing soil
657 landscapes (Calanca et al., 2007). Schnebelen et al. (2004) overestimated soil N absorption
658 with the STICS model. This was probably due to propagation of errors for continuous
659 simulations compared to single-year simulations. More specifically, the underestimation of
660 some parameters in the previous year may have led to errors in the following years.

661

662 **5. New developments/future perspectives**

663 In the above analysis, an indication was given of models' predictive strength, while also
664 hinting at possible limitations in the underlying hypotheses from the literature in the cases
665 where discrepancies between model and observation occurred. Despite this extensive analysis,
666 knowledge basic mechanisms driving C and N cycles in agricultural systems is still far from
667 complete and key questions remain, including: what exactly triggers the cascade of events that
668 finally lead to biological responses? How to differentiate between causes and consequences?
669 How does the knowledge derived from system observations relate to mechanistic events?
670 How does the current knowledge on C and N cycling in agriculture fits with available
671 mechanistic representations? Discrepancies between model outputs and observations can be

672 ascribed to a wide diversity of causes, without any real tendency to associate them with one or
673 another cause. The analysis reported in this work suggested however three (quite large) areas
674 of interest for possible improvements of C and N models: i) soil biology, comprising SOM
675 heterogeneity, decomposition kinetics, and N immobilization; ii) soil physics, including the
676 representation of soil physical properties and the simulation of its effects on reaction rates;
677 and iii) soil management, which indirectly affect soil processes by modifying soil physical,
678 chemical and biological properties.

679 Based on the main issues found in our analysis, despite recognizing the importance of
680 soil management, here we focus on some innovative aspects related to soil biology and soil
681 physics, and interface that requires attention (Blagodatsky and Smith, 2012). This choice is
682 justified in that development of robust predictive frameworks is critical to managing soil
683 biology and its essential functions and services (Thrall et al., 2011). They can help
684 disentangling the causal links between soil biology and structure, physical-chemical factors
685 and ecological processes (e.g. nutrient cycling, soil C sequestration) that contribute to plant
686 community development and function. In addition, how soil communities respond to and
687 impact on plant succession (e.g. via regulatory networks that respond to the availability of
688 fixed N) may be important for predicting the role of plant–soil feedbacks in determining the
689 dynamics of soil microbial communities and the impact of anthropogenic disturbance on soil
690 diversity and function.

691 Soil microbial biomass (SMB) is generally only implicitly modelled by representing it
692 as a C pool not affecting substrate decomposition directly (Manzoni and Porporato, 2009).
693 Approaches of this type mostly implement solutions that are biologically meaningful (e.g.
694 representing realistically SOM turnover) and computationally tractable within a simulation
695 (i.e. with reduced overall complexity of the full model and a limited number of free
696 parameters to be tuned), which make them suitable for analyses in long-term studies
697 (Manzoni and Porporato, 2009, Sierra et al., 2015a). In recent years, researchers have
698 advocated a representation of SOM turnover driven by SMB to gain insight into decomposing
699 SOM-SMB interactions (Schimel and Weintraub, 2003, Lawrence et al., 2009, Blagodatsky et
700 al., 2010, Schmidt et al., 2011). For C and N substrates, concentration constraints driven by
701 microbial allocation patterns could thus be represented in novel biogeochemical models based
702 on microbial physiology (Allison et al., 2014). In this way, models based on microbial
703 biomass-driven SOM decomposition are promising to provide a realistic simulation of SOM
704 turnover in relation to changes in environmental conditions compared to existing models that
705 do not explicitly simulate SMB (Lawrence et al., 2009, Allison et al., 2010, Conant et al.,

706 2011, Sierra et al., 2015b). It is quite common to use classical enzymatic kinetics like
707 Michaelis-Menten or Monod-type kinetics to implement substrate-SMB co-limitation
708 (Blagodatsky and Richter, 1998, Hadas et al., 1998, Wutzler and Reichstein, 2013, Cavalli et
709 al., 2016), even if simpler decomposition kinetics have also been proposed (Manzoni and
710 Porporato, 2007, Withmore, 2007, Wutzler and Reichstein, 2008). Conversely, more general
711 model formulations are described in Neill and Gignoux (2006) and Neill and Guenet (2010) to
712 simulate microbial growth in soil accounting for both positive and negative priming effects.
713 The priming effect is defined as any change (positive or negative) of native SOM
714 decomposition rate following the addition of exogenous organic matter or nutrients, compared
715 to no addition (Fontaine et al., 2007, Kuzyakov et al., 2000, Kuzyakov, 2010, Chen et al.,
716 2014, Perveen et al., 2014).

717 Another important aspect regarding SOM turnover is the effect of N shortage on SOM
718 decomposition. Soil microorganisms are characterised by a narrow range of variation in their
719 C to N ratio (Cleveland and Liptzin, 2007, Xu et al., 2013); thus, they can be approximately
720 considered homeostatic (i.e. they do not change markedly their C to N ratio according to
721 substrate C to N ratio). Mechanisms of adaptation to stoichiometric imbalances between
722 substrates and SMB were reviewed in detail by Mooshammer et al. (2014a). One postulated
723 mechanism of adaptation regards the variation of microbial C use efficiency (CUE, defined as
724 the ratio between newly-formed biomass C and decomposed C) and of N use efficiency
725 (NUE, defined similarly to CUE) to accommodate for excess or deficit of C or N (Manzoni et
726 al., 2012, Sinsabaugh et al., 2013, Mooshammer et al., 2014b). According to this hypothesis,
727 when decomposition is N-limited, excess C is lost through overflow metabolism (Russel and
728 Cook, 1995), either with the synthesis of extracellular C compounds (as polysaccharides)
729 (Hadas et al., 1998, Cavalli et al., 2016), or as CO₂ (Schimel and Weintraub, 2003, Neill and
730 Gignoux, 2006). Conversely, when N is in excess (decomposition is limited by C
731 availability), net N mineralisation occurs. Models usually implement N deficit effects on
732 SOM decomposition with the N inhibition hypothesis (Manzoni and Porporato, 2009), that is,
733 SOM turnover is reduced according to N availability, and thus CUE does not change.
734 Alternatively, other models (Izaurralde et al., 2006, Withmore, 2007) allow SMB to vary its C
735 to N ratio according to stoichiometric imbalances, and thus they consider SMB as non-
736 homeostatic.

737 Decomposition of SOM in soil occurs at microsites showing varying N availability
738 (Schimel and Bennett, 2004). This is caused by heterogeneity of both SOM and of soil
739 physical properties (Schmidt et al., 2011). Thus, N is supposed to flow from micro-sites

740 showing net N mineralisation to others showing net N immobilisation (Schimel and Bennett,
741 2004). Mathematically, the heterogeneity of SOM decomposition in a first approximation can
742 be simulated considering that not all organic N in substrates is available to SMB, according to
743 the parallel hypothesis (Manzoni and Porporato, 2007). The use of a simple lumped SOM
744 model, based on the parallel approach, was shown to provide almost similar results to the
745 same model structure that explicitly took into account the heterogeneity of soil
746 decomposition, and in which all organic N in substrates was available to decomposers,
747 according to a direct assimilation pathway (Manzoni et al., 2008).

748 The heterogeneity of SOM is simulated with models that comprise several pools of
749 different decomposability (Nicolardot et al., 2001, Manzoni and Porporato, 2009, Sierra et al.,
750 2011, Sierra and Müller, 2015). In many models, decomposition constants of model pools
751 incorporate intrinsic chemical recalcitrance of SOM, and availability of SOM to decomposers
752 (Nicolardot et al., 2001, Sierra and Müller, 2015). However, it was recently emphasised that
753 chemically-labile (or high-quality, and thus potentially easily-degradable) molecules can
754 persist in soil for a long time due to constraints on their microbial decomposition not related
755 to intrinsic chemical characteristics (Kleber, 2010, Marschner et al., 2008): biology of
756 decomposers, abiotic reactions and desorption, environmental variables and physicochemical
757 stabilisation processes (Ekschmitt et al., 2005, Kemmit et al., 2008, Kleber et al., 2011,
758 Schmidt et al., 2011, Dungait et al., 2012). Regarding SOM physical and chemical
759 stabilisation, models that explicitly represent protected and unprotected SOM pools of similar
760 chemical characteristics (Kuka et al., 2007) allow separating intrinsic recalcitrance (substrate
761 quality) from availability, and thus enable simulating long-term stabilisation of chemically
762 easily-decomposable high-quality SOM in soil (Dungait et al., 2012). In addition, more
763 sophisticated and realistic approaches to simulate soil physicochemical heterogeneity, and
764 thus variability of SOM decomposition, were implemented in SOM models that represent soil
765 as 3D structure in which decomposition takes place (Garnier et al., 2008, Masse et al., 2007,
766 Monga et al., 2009, 2014).

767 Improving soil biology aspects related to the production and consumption of gases (O_2 ,
768 CO_2 , CH_4 , N_2O , and N_2) will improve the simulation of soil gas concentrations. However, this
769 is not sufficient to achieve proper simulations of GHG emissions, as accounting for gas
770 transport through the soil profile is also important. As pointed out by Blagodatsky and Smith
771 (2012), it is necessary to find the right balance in complexity between biological and soil
772 physical simulations. For example, the higher soil tortuosity the higher the N_2/N_2O ratio,
773 because N_2O has more possibilities to be reduced when the escape pathway from the N_2O

774 production sites to the atmosphere (and thus its diffusion time) is longer. Adequate simulation
775 of gas transport in soil can be achieved using mechanistic models based on water, heat, and
776 gas transport equations, and gas-liquid phase exchange. A further connection among soil
777 biology and soil physics research will be to simulate SOM turnover and gas production,
778 consumption, and transport in a 3D soil structure using the concepts presented above, so as to
779 achieve a more realistic representation of environmental effects (soil temperature and
780 moisture), especially in the context of climate change.

781 One final observation is that all of the model improvements presented above require
782 adequate simulation of initial conditions of inorganic N availability. Thus, it is mandatory that
783 all processes affecting soil ammonium concentration are accurately simulated. Among these,
784 ammonium fixation in non-exchangeable form by clay minerals in fine-textured soils is not
785 frequently considered in modelling practice (Nieder et al., 2011). After its application to soil
786 with fertilisers, a relevant fraction of ammonium can be very rapidly (hours or days) fixed by
787 clay minerals (Nõmmik, 1957) in a form that is very slowly released during the following
788 weeks or months (Steffens and Sparks, 1997). This fraction of applied N is thus not
789 immediately available for nitrification, microbial immobilisation, and plant uptake. Despite its
790 importance, ammonium fixation / release is not commonly simulated by crop/grassland
791 system and SOM models. The rapid fixation can be simulated with well-known isotherms,
792 which represent the static adsorption of an ion onto a surface (Cameron and Kowalenko,
793 1976, Cavalli et al., 2015) as a function of ion concentration. Research is needed to estimate
794 isotherm parameters depending on soil characteristics (such as type of clay, potassium
795 concentration, and soil water content) and to simulate ammonium release over time.

796

797 **6. Summary and concluding remarks**

798 At present, process-based biogeochemical models represent a valuable tool for
799 examining the magnitude and spatial-temporal patterns of C and N fluxes in terrestrial
800 biosphere dynamics. Our analysis shows that there is still great divergence between models in
801 the simulation of C sequestration and GHG source/sink status, in relation to a different
802 interpretation of physical and biogeochemical processes.

803 Representative works have been summarized to provide a general overview of the state-
804 of-the-art of models, and to allow process-based models (the nine identified in this study) to
805 be compared and selected for the simulation of C and N cycles in crop and grassland systems.
806 We classified models into categories according to three levels of knowledge: five general
807 classes (level 1), 20 main processes (level 2), and 196 methods/options/components (level 3),

808 and then we assessed the tools in terms of the comprehensiveness of processes related to
809 pedo-climatic and management options, and their accuracy in a variety of contexts.

810 This review highlighted strengths and weaknesses of the models analysed. Essentially,
811 they involve limitations in simulating the effects of pedo-climatic conditions (46.2%) and
812 different management practices (33.1%). Other weaknesses (i.e. 20.7%) were due to the scale
813 of application in time and space.

814 The major limitations of model structure related to C-cycles were observed under
815 management practices (43.4%), whilst for the scale of application the major weaknesses were
816 due to different pedo-climatic conditions (11.8%). For the N cycle, the main limitations
817 inherent in model structure were found under different pedo-climatic conditions (51.7%),
818 whilst for the scale of application the major weaknesses were due to different pedo-climatic
819 conditions (20.4%).

820 All the models considered here showed positive and negative features and none may
821 necessarily be ideal in any particular circumstance. If the model chosen is not able to
822 reproduce the output required, two or more of these models may be combined to derive upper
823 and lower values for all simulated outputs. Moreover, a decision about which model or
824 models to use should be seen as dynamic, not static. As conditions change, or if one model
825 proves unsuccessful, they can be adapted or replaced with other, more suitable, models.

826 Although the above reported weaknesses were already known due to a wide number of
827 published studies, in the present analysis we have tried to relate them to their causes in the
828 view of using them as an effective basis for improving current modelling approaches.
829 Although different avenues could be considered to improve models (e.g. Coucheney et al.,
830 2015), mainly depending on the purpose of modelling, to overcome the reported limitations
831 and account for the effect of multiple disturbances (i.e. pedo-climatic conditions, management
832 practices, scale of analysis) affecting basic processes, as well as to simplify the decision of
833 which model to choose to understand mechanistically specific study-contexts and to make
834 detailed predictions in a large diversity of situations, some innovative aspects should be
835 considered in the modelling work. Among these, we target the representation of SOM
836 turnover driven by SMB, the effect of N shortage on SOM decomposition, improvement
837 related to the production and consumption of gases (O_2 , CO_2 , CH_4 , N_2O , and N_2), adequate
838 simulations of gas transport in soil, the use of a 3D soil structure in order to achieve a more
839 realistic representation of environmental effects (soil temperature and moisture), especially in
840 the context of climate change.

841 Model improvement thus implies extending the existing body of knowledge on
842 ecological and biogeochemical concepts, to allow them to be incorporated using novel
843 approaches, thus improving the representation of the dynamics of the ecosystems, and the
844 related advantages for stakeholders.

845

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Tables

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Model Name	Version	URL or contact for documentation/description	References
APSIM	7.6	http://www.apim.info	Keating et al., 2003. An overview of APSIM, a model designed for farming systems simulation. <i>European Journal of Agronomy</i> 18, 267-288. ; Holzworth DP, Huth NI, et al. (2014) APSIM – Evolution towards a new generation of agricultural systems simulation. <i>Environmental Modelling & Software</i> 62, 327-350. http://www.apsim.info/Documentation.aspx
CERES-EGC		https://ecosys.versailles-grignon.inra.fr/ceres_mais/ceres.html	Gabrielle et al., 1995. Analysis and field-evaluation of the CERES models' water balance component. <i>Soil Science Society Of America Journal</i> 59, 1402-1411; Gabrielle et al., 1996. Analysis and field evaluation of the CERES models' soil components: Nitrogen transfer and transformations. <i>Soil Science Society of America Journal</i> 60, 142-149; Gabrielle et al., 1998. Development and evaluation of a CERES-type model for winter oilseed rape. <i>Field Crops Research</i> 57, 95-111; Gabrielle et al., 1998. A model of leaf area development and senescence for winter oilseed rape. <i>Field Crops Research</i> 57, 209-222; Hénault et al., 2005. Predicting in situ soil N ₂ O emissions using NOE algorithm and soil data base. <i>Global Change Biology</i> 11, 115-127, 2005
DayCent	DayCent 4.5	http://www.nrel.colostate.edu/projects/daycent-home.html	Parton et al., 1994. A general model for soil organic matter dynamics: Sensitivity to litter chemistry, texture and management. p. 147–167. In: <i>Quantitative modeling of soil forming processes</i> , SSSA Spec. Public. No. 39. Madison, WI, USA; Parton et al., 2001. Generalized model for NO _x and N ₂ O emissions from soils. <i>Journal of Geophysical Research</i> 106(D15), 17403-17419. doi:10.1029/2001JD900101 . Del Grosso et al., 2000. General model for N ₂ O and N ₂ gas emissions from soils due to denitrification. <i>Global Biogeochemical Cycles</i> 14, 1045–1060. doi:10.1029/1999GB001225 ; Del Grosso et al., 2002. Simulated effects of dryland cropping intensification on soil organic matter and greenhouse gas exchanges using the DAYCENT ecosystem model. <i>Environmental Pollution</i> 116, S75-S83. doi:10.1016/S0269-7491(01)00260-3
DNDC	DNDC 95 and Manure DNDC	http://www.dndc.sr.unh.edu/	Li, 2000. Modeling trace gas emissions from agricultural ecosystems. <i>Nutrient Cycling in Agroecosystems</i> 58, 259–276. doi:10.1023/A:1009859006242 ; Li et al., 2012. Manure-DNDC: A biogeochemical process model for quantifying greenhouse gas and ammonia emissions from livestock manure systems. <i>Nutrient Cycling in Agroecosystems</i> 93, 163-200. doi:10.1007/s10705-012-9507-z
DSSAT	4.6	http://dssat.net	Jones, et al., 2003. The DSSAT cropping system model. <i>European Journal of Agronomy</i> 18, 235–265. doi:10.1016/S1161-0301(02)00107-7 ; Thorp et al., 2012. Methodology to evaluate the performance of simulation models for alternative compiler and operating system configurations. <i>Computers and Electronics In Agriculture</i> 81, 62–71. doi:10.1016/j.compag.2011.11.008 ; White et al., 2011. Methodologies for simulating impacts of climate change on crop production. <i>Field Crops Research</i> 124, 357–368. doi:10.1016/j.fcr.2011.07.001 .
EPIC	V.0810	http://epicapex.tamu.edu/	Williams, J.R. 1995. The EPIC model, 1995 V.P. Singh (Ed.), <i>Computer Models of Watershed Hydrology</i> , Water Resources Publications, Highlands Ranch, CO (1995), pp. 909–1000.
PaSim	5.3	https://www1.clermont.inra.fr/urep/modeles/pasim.htm	Ma et al., 2015. Regional-scale analysis of carbon and water cycles on managed grassland systems. <i>Environmental Modelling & Software</i> 72, 356-371. http://dx.doi.org/10.1016/j.envsoft.2015.03.007
RothC	RothC10N	http://www.rothamsted.ac.uk/sustainable-soils-and-grassland-systems/rothamsted-carbon-model-rothc	Coleman, K., Jenkinson, D.S., 1996. RothC-26.3. A model for the turnover of carbon in soil. In: Powlson, D.S, Smith, P., Smith, J.U. (eds) <i>Evaluation of soil organic matter models using existing, long-term datasets</i> . NATO ASI series no. 1, vol 38. Springer, Berlin Heidelberg New York, pp. 237–246; Coleman, K., Jenkinson, D.S., 1996. A Model for the Turnover of Carbon in Soil: Model description and user's guide. Lawes Agricultural Trust, Harpenden, UK; Farina, et al., 2013. Modification of the RothC model for simulations of soil organic C dynamics in dryland regions. <i>Geoderma</i> 200, 18-30. doi:10.1016/j.geoderma.2013.01.021
STICS	8.3.1	http://www6.paca.inra.fr/stics/	Brisson et al., 1998. STICS: a generic model for the simulation of crops and their water and nitrogen balances. I. Theory and parameterization applied to wheat and corn. <i>Agronomie</i> 18, 311–346; Brisson et al., 2003. An overview of the crop model STICS. <i>European Journal of Agronomy</i> 18, 309–332; Brisson et al., 2009. Conceptual basis, formalizations and parameterization of the STICS crop model, ed. Quae, 297 pp.; Coucheny et al., 2015. Accuracy, robustness and behavior of the STICS soil–crop model for plant, water and nitrogen outputs: Evaluation over a wide range of agro-environmental conditions in France. <i>Environmental Modelling & Software</i> 64, 177–190. doi:10.1016/j.envsoft.2014.11.024

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4

5 **Table 1** - The nine biogeochemical models used for the intercomparison.

6

7

General Classes (Lev.1)		% of models able to simulate at least 1 Main process contained within each General Class		
<i>Name of Class</i>	<i>N° of Main Processes contained within each General Class</i>	<i>Able (%)</i>	<i>Not able (%)</i>	<i>N.A *</i>
Plant ecophysiology and partitioning	10	100	0	---
Soil	4	100	0	---
Climate	1	100	0	---
Management	2	100	0	---
GHG emissions and other fluxes	3	100	0	---

8

9

10 **Table 2** - Level 1 of compositional sub-systems: general classes as usually considered in agricultural,
 11 the main processes identified within each general class and the percentage of models able to simulate
 12 at least 1 main process contained within each general class. * No information is available.

13

<i>Name of the Main Processes</i>	<i>N° of methods, options or components contained within each Main Processes</i>	% of models able to simulate at least 1 methods, options or components contained within each Main Processes		
		<i>Able (%)</i>	<i>Not able (%)</i>	<i>N.A *</i>
Carbon allocation mechanism	1	55.6	44.4	---
Carbon assimilation	4	88.9	11.1	---
Stomata	3	33.3	66.7	---
Phenology	4	88.9	11.1	---
Leaf area	3	77.8	22.2	---
Reference evapotranspiration	10	88.9	11.1	---
Root distribution	3	77.8	22.2	---
Plant partitioning	9 (2)	88.9	11.1	---
Yield formation	8	88.9	11.1	---
Limiting factors	9	88.9	11.1	---
Soil carbon	8	100	0.0	---
Soil temperature	4	100	0.0	---
Soil water transport	4	100	0.0	---
Soil N transport and transformation	5	88.9	11.1	---
Data input	14 (19)	100	0.0	---
General options	20 (8)	100	0.0	---
Pastures options	3 (12)	66.7	33.3	---
CO ₂	8	100	0.0	---
Non CO ₂ -gas	6 (19)	88.9	11.1	---
N processes	10	88.9	11.1	---

15

16 **Table 3** – Level 2 of compositional sub-systems: the main processes identified within each general
17 class, the number of methods, options or components contained within each main processes and the
18 percentage of models able to simulate at least 1 methods, options or components contained within each
19 main processes. * No information is available. Numbers in brackets represents specific information
20 related to the modelling approaches (see Tables S1-5).

	APSIM	CERES-EGC	DayCent	DNDC	DSSAT	EPIC	PaSim	RothC	STICS
N° of organic pools	7	4	3	6	5	5	5	5	6
Microbial biomass	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Humus	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Added organic matter labile	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Added organic matter recalcitrante	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
DOC	No	No	Yes	Yes	No	Yes	No	No	No
DON	No	No	No	Yes	No	Yes	No	No	No
Kinetic of conversion of organic pools	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Kinetic of nitrification	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes
Kinetic of nitrification - environmental factors involved	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes
N ₂ O losses from nitrification	Yes	Yes	Yes	Yes	No	Yes *	Yes	No	Yes
Kinetic of denitrification	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes

Kinetic of denitrification - environmental factors involved	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes
Denitrification: N ₂ /N ₂ O ratio	Yes	Yes	Yes	Yes	No	Yes *	Yes	No	Yes
Soil physical properties variation (impact on fluxes)	Yes	No	No	Yes	No	Yes	No	No	No

22

23 **Table 4** – Overview of the C and N approaches used by the CN-MIP models. * Only in the latest version (EPIC V.1102)

Model	Location	Type of environment	Biogeochemical cycles involved	Type of version *	Reference
APSIM	Australia	Plantation forestry	N	O	<i>Snow et al. (1999)</i>
	Australia	Arable	C-N	M	<i>Thorburn et al. (2010)</i>
	Australia	Arable	C-N	O	<i>Huth et al. (2010)</i>
	New Zealand	Arable	N	O	<i>Sharp et al. (2011)</i>
	Australia	Arable	C	O	<i>Luo et al. (2011)</i>
	Australia	Grassland	C	M	<i>Xing et al. (2011)</i>
	New Zealand	Grassland	N	O	<i>Giltrap et al. (2015)</i>
CERES-EGC	France	Arable	N	O	<i>Gabrielle et al. (2006)</i>
	France	Arable	C-N	O	<i>Lehuger et al. (2007)</i>
	France	Arable	N	O/M	<i>Rolland et al. (2008)</i>
	France	Arable	N	O	<i>Lamboni et al. (2009)</i>
	France	Arable	N	O	<i>Rolland et al. (2010)</i>
	France, Germany, Switzerland	Arable	C	O	<i>Wattenbach et al. (2010)</i>
	France	Arable/Grassland	N	O	<i>Drouet et al. (2011)</i>
	France, Germany	Arable	C-N	O	<i>Lehuger (2011)</i>
	France	Arable	N	O	<i>Dufossè et al. (2013)</i>
	France	Arable	N	O	<i>Goglio et al. (2013)</i>
	France	Arable	N	O	<i>Lehuger et al. (2014)</i>
France	Arable	C-N	M	<i>Noirot-Cosson (2016)</i>	
DayCent	Germany, USA, Scotland	Arable/Grassland	N	O	<i>Parton et al. (1998)</i>
	USA	Arable/Grassland	C	O	<i>Del Grosso et al. (2002)</i>
	New Zealand	Grassland	N	O	<i>Stehfest and Muller (2004)</i>
	USA	Arable	N	O	<i>Del Grosso et al. (2005)</i>
	China	Arable	N	O	<i>Li et al. (2005)</i>
	Global	Arable	C-N	O	<i>Stehfest et al. (2007)</i>
	Canada	Arable	N	O	<i>Smith et al. (2008)</i>

	USA	Arable	C-N	O	<i>Del Grosso et al. (2008)</i>
	USA	Arable	N	O	<i>Jarecki et al. (2008)</i>
	USA	Arable/tile drained	N	O	<i>David et al. (2009)</i>
	Ireland	Grassland	N	O	<i>Abdalla et al. (2010)</i>
	USA	Arable	C-N	O	<i>De Gyrze et al. (2010)</i>
	USA	Arable	N	O	<i>Del Grosso et al. (2010)</i>
	USA (Incubation exp).	-----	C-N	O/M	<i>Li et al. (2010)</i>
	Australia	Grassland	C-N	O	<i>Xing et al. (2011)</i>
	USA	Switchgrass	C	O	<i>Chamberlain et al. (2011)</i>
	USA	Grassland	C-N	O	<i>Hartman et al. (2011)</i>
	Canada/USA	Arable	C	O	<i>Smith et al. (2012)</i>
	Canada	Arable	C-N	O	<i>Chang et al. (2013)</i>
	Canada	Arable	N	O	<i>Sansoulet et al. (2014)</i>
	Australia	Arable	N	?	<i>Scheer et al. (2014)</i>
	UK	Arable	C-N	O	<i>Fitton et al. (2014a,b)</i>
	USA	Grassland	C-N	O	<i>Ryals et al. (2015)</i>
	USA	Switchgrass	C-N	O	<i>Field et al. (2016)</i>
DNDC	Costa Rica	Bare soil	C	O	<i>Li et al. (1994)</i>
	Europe/Australia	Arable/Grassland	C	O	<i>Li et al. (1997)</i>
	UK	Grassland	N	M	<i>Brown et al. (2002)</i>
	Canada	Arable	N	O	<i>Smith et al. (2002)</i>
	India	Paddy soil	C-N	O	<i>Pathak et al. (2003)</i>
	China, Japan, Thailand	Paddy soil	C-N	O	<i>Cai et al. (2003)</i>
	New Zealand	Grassland	N	M	<i>Saggar et al. (2004)</i>
	USA, China, Germany	Arable	C-N	O	<i>Li et al. (2005)</i>
	India	Paddy soil	C-N	M	<i>Pathak et al. (2005)</i>
	India	Paddy soil	C-N	O	<i>Babu et al. (2006)</i>
	Belgium	Arable	C	O	<i>Sleutel et al. (2006)</i>
	USA	Arable	N	O	<i>Tomitto et al. (2007)</i>
	Canada	Arable	N	O	<i>Smith et al. (2008)</i>

	China, Japan	Rice	C	M	<i>Fumoto et al. (2008)</i>
	Ireland	Grassland	N	O	<i>Abdalla et al. (2010)</i>
	China	Arable	C-N	O	<i>Li et al. (2010)</i>
	France, Germany, Switzerland	Arable	C	O	<i>Wattenbach et al. (2010)</i>
	Germany	Arable	N	O	<i>Ludwig et al. (2011)</i>
	Canada/USA	Arable	C	M	<i>Smith et al. (2012)</i>
	France, Germany, Belgium, UK, Netherlands, EU-15	Arable/Grassland	N	M	<i>Leip et al. (2011)</i>
	China	Arable	N	M	<i>Wu and Zhang (2014)</i>
	France	Arable	N	O	<i>Gu et al. (2014)</i>
	Canada	Arable/Grassland	N	M	<i>Uzoma et al. (2015)</i>
	Australia	Arable	N	O	<i>Chen et al. (2015)</i>
	USA (Alaska)	Peatland	C	O	<i>Deng et al. (2015)</i>
	China	Arable	C	M	<i>Yu et al. (2015)</i>
	New Zealand	Grassland	N	M	<i>Giltrap et al. (2015)</i>
	China	Arable	N	M	<i>Zhang et al. (2015)</i>
	Canada	Arable	N	M	<i>Congreves et al. (2016)</i>
	Canada	Arable	C	M	<i>Gagnon et al. (2016)</i>
DSSAT	UK, Brasil	Arable/Bare soil	C/N	O	<i>Gijsman et al. (2002)</i>
	Mexico	Arable	C	M	<i>Hartkamp et al. (2004)</i>
	Canada	Arable	N	O	<i>Liu et al. (2011)</i>
	Burkina Faso	Arable	C	M	<i>Soler et al. (2011)</i>
	Italy	Arable	C	O	<i>De Sanctis et al. (2012)</i>
	Spain	Arable	C/N	O	<i>Soldevilla-Martinez et al. (2013)</i>
	China	Arable	C/N	O	<i>Yang et al. (2013)</i>
	China	Arable	C/N	O	<i>Li et al. (2015)</i>
	Canada	Arable	C/N	O	<i>Li et al. (2015)</i>

	USA	Arable	N	O	<i>Prasad et al. (2015)</i>
EPIC	USA	Arable	N	O	<i>Jackson et al. (1994)</i>
	USA	Arable	N	O	<i>Cavero et al. (1996)</i>
	USA	Arable	N	O	<i>Ramanarayanan et al. (1998)</i>
	Canada	Arab	C-N	O	<i>Roloff et al. (1998)</i>
	USA	Arable	N	O	<i>Cavero et al. (1999)</i>
	Argentina	Arable/Grassland	N	O	<i>Bernardos et al. (2001)</i>
	USA	Arable	N	O	<i>Chung et al. (2002)</i>
	USA	Arable/Grassland	C	O	<i>Potter et al. (2004)</i>
	USA	Arab	C-N	O	<i>Wang et al. (2005)</i>
	Lab. Experiment	Lab. Experiment	C-N	O	<i>He et al. (2006)</i>
	USA, Canada	Arable	C-N	O	<i>Izaurrealde et al. (2006)</i>
	USA	Arable	C	O	<i>Causarano et al. (2007)</i>
	USA	Arable	C	O	<i>Abrahamson et al. (2009)</i>
	Argentina	Arable	C	O	<i>Apezteguia et al. (2009)</i>
	Germany	Arable	C	O	<i>Billen et al. (2009)</i>
	Italy	Arable	C	O	<i>Farina et al. (2011)</i>
	USA	Arable	C	O	<i>Zhang et al. (2015)</i>
PaSim	Switzerland	Grassland	N	O	<i>Schmid et al. (2001)</i>
	Scotland	Grassland	N	O	<i>Riedo et al. (2002)</i>
	Ireland	Grassland	C	O	<i>Lawton et al. (2006)</i>
	Hungary, Scotland, Ireland, France, Switzerland	Grassland	C-N	O	<i>Calanca et al. (2007)</i>
	Switzerland, Ireland, France, Scotland	Grassland	C	O	<i>Gottschalk et al. (2007)</i>
	France, Switzerland, Ireland	Grassland	C	O	<i>Vuichard et al. (2007a)</i>
	France	Grassland	C	O	<i>Aulagnier et al. (2013)</i>

	France, Germany, Hungary, Ireland, Italy, Portugal, Spain, Switzerland, The Netherlands, UK	Grassland	C	O	<i>Ma et al. (2015)</i>
	France, Germany, Italy, Switzerland	Grassland	C	O	<i>Sandor et al. (2016)</i>
RothC	Czech republic	Arable	C	O	<i>Coleman et al. (1997)</i>
	Hungary, Sweden, UK	Arable/Grassland	C	O	<i>Falloon and Smith (2002)</i>
	Australia	Arable	C	O	<i>Skjemstad et al. (2004)</i>
	Japan	Paddy soil	C	O/M	<i>Shirato and Yokazawa (2005)</i>
	Syria	Arable	C	O/M	<i>Jenkinson et al., 2005</i>
	China	Arable	C	O	<i>Guo et al. (2007)</i>
	Switzerland	Arable/Grassland	C	O	<i>Zimmermann et al. (2007)</i>
	Kenya	Arable	C	O	<i>Kamoni et al (2007b)</i>
	Zambia	Arable	C	O	<i>Kaonga et al (2008)</i>
	Australia	Arable	C	O	<i>Liu et al. (2009)</i>
	Ireland	Arable	C	O	<i>Dondini et al. (2009)</i>
	Slovakia	Arable/Grassland	C	O	<i>Barancikova et al. (2010)</i>
	Spain	Orchard	C	O	<i>Nieto et al. (2010)</i>
	Austria	Arable	C	O	<i>Rampazzo Todorovic et al. (2010)</i>
	Australia	Grasslands	C	O	<i>Liu et al. (2011)</i>
	Ireland	Grassland	C	O	<i>Xu et al. (2011)</i>
	Mexico	Arable/Grassland/Forest/Rangeland	C	O	<i>Gonzalez-Molina et al. (2011)</i>
China	Arable	C	O	<i>Wang et al. (2013)</i>	
	Italy, Spain, Australia, Syria, UK	Arable	C	O/M	<i>Farina et al. (2013)</i>
STICS	France	Arable	N	O	<i>Schnebelen et al. (2004)</i>
	France	Arable	N	O	<i>Corre-Hellou et al. (2009)</i>

France	Arable	C-N	O	<i>Justes et al. (2009)</i>
France	Arable	N	O	<i>Jego et al. (2012)</i>
France	Arable	N	O	<i>Constantin et al. (2012)</i>

24

25 **Table 5** – Overview of the studies carried out using the CN-MIP models for a broad gradient of
 26 geographic and climatic conditions, as well as a variety of soil types and management practices. * O =
 27 original version; M = modified version.

Model	N° of Ref.	Factor of weaknesses	N° of weaknesses per each model				% of weaknesses per each model			
			C-Cycle		N-Cycle		C-Cycle		N-Cycle	
			Modelling	Scale of analysis	Modelling	Scale of analysis	Modelling	Scale of analysis	Modelling	Scale of analysis
APSIM	6	Pedo-climatic	0	0	5	1	0.0	0.0	62.5	12.5
		Management	1	0	1	0	12.5	0.0	12.5	0.0
CERES-EGC	8	Pedo-climatic	1	0	6	2	7.7	0.0	46.2	15.4
		Management	1	0	3	0	7.7	0.0	23.1	0.0
DayCent	17	Pedo-climatic	4	0	14	8	11.8	0.0	41.2	23.5
		Management	3	1	4	0	8.8	2.9	11.8	0.0
DNDC	23	Pedo-climatic	10	6	13	6	18.5	11.1	24.1	11.1
		Management	9	3	6	2	16.7	5.6	9.3	3.7
DSSAT	7	Pedo-climatic	4	0	2	1	40.0	0.0	20.0	10.0
		Management	2	0	1	0	20.0	0.0	10.0	0.0
EPIC	13	Pedo-climatic	3	1	5	1	14.3	4.8	23.8	4.8
		Management	7	0	4	0	33.3	0.0	19	0.0
PaSim	7	Pedo-climatic	4	2	2	0	33.3	16.7	16.7	0.0
		Management	2	0	2	0	16.7	0.0	16.7	0.0
RothC	11	Pedo-climatic	5	0	0	0	35.7	0.0	0.0	0.0
		Management	9	0	0	0	64.3	0.0	0.0	0.0
STICS	3	Pedo-climatic	0	0	1	0	0.0	0.0	20.0	0.0
		Management	0	0	3	1	0.0	0.0	60.0	20.0
Total	95	Pedo-climatic	31	9	48	19	18	5.2	27.9	11
		Management	34	4	24	3	19.8	2.3	14	1.7

Table 6 – Number of weaknesses and the relative percentage emerged in **95** modelling studies. Model performances were mainly unsatisfactory due to erroneous accounting of pedo-climatic conditions (**45.9 %**) and management practices (**33.8 %**).

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
APSIM	<i>Snow et al. (1999)</i>	Pedo-climatic	0	0	1	0	Underestimation of soil N supply	Soil properties (C)	Modelling HUM decomposition too slow
		Management	0	0	0	0	----	----	----
	<i>Thorburn et al. (2010)</i>	Pedo-climatic	0	0	1	0	General discrepancies (Underestimation of Denitrification, Unpredicted N ₂ O emissions peaks)	Soil properties (N) - Climate	Model parametrization: Default value of denitrification coefficient within the model was much lower than the optimized - Errors in rainfall data used (i.e. spatially averaged rainfall data were used vs specific test site rainfall data)
		Management	0	0	0	0	----	----	----
	<i>Sharp et al. (2011)</i>	Pedo-climatic	0	0	1	0	Overestimation of annual leaching	Soil properties (N)	Overestimation of soil solution nitrate concentration
		Management	0	0	0	0	----	----	----
	<i>Xing et al. (2011)</i>	Pedo-climatic	0	0	1	1	Underestimation of N ₂ O emissions	Soil properties (N)	Underestimation of denitrification (response of denitrification rate to soil temperature and moisture (or WFPS) were the two primary factors leading to the underestimation of denitrification)
		Management	0	0	0	0	----	----	----
		Pedo-climatic	0	0	0	0	----	----	----
	<i>Luo et al. (2011)</i>	Management	1	0	0	0	Underestimation of SOC decomposition	Management (Tillage - Crop type)	Tillage: effect on soil features can lead to possible acceleration in soil C decomposition due to changes in soil environment. Tillage effects in APSIM is very simple and could not take in account the real effect on soil - Crop type: crop varietal changes could have significant effect on crop production and, in turn, on C input.
		Pedo-climatic	0	0	1	0	Under/Overestimation of N ₂ O emissions	Soil properties (general) - Climate	Average field soil properties used for running the model rather than specific values
	<i>Giltrap et al. (2015)</i>	Management	0	0	1	0		Management (Fertilization)	Fertilization type: urine patches is much more extreme than typical fertilization as NH ₄ ⁺
CERES-EGC	<i>Gabrielle et al. (2006)</i>	Pedo-climatic	0	0	0	1	Under/Overestimation of N ₂ O emission peaks	Soil properties (SWD - BD)	Soil water retention properties and bulk density. Different parametrization lead to differences in N outputs from test site to regional scale
		Management	0	0	0	0	----	----	----

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation	
	<i>Lamboni et al. (2009)</i>	Pedo-climatic	0	0	1	0	General discrepancies (N ₂ O emissions)	Soil properties (N)	Sensitivity of N ₂ O emissions: Denitrification, Potential denitrification rate, Fraction of denitrified N.	
		Management	0	0	0	0	----	----	----	
	<i>Wattenbach et al. (2010)</i>	Pedo-climatic	1	0	0	0	Overestimation NEE peaks	Climate	Climate Model was developed for Northern regions. Main issues in Southern regions of Europe. Issues in coupling water and carbon fluxes	
		Management	1	0	0	0		Phenology	Possible mismatch due to ecophysiology: overestimation NEE peaks and fluxes during senescence and mismatch in the cumulative NEE for the year. Poor performance in reproducing LE flux	
	<i>Drouet et al. (2011)</i>	Pedo-climatic	0	0	1	0	General discrepancies (N ₂ O emissions)	Soil properties (N - BD)	Sensitivity of N ₂ O emissions: N ₂ O emissions from denitrification; Max. rate of nitrification, Soil Bulk Density	
		Management	0	0	1	0		Management (Crop type)	Sensitivity of N ₂ O emissions: Cropland area (crop variety and management)	
	<i>Lehuger et al. (2011)</i>	Pedo-climatic	0	0	1	1	Overestimation of N ₂ O emissions	Soil properties (N)	N ₂ O emission peak was produced in response of the high ammonium content in topsoil - Possible time lag in N ₂ O emissions	
		Management	0	0	0	0	----	----	----	
	<i>Goglio et al. (2013)</i>	Pedo-climatic	0	0	1	0	Underestimation of N ₂ O emissions peaks	Climate	Inter-annual variability	
		Management	0	0	1	0		Management (Fertilization - water conservation)	Legumes incorporation and mulching	
	<i>Lehuger et al. (2014)</i>	Pedo-climatic	0	0	1	0	General discrepancies (N ₂ O emissions)	Climate (Rainfall)	Rainfall	
		Management	0	0	0	0	----	----	----	
	<i>Noirot-Cosson (2016)</i>	Pedo-climatic	0	0	1	0	Overestimation of mineral N	Soil properties (T - SWD)	Temperature and water on mineralization dynamics	
		Management	0	0	1	0		Management (Fertilization)	Effect of N fertilizer	
	DayCent	<i>Parton et al. (2001)</i>	Pedo-climatic	0	0	1	1	General discrepancies (N ₂ O and NO _x emissions)	Soil properties (Texture)	Texture
			Management	0	0	0	0	----	----	----

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>Stehfest and Muller (2004)</i>	Pedo-climatic	0	0	1	0	Overestimation of N ₂ O emissions	Soil properties (N - WFPS) - Climate	WFPS overestimation and issues in the ratio Denitrification/Nitrification - Rainfall
		Management	0	0	1	0		Management (Fertilization)	Urine application
	<i>Del Grosso et al. (2005)</i>	Pedo-climatic	0	0	1	1	General discrepancies (N ₂ O emissions)	Soil properties (general) - Climate	Soil properties
		Management	0	0	0	0	----	----	----
	<i>Li et al. (2005)</i>	Pedo-climatic	0	0	1	1	Underestimation of NH ₄	Soil properties (N)	Overestimation nitrification rate and underestimation Nitrification (mainly due to temperature effect)
		Management	0	0	0	0	----	----	----
	<i>Smith et al. (2008)</i>	Pedo-climatic	0	0	1	1	Underestimation of N ₂ O emissions	Soil properties (N - SWD)	Under prediction of Mineralization and soil properties (SWC, soil N and soil ammonium)
		Management	0	0	0	0	----	----	----
	<i>Jarecki et al. (2008)</i>	Pedo-climatic	0	0	1	0	Underestimation of N ₂ O emissions	Soil properties (N - SWD) - Climate	Soil properties (inorganic N, soil moisture) - Rainfall
		Management	0	0	0	0	----	----	----
	<i>Del Grosso et al. (2008)</i>	Pedo-climatic	0	0	1	1	Overestimation of N ₂ O emissions	Soil properties (N)	Nitrification rates too high, NO ₃ too low, N ₂ O too high.
		Management	0	0	0	0	----	----	----
	<i>David et al. (2009)</i>	Pedo-climatic	0	0	1	1	Overestimation of N ₂ O emissions	Soil properties (general)	Crop evapotranspiration and the impact of tile drainage
		Management	0	0	0	0	----	----	----
	<i>Li et al. (2010)</i>	Pedo-climatic	1	0	1	0	General discrepancies (CO ₂ , N mineralization and Nitrification)	Soil properties (SWD)	Soil moisture
		Management	0	0	0	0	----	----	----
	<i>Abdalla et al. (2010)</i>	Pedo-climatic	0	0	1	0	General discrepancies (Overestimation N ₂ O emissions, underestimation N ₂ O emissions)	Soil water flows (WFPS)	Overestimation WFPS
		Management	0	0	1	0		Management (Fertilization - Crop type)	Fertilization maintained high mineral N along with secondary peaks compared to field data, underestimated biomass.
	<i>Del Grosso et al. (2010)</i>	Pedo-climatic	0	0	1	1	Overestimation of N ₂ O emissions	Soil properties (N)	N mineralization rates too high and too responsive to climate drivers

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>De Gyrze et al. (2010)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	1	0	1	0	General discrepancies (SOC; underestimation N ₂ O emissions)	Soil properties (C - BD - texture) - Climate	Texture, decomposition rate, Bulk Density - Rainfall
		Management	1	0	1	0		Management (Tillage - Crop type)	Tillage and cover crop
		Pedo-climatic	1	0	0	0	General discrepancies (CO ₂ emissions)	Soil properties (SWD - WFPS)	Soil moisture variations, high sensitivity to WFPS
	<i>Xing et al. (2011)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	0	0	0	0	----	----	----
	<i>Smith et al. (2012)</i>	Management	1	1	0	0	Underestimation of SOC	Management (Fertilization)	Slight overestimation of residue removal impact on SOC partly because of the inherent variability in SOC measurements and also partly due to imperfections in the models themselves
		Pedo-climatic	0	0	1	1	General discrepancies (Overestimation N ₂ O emissions and soil NH ₄ ; Underestimation NO ₃ emissions)	Climate	Drying out periods
	<i>Scheer et al. (2014)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	0	0	1	0	Underestimation of N ₂ O emissions	Soil properties (N) - Climate	N subroutine heavily affected by soil parameters. Mineralization and denitrification rates may be too low, freeze-thaw fluxes need work - N subroutine heavily affected by climate
	<i>Fitton et al. (2014a,b)</i>	Management	0	0	1	0	Management (Fertilization)	Management (Fertilization)	Model sensitive at low N application rates
		Pedo-climatic	1	0	0	0	Underestimation of CO ₂ emissions	Soil properties (N - WFPS)	N mineralization rates may be off, underestimated WFPS
	<i>Ryals et al. (2014, 2015)</i>	Management	1	0	0	0	Management (Fertilization)	Management (Fertilization)	No soil water benefits provided by adding of compost
		Pedo-climatic	0	0	1	1	Overestimation of N ₂ O emissions	Soil properties (general)	Overestimation N ₂ O emissions from shoulder position (upper landscape). Inability to characterize differences in soil properties and water/nutrient flow for 3-D landscape
DNDC	<i>Smith et al. (2002)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	1	0	1	0	General discrepancies (CH ₄ , N ₂ O and NO emissions)	Soil properties (general)	Soil properties
	<i>Cai et al. (2003)</i>	Pedo-climatic	1	0	1	0	General discrepancies (CH ₄ , N ₂ O and NO emissions)	Soil properties (general)	Soil properties

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>Pathak et al. (2003)</i>	Management	1	0	0	0	Overestimations of CH ₄ emissions	Management (Crop type)	Type of cultivar (crop parameters) - daily timescale
		Pedo-climatic	1	0	0	0		Soil properties (N)	Leaking rate
	<i>Saggar et al. (2004)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	0	0	1	1	Underestimation of N ₂ O emissions	Soil properties (T - SWD)	Under prediction of Temperature effect and moisture after rainfall (size and timing)
	<i>Pathak et al. (2005)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	1	0	0	0	Overestimations of CH ₄ emissions	Soil properties (C - pH)	Initial SOC content and soil redox potential
	<i>Babu et al. (2006)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	1	1	0	1	General discrepancies (CH ₄ and N ₂ O peaks)	Soil properties (SWD)	Soil shrinking and swelling - daily timescale
	Management	1	0	0	1	Management (Crop type)		CH ₄ and N ₂ O peaks not well captured at the beginning and end of growing season. Type of cultivar (crop parameters)	
	<i>Sleutel et al. (2006)</i>	Pedo-climatic	1	1	0	0	Under/Overestimation of SOC	Soil properties (general)	Soil type
		Management	1	0	0	0	Overestimation of SOC	Management (Fertilization)	Residues incorporation
	<i>Liu et al. (2006)</i>	Pedo-climatic	1	1	0	0	General discrepancies (SOC)	Climate	Spatial heterogeneity in environmental parameters
		Management	1	1	0	0		Management (general)	Spatial heterogeneity in farm management practices
	<i>Tonitto et al. (2007)</i>	Pedo-climatic	0	0	1	1	Overestimation of N leaching	Soil properties (N)	The base DNDC model greatly over predicted N leaching: calibration of 4 leaching parameters (within code) was required to improve model performance.
		Management	0	0	0	0	----	----	----
	<i>Smith et al. (2008)</i>	Pedo-climatic	0	0	1	1	General discrepancies (timing of N ₂ O emissions).	Soil properties (N - SWD)	Soil water content and soil N underestimated. Too few chamber measurements of N ₂ O emissions available for detailed temporal testing.
		Management	0	0	1	1	Underestimation of N ₂ O emissions	Management (Fertilization)	Error in plant N uptake equation. Highest slurry rate
	<i>Fumoto et al. (2008)</i>	Pedo-climatic	1	1	0	0	Under/Overestimation of CH ₄ emissions	Soil properties (general)	Soil properties and effect of temperature on Leaf Area development
		Management	1	0	0	0		Management (Crop type) - Phenology	Type and stage of cultivar

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>Abdalla et al. (2010)</i>	Pedo-climatic	0	0	1	0	Overestimation of N ₂ O emissions	Soil properties (C - WFPS)	Overestimation WFPS and SOC content
		Management	0	0	0	0	----	----	----
	<i>Li et al. (2010)</i>	Pedo-climatic	0	0	1	0	Underestimation of N ₂ O emissions	Soil properties (SWD)	Impact of soil freezing and thawing
		Management	0	0	0	0	----	----	----
	<i>Wattenbach et al. (2010)</i>	Pedo-climatic	1	0	0	0	General discrepancies (cumulative NEE and Reco, overestimation NEE peaks).	Climate	Issues in coupling water and carbon fluxes, air temperature (i.e. mild winter)
		Management	1	0	0	0		Management (Fertilization - Tillage - Crop type)	Overestimation NEE peaks and general discrepancies at senescence and post-harvesting, (cumulative NEE and Reco). Crop rotation, fertilization and tillage
	<i>Ludwig et al. (2011)</i>	Pedo-climatic	0	0	1	0	Under/Overestimation of N ₂ O emissions	Soil properties (general) - Climate	Soil properties - Rainfall
		Management	0	0	0	0	----	----	----
	<i>Leip et al. (2011)</i>	Pedo-climatic	0	0	1	1	Under/Overestimation of N ₂ O emissions	Soil properties (general) - Climate	Soil properties - Rainfall
		Management	0	0	0	0	----	----	----
	<i>Smith et al. (2012)</i>	Pedo-climatic	1	1	0	0	Overestimation of SOC following residue removal	Soil properties (C)	High spatial heterogeneity in SOC measurements. The conceptual SOC "passive fraction" may have been set too high in DNDC from some locations/soil types.
		Management	1	1	0	0		Management (Fertilization)	DNDC tended to underestimate the rate of decomposition. SOC change as affected by residue removal at some sites
	<i>Yu et al. (2015)</i>	Pedo-climatic	0	0	0	0	----	----	----
		Management	1	0	0	0	Underestimation of CO ₂ emissions and heterotrophic respiration	Phenology	Use of generalized crop growth curve resulted in underestimation of duration of root growth and N uptake
	<i>Uzoma et al. (2015)</i>	Pedo-climatic	0	0	1	0	Under/Overestimation of N ₂ O emissions	Soil properties (SWD) - Climate	Inability of cascade flow hydrology model to effectively simulate water content above field capacity - N ₂ O emissions overestimated during alfalfa production and underestimated during long periods of episodic rainfall.
		Management	0	0	1	0		Phenology	Interception and uptake of water by alfalfa was likely underestimated.

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>Zhang et al. (2015)</i>	Pedo-climatic	0	0	1	0	General discrepancies (timing of daily N ₂ O and NO emissions)	Soil properties (SWD)	Soil water content was not well simulated
		Management	0	0	1	0	Overestimation of N ₂ O and NO emissions	Management (Fertilization)	High fertilizer treatments: Need to better simulate the limitation of dissolved organic carbon on denitrification
	<i>Gu et al. (2014)</i>	Pedo-climatic	0	0	1	0	Overestimation of N ₂ O emissions, soil nitrate and ammonia concentrations.	Soil properties (N)	The model had incorrect nitrogen partitioning for urea ammonium nitrate applications.
		Management	0	0	1	0		Management (Fertilization)	Model doesn't include canopy interception and foliar N uptake when spraying liquid fertilizer.
	<i>Congreves et al. (2016)</i>	Pedo-climatic	0	0	1	0	Underestimation of NH ₃ emissions	Soil properties (Texture - SWD)	NH ₃ emissions were greatly improved for a newly develop NH ₃ sub-model but emissions were still largely underestimated for one treatment. The model could not simulate a heterogeneous soil profile.
		Management	0	0	1	0		Management (Fertilization)	Due to simple cascade water flow DNDC had limited ability to simulate slurry infiltration rates.
	<i>Gagnon et al. (2016)</i>	Pedo-climatic	1	1	0	0	General discrepancies (soil CO ₂ respiration).	Soil properties (C - texture)	Inputs data describing long-term field history was not available. Thus the initial assumed fractions of litter, humads and humus may have been wrong.
		Management	1	1	0	0		Management (Fertilization)	DNDC could not simulate the differences in soil CO ₂ respiration between soil textures and produced opposite values than was observed when N fertilizer was added (respiration was increased rather than decreased). DNDC does not include soil processes which reduce soil CO ₂ respiration after fertilizer addition (these processes are not well understood).
DSSAT	<i>Gijsman et al. (2002)</i>	Pedo-climatic	1	0	1	0	General discrepancies (SOC dynamics and soil mineral N)	Soil properties (C - texture)	Relative proportion of SOM pools and the rate of some pools were not likely to be well simulated. Other factor can be that the soil texture data used as inputs for the simulation were expressed in ISSS textural units, in which silt is the 2- to 20-µm class, while DSSAT use the American unit system with silt equals to 2 to 50 µm. This has likely affected also soil retention characteristics.
		Management	0	0	0	0	----	----	----
	<i>Liu et al. (2011)</i>	Pedo-climatic	0	0	1	1	Overestimation of N losses	Soil properties (N - texture)	Consistently overestimation of nitrate loss from no fertilization treatment in long term experimental sites. This overestimation may reflect inadequate model representation of degraded soil profile for long-term simulations
		Management	0	0	0	0	----	----	----

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation	
	<i>Hartkamp et al. (2004)</i>	Pedo-climatic	0	0	0	0	----	----	----	
		Management	1	0	0	0	Overestimation of SOC	Management (Fertilization)	Fertilization: Overestimation SOC (SOC was overestimated in the crop rotations with N fertilization) Initial values for SOC not accurately defined. SOC overestimation associated to overestimation of the biomass incorporated into the soil. In fact, SOC in the fallow quite well simulated.	
	<i>De Sanctis et al. (2012)</i>	Pedo-climatic	1	0	0	0	Underestimation of SOC	Soil properties (SWD)	The long-term increase of SOC in the top soil layers can have a relevant influence on soil hydraulic properties but this is not automatically simulated by DSSAT	
		Management	0	0	0	0	----	----	----	
	<i>Li et al. (2015)</i>	Pedo-climatic	1	0	0	0	General discrepancies (SOC)	Soil properties (C) - Climate	Overestimation of the rate of soil C decomposition and the underestimation of the efficiency of conversion of crop residue C to soil C set in the model - Soil C decomposition rates set in the CENTURY model may be too high for semi-arid Canadian soils.	
		Management	1	0	0	0		Management (Crop type)	Improvements in the cultivar coefficients are required, in fact deviations in straw and root yields were highlighted	
	<i>Li et al. (2015)</i>	Pedo-climatic	1	0	0	0	Overestimation of SOC	Soil properties (C - N)	Differences between the model soil C/N ratio and the measured C/N ratio parameter	
		Management	0	0	0	0	----	----	----	
		Pedo-climatic	0	0	0	0	----	----	----	
	<i>Prasad et al. (2015)</i>	Management	0	0	1	0	General discrepancies (leaching loss and gaseous loss of N via volatilization and denitrification).	Management (Fertilization) - Phenology	High soil mineral N concentrations that might have resulted from late application of large amounts of N that were not utilized by potato plants - During the tuber bulking phase, the potato plant slows down N uptake and starts N translocation from leaves to tubers. The presence of large amount of mineral N might have created hot spot area in the potato beds where soil sampling was carried out.	
	EPIC	<i>Jackson et al. (1994)</i>	Pedo-climatic	0	0	0	0	----	----	----
			Management	0	0	1	0	Underestimation of soil NO ₃ content	Management (Irrigation)	Leached or denitrified during the irrigated crop period.
<i>Cavero et al. (1996)</i>		Pedo-climatic	0	0	0	0	----	----	----	
		Management	0	0	1	0	Overestimation of inorganic N concentration	Management (Fertilization)	Crop residues incorporation (i.e. overestimation N uptake at harvest)	
<i>Ramanarayanan et al. (1998)</i>		Pedo-climatic	0	0	1	0	Overestimation of soil NO ₃ content	Climate	Weather condition	
		Management	0	0	0	0	----	----	----	

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>Roloff et al. (1998)</i>	Pedo-climatic	0	0	1	0	Underestimation of soil N content	Soil properties (N - SWD)	N transformation, water dynamics and soil water balance routine (PET and water distribution within profile) are probably the main issues
		Management	0	0	0	0	----	----	----
	<i>Cavero et al. (1999)</i>	Pedo-climatic	0	0	1	0	Underestimation of inorganic N concentration, N losses	Soil properties (N)	N distribution in the bed
		Management	0	0	1	0		Management (Fertilization - Crop type - Irrigation)	Crop (Access of roots to inorganic N), irrigation
	<i>Chung et al. (2002)</i>	Pedo-climatic	0	0	1	1	Overestimation NO ₃ -N losses	Soil properties (SWD) - Climate	Simplistic tile drainage routine/lack of a flow component - Storm events
		Management	0	0	0	0	----	----	----
	<i>Potter et al. (2004)</i>	Pedo-climatic	1	0	0	0	Underestimation of soil C	Soil properties (general)	Soil properties
		Management	1	0	0	0		Management (Tillage)	Rate of C losses in tilled management too high or C accumulation in grassed area reaching a plateau after "quick" increase (possible cause: lack of available N)
	<i>Wang et al. (2005)</i>	Pedo-climatic	0	0	0	0	----	----	----
		Management	1	0	0	0	Underestimation (SOC content)	Management (Fertilization)	Issues in observations and model structural error in underestimating the return of corn residues. Disturbance of the soil sample (consequent increase of mineralization) - N mineralization algorithms may underpredict Net Nitrogen Mineralization (NMN) observable under field conditions - Problem in reproducing the lab. Experiment.
	<i>He et al. (2006)</i>	Pedo-climatic	1	0	1	0	General discrepancies (soil C, Overestimation of N mineralization)	Soil properties (C)	Underestimation of the soil capacity to transform crop residue in SOC
		Management	1	0	1	0	General discrepancies (Overestimation of microbial biomass C and total organic C, Underestimation particulate organic C)	Management (Fertilization)	Spatial differences in C fraction due to differing soil landscapes
	<i>Causarano et al. (2007)</i>	Pedo-climatic	0	1	0	0		Management (Fertilization - Tillage)	Soil properties (C)
		Management	1	0	0	0	----		----
	<i>Apezteguia et al. (2009)</i>	Pedo-climatic	0	0	0	0	General discrepancies (SOC content)	Phenology	Inability of the model to capture the yield trends as well to the overestimation of the contribution of monoculture to TOC.
		Management	1	0	0	0			
	<i>Billen et al. (2009)</i>	Pedo-climatic	0	0	0	0	----	----	----

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>Zhang et al. (2015)</i>	Management	1	0	0	0	General discrepancies (SOC content)	Management (Tillage)	Tillage effect
		Pedo-climatic	1	0	0	0	General discrepancies (differences in the magnitude of NPP and NEE, and in the spatial pattern of SOC change).	Soil properties-Climate	Errors in climate records, inaccurate soil parameters, incomplete management information, and interactions among these factors, inaccurate representation of crop rotations
		Management	1	0	0	0		Management	
PaSim	<i>Schmid et al. (2001)</i>	Pedo-climatic	0	0	1	0	Underestimation of N ₂ O emission peaks	Climate	Wet conditions
		Management	0	0	1	0		Phenology	Overestimation transpiration and N uptake by plants;
		Pedo-climatic	0	0	0	0		----	----
	<i>Riedo et al. (2002)</i>	Management	0	0	1	0	Underestimation of NH ₃ emission peaks	Management (Fertilization - Cutting)	Soil ammoniacal nitrogen pool is partitioned between soil surface and soil layers with the NH ₃ emissions being driven by NH ₄ in the 0-3 mm soil layer. The drawback here is that models does not consider the form of N taken up by roots, Accordingly high NH ₄ absorption by plants leads to high NH ₃ emissions and vice versa - explaining some discrepancies between simulations and measurements during the period after fertilisation
		Pedo-climatic	1	0	0	0	Overestimation of NEE	Climate	Over prediction of the uptake due to the oversensitivity of PaSim to initial conditions/winter conditions.
	<i>Lawton et al. (2006)</i>	Management	0	0	0	0	General discrepancies (Under/Overestimation of GPP, Reco and N ₂ O emissions; daily CO ₂ emissions)	Management	Type of management (intensive vs extensive)
		Pedo-climatic	1	1	1	0		Soil properties (C - SWD)	Inappropriate setting of initial parameters, SOM stock initialization, over emphasis of water stress effect on assimilation
	<i>Vuichard et al. (2007a)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	0	0	0	0	----	----	----
	<i>Ma et al. (2015)</i>	Management	1	0	0	0	Under/Overestimation of NEE	Management	Grazing effect
		Pedo-climatic	1	0	0	0	Under/Overestimation of GPP and Reco	Soil properties (T - SWD)	SWC and soil temperature
		Management	1	0	0	0	General discrepancies (NEE)	Management	Type of management (intensive vs extensive)
	Pedo-climatic	1	1	0	0	Soil properties (T - SWD)		Improper representation of soil water content and soil temperature	
	<i>Sandor et al. (2016)</i>	Management	0	0	0	0	----	----	----
Pedo-climatic		0	0	0	0	----	----	----	
RothC	<i>Skjemstad et al. (2004)</i>	Pedo-climatic	0	0	0	0	----	----	----

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>Shirato and Yokazawa (2005)</i>	Management	1	0	0	0	General discrepancies (C)	Management	Disturbances (i.e. clearing and burning of pulled vegetation)
		Pedo-climatic	0	0	0	0	----	----	----
	<i>Zimmermann et al. (2007)</i>	Management	1	0	0	0	Underestimation of SOC content	Management	Slow decomposition rate of SOM in Rice when submerged soils are waterlogged and subjected to anaerobic conditions (RothC is not usable for waterlogged soil, Rice)
		Pedo-climatic	1	0	0	0	General discrepancies (SOC)	Soil properties (general) - Climate	Soil properties - Air temperature
	<i>Liu et al. (2009)</i>	Management	0	0	0	0	----	----	----
		Pedo-climatic	0	0	0	0	----	----	----
	<i>Rampazzo Todorovic et al. (2010)</i>	Management	1	0	0	0	Overestimation of SOC content	Management (Fertilization)	Stubble (i.e. using the conventional setting of stubble retention factor)
		Pedo-climatic	1	0	0	0	General discrepancies (SOC content)	Soil properties (general) - Climate	Soil properties
		Management	1	0	0	0		Management (Fertilization - Crop type)	Type of crop and straw
	<i>Nieto et al. (2010)</i>	Pedo-climatic	0	0	0	0	----	----	----
		Management	1	0	0	0	Overestimation of SOC content	Management (Tillage)	C losses due to soil erosion
	<i>Xu et al. (2011)</i>	Pedo-climatic	1	0	0	0	General discrepancies (SOC content)	Soil properties (general) - Climate	Soil properties
		Management	0	0	0	0	----	----	----
	<i>Gonzalez-Molina et al. (2011)</i>	Pedo-climatic	1	0	0	0	Overestimation of SOC content	Soil properties (general) - Climate	Type of ecosystem (rangelands complexity, erosion, type of soil, etc.)
		Management	1	0	0	0		Management (general)	Residues, overgrazing, etc.
	<i>Nieto et al. (2013)</i>	Pedo-climatic	0	0	0	0	----	----	----
		Management	1	0	0	0	Overestimation of SOC content	Management (Tillage)	Tillage (erosion)
	<i>Wang et al. (2013)</i>	Pedo-climatic	0	0	0	0	----	----	----
		Management	1	0	0	0	Overestimation of SOC content	Management (Fertilization)	Fertilization (N + straw)

Model Name	References	Factor of weaknesses	C-Cycle Model structure	C-Cycle Scale of analysis	N-Cycle Model structure	N-Cycle Scale of analysis	Type of weaknesses	Cause of weaknesses	Possible explanation
	<i>Farina et al. (2013)</i>	Pedo-climatic	1	0	0	0	Under/Overestimation of GPP and Reco	Climate Management (general)	Dry condition
		Management	1	0	0	0			Rotation with fallow
STICS	<i>Schnebelen et al. (2004)</i>	Pedo-climatic	0	0	1	0	Overestimation of soil N absorption	Soil properties (general)	Type of soil (soil lying on cryoturbated material cannot be parametrized).
		Management	0	0	1	1		Management (Crop type)	Type of crop (inadequate predication root density in some particular soil i.e. cryot.)
	<i>Justes et al. (2009)</i>	Pedo-climatic	0	0	0	0	----	----	----
		Management	0	0	1	0	Underestimation of N mineralization	Management (Fertilization)	Default values of the decomposition module (Analysis on 25 catch crops residues).
	<i>Constantin et al. (2012)</i>	Pedo-climatic	0	0	0	0	----	----	----
		Management	0	0	1	0	General discrepancies (N mineralization and organic N sequestered in soil)	Management (Fertilization)	Lack of sensitivity of N uptake to N mineralization (lack of synchrony between extra mineralization due to catch crops and crop N demand in the model).

Table 7 – Analysis of type and cause of modelling weaknesses and the relative possible explanation for single modelling study. For each study, the specific factor of weaknesses and the biogeochemical cycle involved (i.e. C or N) **have** been considered

Figure captions

Figure 1 – Top-down approach focused at gaining insight into compositional sub-systems of the most important processes and approaches implemented into the 9 biogeochemical models used in the analysis. Classification was built according to three levels of detail: i) Low: five general classes (level 1); ii) Medium: 20 main processes (level 2); iii) High: 196 approaches (methods/options/components, level 3).

Level 1 – General Classes		
Mostly simulated discrete units considered in agricultural modelling N° of units: 5 Level of detail: LOW	Level 2 – Main Processes	
	Mostly simulated main processes considered in agricultural modelling N° of processes: 20 Level of detail: MEDIUM	Level 3 – Main approaches Mostly simulated modelling approaches considered in agricultural modelling N° of approaches: 196 Level of detail: HIGH

Fig. 1

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