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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 (CO_2), and nitrate (NO_3))
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 makinges 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. Izaurralde 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. Willianms. 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., Izaurralde, 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.
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, 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 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.faccejpi.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 "CO_2" rather than "CO_2-GHG", and use "Non CO_2-Gas" instead of "Non CO_2-GHG" because N_2 and NH_3 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 (^{13}C-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 theat 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 makinges 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.faccejpi.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. Izaurralde 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. Willianms. 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., Izaurralde, 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.

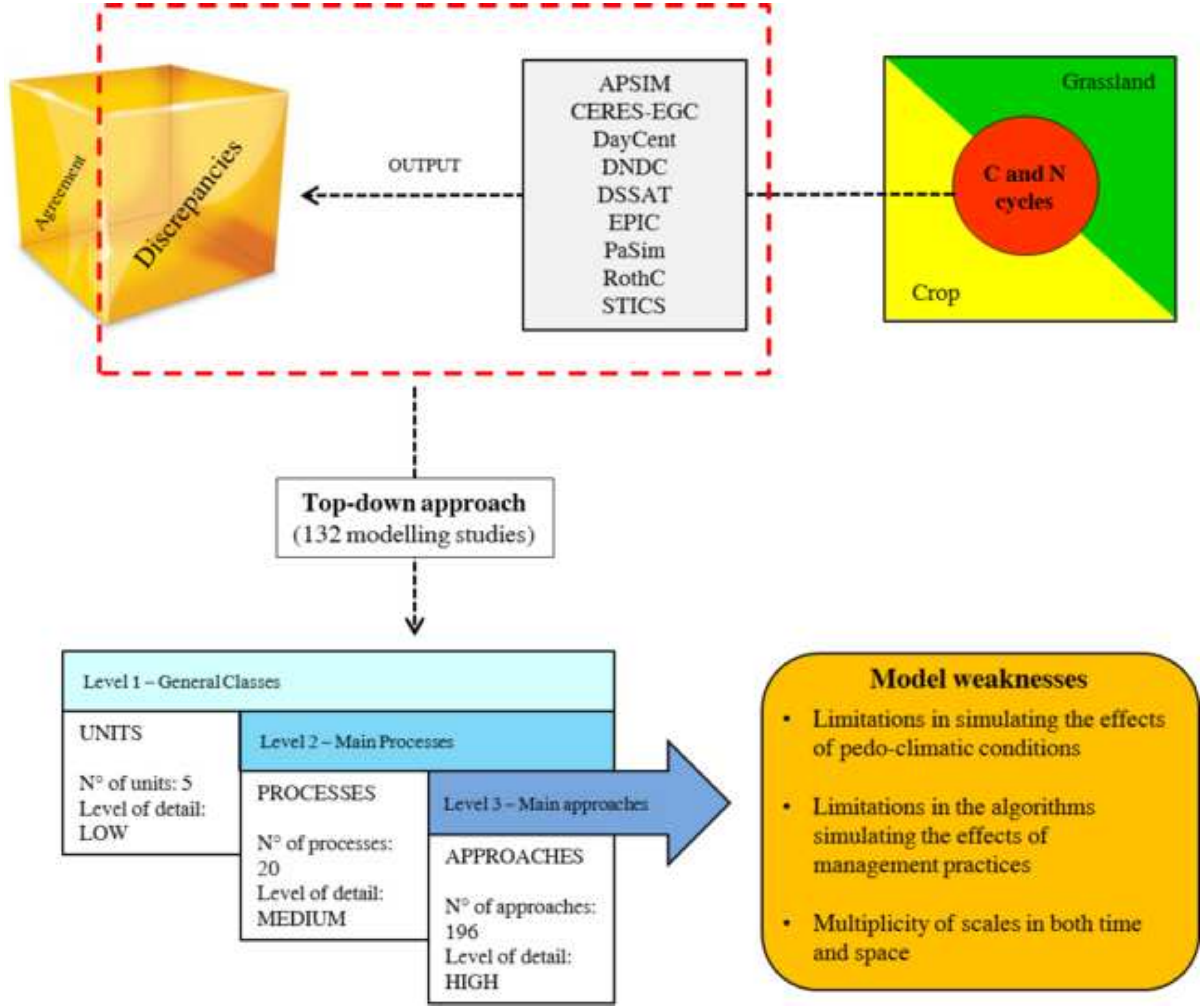
We thank the reviewer for these comments. We modified the text (see L176-183: "EPIC (Environmental Policy Integrated Climate) (Williams, 1995, Izaurralde et al., 2012) can simulate about 130 crop and grass species through its plant growth model, which uses unique parameter values for each species. It 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 CO_2. Moreover, novel algorithms were recently implemented (Izaurralde et al., 2012) to improve the simulation of C and N transformations, gas (O_2, CO_2, and N_2O) and solute (NO_3^-, NO_2^-) 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 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.
   We thank the reviewer for the comment. The information reported in table 4 has been modified accordingly.

*Graphical Abstract



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

*Revised manuscript with changes marked
Click here to view linked References

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 carbon sequestration and greenhouse gas 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 carbon and nitrogen 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 (https://www6.inra.fr/cnmip/Project): 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 carbon and nitrogen models. They include the explicit representation of soil microbial biomass to drive soil organic matter turnover, the effect of nitrogen shortage on soil organic matter decomposition, the improvements related to the production and consumption of gases and an adequate simulation of gas transport in soil. Given these conditions, the assessment of trends and gaps in the modelling approaches currently employed to represent biogeochemical cycles in crop and grassland systems appears to be an essential step for future research.

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

1. Introduction

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

Process-based ecosystem models take the approach of simulating underlying biogeochemical processes, such as plant photosynthesis and respiration, using mathematical equations that determine the allocation of C from atmospheric CO_2 into biomass down to the soil organic matter (SOM). A relatively complete suite of biogeochemical processes (e.g. plant growth, organic matter decomposition, fermentation, ammonia volatilisation, nitrification and denitrification) is generally embedded in these models, enabling computation of transport and transformations in plant–soil ecosystems. Sub-models are designed to interact with each other to describe cycles of water, C and N for target ecosystems, thus any change in the environmental factors collectively affect a group of biogeochemical reactions. Extensively tested biogeochemical models (with the coupled C-N cycling) are effective tools for examining the magnitude and spatial-temporal patterns of C and N fluxes, and play an important role in designing specific policies appropriate to the soils, climate, and agricultural conditions of a location or region. In recent decades, these tools have also been used for assessing the expected impacts of future climate, as represented by several climate change scenarios (Graux et al., 2013). However, results of state-of the-art terrestrial biogeochemical models, describing the contribution of agricultural systems to C sequestration and GHG source/sink status, may diverge significantly even when models are run under the same conditions of climate, soil and management (Palosuo et al., 2011, Rotter et al., 2012, Asseng et al., 2013, Sándor et al., 2016; Sandor et al., 2017). Such differences between model results are often attributed to physical and biogeochemical processes being inadequately resolved and, for these models, the improvement of algorithms and structure is recommended beyond parameter optimization (Tian et al., 2011, Lu and Tian, 2013).

It is the goal of this paper to examine the strengths and weaknesses of nine crop and grassland models that incorporate C and N fluxes into biogeochemical frameworks and fully assess C and GHG dynamics in agricultural soils. These models are commonly applied worldwide and are used to simulate biogeochemical and related outputs by the 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.faccejpi.com), which brings together 10 organizations from six countries. With this analysis we are not arguing against the quality of models. While highlighting weaknesses and limits of current modelling approaches as documented in several published studies, we intend to offer a general overview as a basis for new ways of improving current modelling approaches.

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

2. Modelling approaches

2.1. The CN-MIP models

The nine models considered for the CN-MIP exercise are process-based models mainly developed for crop or grassland ecosystems. They attempt to reproduce the most relevant ecological and physiological process through a theoretical understanding grounded in state of the art knowledge. In this way, they reproduce specific agro-ecological dynamics under prescribed conditions of climate, soil and management, thanks to the concepts and relationships that interlink entities of the real world. Most models represent plant phenology and yield-formation processes, together with functional processes at the basis of SOM (Soil Organic Matter) turnover, gas exchange at the soil-plant-atmosphere interface and soil water dynamics.

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

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

ii) *CERES-EGC* (Crop Environment REsource Synthesis - Environnement et Grandes Cultures) (Gabrielle et al., 1995) simulates the biogeochemical cycles of water, C and N in agro-ecosystems. The model predicts crop production and the environmental impacts related to the agricultural activity (e.g. nitrous oxide (N_2O), nitrogen oxide (NO), ammonia (NH_3), carbon dioxide (CO_2), and nitrate (NO_3)) based on management for a wide range of arable crops (e.g. wheat, barley, maize, sorghum, sunflower, pea, sugar-beet, oilseed rape and miscanthus). Crop-specific modules include approaches for plant growth and development, coupled to a generic soil sub-model.

iii) *DayCent* (Parton et al., 1994) is a biogeochemical model able to simulate crop growth, soil C dynamics, N leaching, gaseous emissions (e.g. N_2O, NO, nitrogen (N_2), NH_3, methane (CH_4) and CO_2) and C fluxes - e.g. net primary production (NPP), net ecosystem exchange (NEE) - in crop fields, grassland, forest, and savanna ecosystems. Also, the model can simulate several management practices (i.e. fertilization, tillage, pruning, cutting, grazing, etc.) as well as specific external disturbances (i.e. fires).

iv) *DNDC* (DeNitrification-DeComposition) (Li et al., 1992a) simulates C and N biogeochemistry in agro-ecosystems. The model predicts crop growth, soil regimes (i.e. temperature and moisture), soil C dynamics, N leaching, and trace gases emissions (e.g. N_2O, NO, N_2, NH_3, CH_4 and CO_2). The model was expanded in 2012 to include biophysical processes in whole-farm systems (Li et al., 2012).

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

vi) *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 CO_2. Moreover, novel algorithms were recently implemented (Izaurralde et al., 2012) to improve the simulation of C and N transformations, gas (O_2, CO_2, and N_2O) and solute (NO_3^-, NO_2^-) movement, and ecosystem C balance and fluxes (Izaurralde et al., 2012).

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

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

ix) *STICS* (Simulateur mulTIdiscplinaire pour les Cultures Standard) (Brisson et al., 1998) is a soil-crop model, which is built on a generic framework for plant description. Within this framework, the selection of adequate options and parameters values allows the simulation of a wide range of plants, from annual crops to perennial grasses or trees. The model simulates plant growth as well as water, C and N fluxes. It allows consideration of the effect of a large range of management options on agronomic (biomass or grain productivity and quality) and environmental (C and N storage, nitrate leaching, N_2O emissions) outputs.

Most of the models included in this review are in active development and use, and this activity can result in a temporal fluidity of model descriptions. The information provided in this section is based on the authors' knowledge of the state of the models at the beginning of the project CN-MIP as well as on published material.

2.2. *Model analysis*

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

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

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

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

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

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

3. Results

3.1. Meteorological variables

Meteorological inputs strongly influence model outputs since they affect plant growth, plant development stages, and soil turnover/balances, including flux exchanges at the soil-plant-atmosphere interface. The number and type of climatic variables required by each model informs us about the relationship between model outputs and climate drivers. In principle, for the modelling of surface reactions and diffusion of volatile products (e.g. N_2O emissions, soil water content dynamics), the higher the resolution in the climate information (e.g. hourly to sub-hourly weather inputs), the more accurate the model response is for short-term processes but the higher the probability that missing data may be present in the weather series used. For longer-term processes such as soil organic carbon (SOC) decomposition, higher temporal resolution data may not improve the accuracy of the model response.

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

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

Relative humidity (daily mean) and global solar radiation are also used by 67% and 56% of the models, respectively. The atmospheric concentration of CO_2 is an optional input for many models (78%), with the exception of CERES-EGC and RothC.

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

3.2. Soil

Similarly to climate inputs, soil characteristics also have a great influence on model outputs. These characteristics strongly influence crop growth and fluxes related to the gaseous biogeochemical cycles as water, C and N. Some soil inputs are assumed as constant values (i.e. parameters), not changing during the simulation. Different soil properties (e.g. texture, pH, bulk density, etc.) can affect plant growth and the environmental conditions for the microbial activity driving the formation and decomposition of SOM and mediating biochemical processes.

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

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

For the transport and transformation of N in the soil profile, most models estimate pools and fluxes of NO_3-N (78%) and/or NH_4-N (89%).

3.3. *Plant ecophysiology and partitioning*

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

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

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

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

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

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

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

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

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

3.4. *GHG emissions and other fluxes*

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

The most important C-fluxes from the ecosystems were considered in the main process called "CO_2". More specifically, they include the gross primary production (GPP), NPP, NEE, the net biome production (NBP) and several types of respiration processes, e.g. ecosystem respiration (RECO), heterotrophic respiration from both soil and grazing animals, and autotrophic respiration.

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

Among all of the models analysed only DNDC is able to simulate all the CO_2 fluxes considered. More than 70% of CO_2-GHG can be simulated also by APSIM, DayCent and PaSim. The CO_2 simulated by the highest number of models (i.e. six models) are NPP, NEE and soil respiration.

The main non-CO_2 fluxes (for simplicity called non CO_2-gas) include CH_4, N_2O, several N emissions (i.e. NH_3, NO_x, N_2) and O_3.

N_2O emissions are most commonly simulated (78%), followed by NH_3 (56%). By contrast, only a few models generate CH_4 and N_2 emission outputs (44%) and NO_x (33%). None of the models provide ozone (O_3) emissions output.

N_2O emissions provided by the models are mostly generated by denitrification and nitrification (78%), mainly based (i.e. >70% of the models) on a soil N pools (e.g. nitrate pool, NH_4 pool) with soil water and temperature acting as main drivers of change on mineral N pools.

Among all models analysed DayCent and DNDC were able to simulate all non CO_2-gas considered in our analysis. However, more than 70% of non CO_2-gas can be simulated also by APSIM, PaSim and CERES-EGC. The non CO_2-GHG simulated by the highest number of models (i.e. seven models) was N_2O. The models able to simulate the highest number of variables (i.e. CH_4, N_2O and N_2) were APSIM, DayCent, DNDC and PaSim.

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

Among the models analysed, only RothC does not take into account any N process. All the remaining models are able to simulate each of the N processes considered in our analysis, with the only exceptions being APSIM, which does not consider NH_3 volatilization, and PaSim and STICS, which only take account of assimilation indirectly (C:N-driven).

3.5. Management

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

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

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

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

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

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

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

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

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

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

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

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

4.1. Model structures and pedo-climatic conditions

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

Concerning soil physical characteristics, a primary role in modelling issues was played by the soil water properties. Errors in the simulation of soil water content (SWC) were the main cause of general discrepancies concerning C and N emissions in many studies (Table 7). Discrepancies in C and N outputs were also observed under specific soil water conditions such as the impact of soil freezing and thawing (Li et al., 2010) or soil shrinking and swelling (Babu et al., 2006). Again, an inappropriate setting of initial state variables determined discrepancies in N emissions (i.e. under- or over-estimation of N_2O emissions peaks, Gabrielle et al., 2006). Considerable overestimations of N_2O emissions were found to be closely related to overestimation of WFPS. WFPS is indeed one of the most important soil variables influencing C and N cycles. For instance, microbially-mediated soil respiration and N cycling processes tend to be higher or lower with increasing soil water content (e.g.

increased nitrification under aerobic conditions, increased denitrification under anaerobic conditions, e.g. Bollmann. As WFPS reaches high values, soil respiration tends to decline and denitrification occurs, resulting in N losses via N_2O and N_2 emissions. This condition was observed especially for DayCent (Stehfest and Muller, 2004, Abdalla et al., 2010, Xing et al., 2011, Ryals et al., 2014, 2015) and DNDC (Saggar et al., 2004, Abdalla et al., 2010). Fast drainage is a particular issue for both the DayCent and DNDC models which drain water in excess of field capacity immediately. This condition makes these models unable to accurately predict N emissions at sites that consistently show soil moisture above FC (e.g. Uzoma et al., 2015).

Soil bulk density (BD) was also a source of modelling error in simulating C and N cycles. For CERES-EGC, Gabrielle et al. (2006) found a discrepancy in N_2O emission peaks due to inappropriate parametrization of soil water retention properties and bulk density from test site to regional scales. Drouet et al. (2011) confirmed that BD was one of the most influential factors for N_2O emissions in CERES-EGC. The effect of BD increase was also reported for DayCent by De Gryze et al. (2010) and Abdalla et al. (2009), respectively, which observed an underestimation of N_2O emissions in a conservation tillage treatment due to the increase in BD, and an associated decrease in pore space over time as DayCent maintains a steady BD and simulation compaction, while the conservation tilled field site resulted in increased BD and reduced N_2O emissions (Pisante et al., 2015). In fact, most of the selected models, with the exception of EPIC, DNDC and STICS, do not simulate soil compaction or loosening, as BD remains constant over time.

Texture was also found to be an influential soil physical characteristic. Congreves et al. (2016) found an underestimation in NH_3 emissions with the DNDC model, which is unable to simulate a heterogeneous soil profile. Similarly, Gagnon et al. (2016) confirmed that DNDC does not effectively discriminate across soil textures to simulate soil CO_2 respiration. Clay concentration affects SOC accumulation in different ways. According to some studies (Nichols, 1984, Burke et al., 1989), SOC increases with increasing clay content due to the bonds between the surface of clay particles and organic matter that retard the decomposition process. 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). The amount of bound enzymes increases with the 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 affect the amount of soil enzymes through reduction in the number of enzyme-producing microorganisms (Inglett et al., 2005). Finally, 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 textured soils is expected due to reduced substrate availability and overall microbial activity.

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

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

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

Nitrification is a two-stage process, performed by different groups of Archaea, bacteria and fungi, consisting in the oxidation of ammonia or ammonium to nitrite (step 1) followed by the oxidation of the nitrite to nitrate (step 2). For DayCent, Li et al. (2005) and Del Grosso et al. (2008) found that overestimation in the nitrification rate was one of the main sources of error for N emissions estimation. This was also found by Drouet et al. (2011), showing that discrepancies in N_2O emissions simulated by CERES-EGC were due to the high sensitivity of the model to the maximum rate of nitrification. The nitrification rate, however, is usually associated with a number of environmental factors including the substrate and oxygen (O_2) concentration, moisture, temperature and pH. For instance, this was observed by Li et al. (2005), who pointed out that poor simulation of NH_4^+ was caused by the inaccurate regulation of the effect of temperature on nitrification in DayCent.

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

Another important source of modelling error resulted from the inaccurate estimation of the immobilization-mineralization processes. N immobilization or mineralization depends on the C:N ratio of the organic materials. The C:N ratio generally tends to decrease as the organic matter becomes more decomposed. Inaccurate C:N parametrization can easily lead to errors in C and N cycle related outputs. For instance, Li et al. (2015) observed for the DSSAT model that differences between the modelled and measured soil C:N ratios led to SOC overestimation. In the EPIC model, He et al. (2006) observed that general discrepancies in C and N dynamics (i.e. lower net N mineralization rate, humification, etc.) were likely due to N mineralization algorithms which may have underpredicted net N mineralization (NMN) observable under field conditions. Smith et al. (2008) and Fitton et al. (2014a, b) found that the underestimation in mineralization rate led to underestimation of N_2O emissions. In the same way, Del Grosso et al. (2010) indicated that overestimation of N_2O emissions was due to N mineralization rates that were too high and too responsive to climate drivers.

Finally, climate conditions influence the C and N outputs in several studies analysed. Some issues were related to how the climate data have been used. For instance, in APSIM, Thorburn et al. (2010) found discrepancies in N emissions (i.e. underestimation of denitrification and N_2O peaks) due to the application of spatially averaged rainfall data instead of the use of specific test-site rainfall data. In other cases, the main issues were due to the sensitivity of the model subroutines. For instance, Wattenbach et al. (2010) observed overestimation in NEE peaks in southern European regions due to issues in coupling water and C-fluxes. These issues were probably caused by the fact that the model was originally developed to represent conditions typical of Northern regions. Again, Lawton et al. (2006)

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

4.2. Model structure and management

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

In the models, fertilization, which influences soil C and N transformations (e.g. acidification following fertilization) and trace gas emissions, was often not well represented (Table 7). For DayCent, Fitton et al. (2014a, b) indicated an underestimation of N_2O emissions due to the low sensitivity of the model at low N application rates. In DNDC, Congreves et al. (2016) found that NH_3 emissions were underestimated due to a simple modelled cascade water flow, which may have limited the ability of the model to simulate slurry infiltration rates. Also, Causarano et al. (2007) observed general discrepancies in C-dynamics (i.e. overestimation of microbial biomass C and total organic C, underestimation of particulate organic C), due to inadequate representation of the effects of tillage and manure in the EPIC model. Another issue related to fertilization was the inability of many models to replicate the effect of specific types of fertilizer. For instance, using DayCent Stehfest and Muller (2004) found overestimation of N_2O emissions under urine application, where N was concentrated in small hotspots. For the same model, Ryals et al. (2014 and 2015) underestimated CO_2 emissions since no soil water benefits were provided by adding compost. This condition was likely due to the lack of increased modelled decomposition because the model was not able to increase soil water contents when compost was added. Gu et al. (2014) overestimated N_2O emissions, soil nitrate and ammonia concentrations due to the inability of DNDC to include canopy interception and foliar N uptake when spraying liquid fertilizer.

Finally, residue management was one of the main weaknesses related to N management (Cavero et al., 1996, Sleutel et al., 2006, Rampazzo Todorovic et al., 2010, Wang et al., 2013). The amount of N applied with residues depends on the quantity of residues and their N concentration. These two factors affect the mineralization-immobilization turnover, whilst their net balance varies with environmental conditions (mainly soil moisture and temperature) and the characteristics of the organic matter (i.e. C:N and the decomposition rate). Since residues directly influence soil C and N processes, residue management in the models resulted in consistent modelling weaknesses. For instance, Justes et al. (2009) underestimated the N mineralization in STICS due to inappropriate parametrization of the model (i.e. default values of the decomposition module were used). In a similar way, Liu et al. (2009) overestimated the SOC content when stubble (wheat and lupine) was applied due to the use of the conventional setting of the stubble retention factor in RothC. Using DayCent and DNDC, Smith et al. (2012) underestimated SOC due to a slight overestimation of residue removal impact. However, the authors indicated that this could have been partly due to the inherent variability in SOC measurements. Smith et al. (2012) also found that DNDC tended to underestimate the rate of SOC change as affected by residue removal at some sites. Using DSSAT, Hartkamp et al. (2004) overestimated SOC in the crop rotations with N fertilization. This overestimation was due to inaccurate initial SOC (i.e. overestimated SOC values) which was related to an overestimation of the biomass incorporated into the soil. Similarly, Wang et al. (2005) underestimated the SOC content using the EPIC model due to a structural error in underestimating the return of corn residues. He et al. (2006) found general discrepancies in C and N dynamics because the EPIC model underestimated the capacity of the soil to transform crop residues into SOM.

Tillage is one of the agricultural practices most commonly simulated by the models and an issue in most modelling applications. The use of tillage or reduced tillage can greatly affect soil properties, and since the models do not adjust some soil properties overtime (such as bulk density) which results in inaccuracies in simulations. Compared with conventional tillage, no/reduced tillage may lead to increasing rather than decreasing emissions (e.g. due to higher density and WFPS, more SOM near the soil surface thus higher denitrification potential, tendency to acidification and thus lower reduction of N_2O to N_2, etc.). Identifying mechanisms which help understand simulate emissions with no tillage is thus a key issue. In our analysis management effects (i.e. tillage) which influences topsoil erosion emerged as a point of weakness. This is because many models do not take into account adequately C-losses due to erosion. For instance, Nieto et al. (2010, 2013) overestimated SOC content using RothC, whilst Billen et al. (2009) observed general discrepancies in SOC content with EPIC.

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

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

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

4.3. *Time-scale*

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

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

Concerning time-scale weaknesses, Xing et al. (2011) underestimated N_2O emissions at the daily time step using APSIM, while the use of the hourly time step may have likely improved the estimate of predicted total daily emissions. This is because, in the APSIM model, as in most models, N_2O emissions were released immediately to the atmosphere without delay upon change in environmental conditions whereas the observations indicated that there was a 1-10 hour lag between peaks of soil moisture and gaseous emissions. Similarly, Lehuger et al. (2011) using CERES-EGC indicated an overestimation in N_2O emissions, probably due to a possible time lag between the production of gaseous N_2O in the soil and its emission to the atmosphere. Also, several studies carried out using DayCent (Parton et al., 2001, Del Grosso et al., 2005, 2010) observed some discrepancies in simulated N emissions due to time-lag. This was found to agree with the results of Li et al. (2005), which indicated that DayCent often has a 1-day lag before emissions occur. In all these cases, the use of hourly time step may result in better predictions especially in conjunction with the addition of a description of gas diffusion into soil, which could result in a delay between N_2O production and emission.

Concerning spatial-scale weaknesses, Gabrielle et al. (2006) found discrepancies in N_2O emission peaks using CERES-EGC. This was probably due to soil property parametrization (i.e. soil water retention properties and bulk density) which may have led to differences in N outputs from test sites to the regional scale. Using EPIC, general discrepancies in C-fluxes (i.e. overestimation of microbial biomass C and total organic C, underestimation of particulate organic C) were likely caused by spatial differences in C fraction due to differing soil landscapes (Calanca et al., 2007). Schnebelen et al. (2004) overestimated soil N absorption with the STICS model. This was probably due to propagation of errors for continuous simulations compared to single-year simulations. More specifically, the underestimation of some parameters in the previous year may have led to errors in the following years.

5. New developments/future perspectives

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

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

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

Even in models with explicit SMB, microbial community is usually simulated with one or few pools, each representing microorganisms belonging to a different functional group (Moorhead and Sinsabaugh, 2006). However, further model developments could be achieved if diversity in soil microbial traits is included in the model, allowing microorganisms with optimal strategies to outperform other microorganisms with less favorable traits in a given environment (Allison et al., 2012, 2014). In such models, genomic and metagenomics data can be integrated with other sources of information to define distributions of microbial traits that are used to characterize the microbial community (Vereeken et al., 2016).

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

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

Another mechanism of CUE regulation by SMB when SOM decomposition is N-limited is overflow metabolism (Russel and Cook, 1995): excess C is excreted as extracellular C compounds (like polysaccharides) (Hadas et al., 1998, Cavalli et al., 2016), or lost as CO_2 (Schimel and Weintraub, 2003, Neill and Gignoux, 2006). Conversely, when N is in excess relative to C (decomposition is limited by C availability), net N mineralisation occurs. Models usually implement N deficit effects on SOM decomposition with the N inhibition hypothesis (Manzoni and Porporato, 2009), that is, SOM turnover is reduced according to N availability, and thus CUE does not change. Alternatively, other models (Izaurralde et al., 2006, Withmore, 2007) allow SMB to vary its C to N ratio according to stoichiometric imbalances, and thus they consider SMB as non-homeostatic.

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

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

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

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

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

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

6. Summary and concluding remarks

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

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

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

The major limitations of model structure related to C-cycles were observed under management practices (43.6%), whilst for the scale of application the major weaknesses were due to different pedo-climatic conditions (11.5%). 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).

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

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.

Although different avenues could be considered to improve models (e.g. Coucheney et al., 2015), mainly depending on the purpose of modelling, to overcome the reported limitations and account for the effect of multiple disturbances (i.e. pedo-climatic conditions, management practices, scale of analysis) affecting basic processes, as well as to simplify the decision of which model to choose to understand mechanistically specific study-contexts and to make detailed predictions in a large diversity of situations, some innovative aspects should be considered in the modelling work. Among these, we target the representation of SOM turnover driven by SMB, the effect of N shortage on SOM decomposition, improvement related to the production and consumption of gases (O_2, CO_2, CH_4, N_2O, and N_2), adequate simulations of gas transport in soil, the use of a 3D soil structure in order to achieve a more realistic representation of environmental effects (soil temperature and moisture), especially in the context of climate change.

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

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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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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 (46.2%), followed by limitations in the algorithms simulating the effects of management practices (33.1%). The multiplicity of scales in both time and space is a fundamental feature, which explains the remaining weaknesses (i.e. 20.7%). 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.

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

1. Introduction

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

Process-based ecosystem models take the approach of simulating underlying biogeochemical processes, such as plant photosynthesis and respiration, using mathematical equations that determine the allocation of C from atmospheric CO_2 into biomass down to the soil organic matter (SOM). A relatively complete suite of biogeochemical processes (e.g. plant growth, organic matter decomposition, fermentation, ammonia volatilisation, nitrification and denitrification) is generally embedded in these models, enabling computation of transport and transformations in plant–soil ecosystems. Sub-models are designed to interact with each other to describe cycles of water, C and N for target ecosystems, thus any change in the environmental factors collectively affect a group of biogeochemical reactions. Extensively tested biogeochemical models (with the coupled C-N cycling) are effective tools for examining the magnitude and spatial-temporal patterns of C and N fluxes, and play an important role in designing specific policies appropriate to the soils, climate, and agricultural conditions of a location or region. However, results of state-of the-art terrestrial biogeochemical models, describing the contribution of agricultural systems to C sequestration and GHG source/sink status, may diverge significantly. Such differences between model results are often attributed to physical and biogeochemical processes being inadequately resolved and, for these models, the improvement of algorithms and structure is recommended beyond parameter optimization (Tian et al., 2011, Lu and Tian, 2013).

It is the goal of this paper to examine the strengths and weaknesses of nine crop and grassland models that incorporate C and N fluxes into biogeochemical frameworks and fully assess C and GHG dynamics in agricultural soils. These models are commonly applied worldwide and are used to simulate biogeochemical and related outputs by the 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.faccejpi.com), which brings together 10 organizations from six countries. With this analysis we are not arguing against the quality of models. While highlighting weaknesses and limits of current modelling approaches as documented in several published studies, we intend to offer a general overview as a basis for new ways of improvement current modelling approaches.

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

2. Modelling approaches

2.1. Basic model assumptions

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

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

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

2.2. The CN-MIP models

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

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

ii) *CERES-EGC* (Crop Environment REsource Synthesis - Environnement et Grandes Cultures) (Gabrielle et al., 1995) simulates the biogeochemical cycles of water, C and N in agro-ecosystems. The model predicts crop production and the environmental impacts related to the agriculture activity (e.g. N_2O, NO, NH_3, CO_2, NO_3) based on management for a wide range of arable crops (e.g. wheat, barley, maize, sorghum, sunflower, pea, sugar-beet, oilseed rape and miscantus). Crop-specific modules include approaches for plant growth and development, coupled to a generic soil sub-model.

iii) *DayCent* (Parton et al., 1994) is a biogeochemical model able to simulate crop growth, soil C dynamics, N leaching, gaseous emissions (e.g. N_2O, NO, N_2, NH_3, CH_4 and CO_2) and C fluxes (e.g. NPP, NEE) in crop fields, grasslands, forests, and savanna ecosystems. The model allows to simulate also several management practices (i.e. fertilization, tillage, pruning, cutting, grazing, etc.) as well as specific external disturbances (i.e. fires).

iv) *DNDC* (DeNitrification-DeComposition) (Li et al., 1992a) simulates C and N biogeochemistry in agro-ecosystems. The model predicts crop growth, soil regimes (i.e. temperature and moisture), soil C dynamics, N leaching, and trace gases emissions (e.g. N_2O, NO, N_2, NH_3, CH_4 and CO_2). The model was expanded in 2012 to include biophysical processes in whole-farm systems (Li et al., 2012).

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

vi) *EPIC* (Environmental Policy Integrated Climate) (Williams, 1995) can simulate about 80 crops through its crop growth model which uses unique parameter values for each crop. It can predict changes in soil, water, nutrient, pesticide movements, and crop yields due to effects of management decisions. Moreover, it can also assess water quality, N and C cycling, climate change impacts, and the effects of atmospheric CO_2.

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

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

ix) *STICS* (Simulateur mulTIdiscplinaire pour les Cultures Standard) (Brisson et al., 1998) is a soil-crop model which is built on a generic framework for plant description. Within this framework, the selection of adequate options and parameters values allows to simulate a wide range of plants, from annual crops to perennial grasses or trees. The model simulates plant growth as well as water, C and N fluxes. It allows to consider the effect of a large range of management options on agronomic (biomass or grain productivity and quality) and environmental (C and N storage, nitrate leaching, N_2O emissions) outputs.

3. Results

3.1. Model analysis

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

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

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

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

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

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

3.1.1. Meteorological variables

Meteorological inputs strongly influence model outputs since they affect plant growth, plant development stages, and soil turnover/balances, including flux exchanges at the soil-plant-atmosphere interface. The number and type of climatic variables required by each model informs us about the relationship between model outputs and climate drivers. In principle, for the modelling of surface reactions and diffusion of volatile products (e.g. N_2O emissions, soil water content dynamics), the higher the resolution in the climate information (e.g. hourly to sub-hourly weather inputs), the more accurate the model response is for short-term processes but the higher the probability that missing data may be present in the weather series used. For longer term processes such as soil organic carbon (SOC) decomposition, higher temporal resolution data may not improve the accuracy of the model response.

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

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

Relative humidity (daily mean) and global solar radiation are also used by 67% and 56% of the models, respectively. The atmospheric concentration of CO_2 is an optional input for many models (78%), with the exception of CERES-EGC and RothC.

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

3.1.2. Soil

Similarly to climate inputs, soil characteristics also have a great influence on model outputs. These characteristics strongly influence crop growth and fluxes related to the gaseous biogeochemical cycles as water, C and N. Some soil inputs are assumed as constant values (i.e. parameters), not changing during the simulation. Different soil properties (e.g. texture, pH, bulk density, etc.) can affect plant growth and the environmental conditions for the microbial activity driving the formation and decomposition of SOM and mediating biochemical processes.

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

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

For the transport and transformation of N in soil profile, most models estimate pools and fluxes of NO_3-N (78%) or/and NH_4-N (89%).

3.1.3. Plant ecophysiology and partitioning

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

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

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

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

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

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

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

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

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

3.1.4. GHG emissions and other fluxes

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

In general from our analysis 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.

In the main process called CO_2-GHG the most important C-fluxes from the ecosystems were considered. More specifically, they include the Gross Primary Production (GPP), the Net Primary Production (NPP), the Net Ecosystem Exchange (NEE), the Net Biome Production (NBP) and several types of respiration processes (i.e. Ecosystem respiration or RECO), heterotrophic respiration from both soil and grazing animals, and autotrophic respiration.

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

Among all of the models analysed only DNDC is able to simulate all the CO_2-GHG fluxes considered. More than 70% of CO_2-GHG can be simulated also by APSIM, DayCent and PaSim. The CO_2-GHG simulated by the highest number of models (i.e. six models) are NPP, NEE and soil respiration.

The main non-CO_2 fluxes (for simplicity called Non CO_2-GHG) include CH_4, N_2O, several N emissions (i.e. NH_3, NO_x, N_2) and O_3.

N_2O emissions are most commonly simulated (78%), followed by NH_3 (56%). By contrast, only a few models generate CH_4 and N_2 emission outputs (44%) and NO_x (33%). None of the models provide O_3 emissions output.

N_2O emissions provided by the models are mostly generated by denitrification and nitrification (78%), mainly based (i.e. >70% of the models) on a soil N pools (e.g. nitrate pool, NH_4 pool) with soil water and temperature acting as main drivers of change on mineral N pools.

Among all models analysed DayCent and DNDC were able to simulate all non CO_2-GHG considered in our analysis. However, more than 70% of non CO_2-GHG can be simulated also by APSIM, PaSim and CERES-EGC. The non CO_2-GHG simulated by the highest number of models (i.e. seven models) was N_2O. The models able to simulate the highest number of variables (i.e. CH_4, N_2O and N_2) were APSIM, DayCent, DNDC and PaSim.

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

Among the models analysed, only RothC does not take into account any N process. All the remaining models are able to simulate each of the N processes considered in our analysis, with the only exceptions being APSIM, which does not consider NH_3 volatilization, and PaSim and STICS, which only take account of assimilation indirectly (C:N-driven).

3.1.5. Management

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

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

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

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

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

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

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

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

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

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

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

Several types of weaknesses emerged in 94 modelling studies (Tab. 6), where criticalities in assessing the impact of pedo-climatic conditions (46.2%) and management practices (33.1%) on environmental variables are reflected in unsatisfactory model performances. These latter were mostly related to limitations of model structure with respect to difficulties of the algorithms in simulating the effects of different management practices on C and N cycling. By contrast, only a few weaknesses were due to the scale of application, strictly related to the high variability in time and space of C and N cycles (16.5% and 4.2% for pedo-climatic conditions and management practices, respectively). For the C cycle, major limitations of model structure were related to management practices (43.4%), whilst for the scale of application, the major weaknesses were due to different pedo-climatic conditions (11.8%). For the N cycle, however, limitations inherent in model structure were predominant under different pedo-climatic conditions (51.7%), whilst for the scale of application, major weaknesses were due to different pedo-climatic conditions (20.4%).

4.1. Model structures and pedo-climatic conditions

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

Concerning soil physical characteristics, a primary role in modelling issues was played by the soil water properties. Errors in the simulation of soil water content (SWC) were the main cause of general discrepancies concerning C and N emissions in many studies (Tab. 7). Discrepancies in C and N outputs were also observed under specific soil water conditions such as the impact of soil freezing and thawing (Li et al., 2010) or soil shrinking and swelling (Babu et al., 2006). Again, an inappropriate setting of initial state variables determined discrepancies in N emissions (i.e. under- overestimation of N_2O emissions peaks, Gabrielle et al., 2006). Considerable overestimations of N_2O emissions were found to be closely related to overestimation of water-filled pore space (WFPS). WFPS is indeed one of the most important soil variables influencing C and N cycles. For instance, microbially-mediated soil respiration and N cycling processes tend to be higher or lower with increasing soil water content (e.g. increased nitrification under aerobic conditions, increased denitrification under anaerobic conditions, e.g. Bollmann, 1988). As WFPS reaches high values, soil respiration tends to decline and denitrification occurs, resulting in N losses via N_2O and N_2 emissions. This condition was observed especially for DayCent (Stehfest and Muller, 2004, Abdalla et al., 2010, Xing et al., 2011, Ryals et al., 2014, 2015) and DNDC (Saggar et al., 2004, Abdalla et al., 2010). Fast drainage is a particular issue for both the DayCent and DNDC models which drain water in excess of field capacity immediately. This condition makes these models unable to accurately predict N emissions at sites that consistently show soil moisture above FC (e.g. Uzoma et al., 2015).

Soil bulk density (BD) was also a source of modelling error in simulating C and N cycles. For CERES-EGC, Gabrielle et al. (2006) found a discrepancy in N_2O emission peaks due to inappropriate parametrization of soil water retention properties and bulk density from test site to regional scales. Drouet et al. (2011) confirmed that BD was one of the most influential factors for N_2O emissions in CERES-EGC. The effect of BD increase was also reported for DayCent by De Gryze et al. (2010) and Abdalla et al. (2009), respectively, which observed an underestimation of N_2O emissions in a conservation tillage treatment due to the increase in BD, and an associated decrease in pore space over time as DayCent maintains a steady BD and simulation compaction, while the conservation tilled field site resulted in increased BD and reduced N2O emissions (Pisante et al, 2015). In fact, most of the selected models, with the exception of EPIC, DNDC and STICS, do not simulate soil compaction or loosening, as BD remains constant over time.

Texture was also found to be an influential soil physical characteristic. Congreves et al. (2016) found an underestimation in NH_3 emissions with the DNDC model, which is unable to simulate a heterogeneous soil profile. Similarly, Gagnon et al. (2016) confirmed that DNDC does not effectively discriminate across soil textures to simulate soil CO_2 respiration. Clay concentration affects SOC accumulation in different ways. According to some studies (Nichols, 1984, Burke et al., 1989), SOC increases with increasing clay content due to the bonds between the surface of clay particles and organic matter that retard the decomposition process. Also, 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). However, a recent study (Gregorich et al., 2016) indicated that only temperature (not soil texture or other soil properties) was a driver of decomposition for 10 sites in Canada (^{13}C-labelled study), thus suggesting as the effect of texture on SOC decomposition is controversial. Furthermore, texture parametrization is another possible source of error. For instance, Gijsman et al. (2002) indicated that inaccuracies in soil texture data used as inputs may have affected soil retention characteristics, thus resulting in discrepancies in SOC and soil mineral N dynamics.

Soil chemical processes are generally similar between the models and all models considered showed difficulty in reproducing the observed C and N cycles. The processes influencing soil organic matter (SOM) in the models include nitrification, denitrification, immobilization and mineralization.

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

Nitrification is a two-stage process, performed by different groups of Archaea, consisting in the oxidation of ammonia or ammonium to nitrite (step 1) followed by the oxidation of the nitrite to nitrate (step 2). For DayCent, Li et al. (2005) and Del Grosso et al. (2008) found that overestimation in the nitrification rate was one of the main sources of error for N emissions estimation. This was also found by Drouet et al. (2011), showing that discrepancies in N_2O emissions simulated by CERES-EGC were due to the high sensitivity of the model to the maximum rate of nitrification. The nitrification rate, however, is usually associated with a number of environmental factors including the substrate and oxygen concentration, temperature and pH. For instance, this was observed by Li et al. (2005), who pointed out that poor simulation of NH_4^+ was caused by the inaccurate regulation of the effect of temperature on nitrification in DayCent.

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

Another important source of modelling error resulted from the inaccurate estimation of the immobilization-mineralization processes. In the EPIC model, He et al. (2006) observed that general discrepancies in C and N dynamics (i.e. lower net N mineralization rate, humification, etc.) were likely due to N mineralization algorithms which may have underpredicted net N mineralization (NMN) observable under field conditions. Smith et al. (2008) and Fitton et al. (2014a, 2014b) found that the underestimation in mineralization rate led to underestimation of N_2O emissions. In the same way, Del Grosso et al. (2010) indicated that overestimation of N_2O emissions was due to N mineralization rates that were too high and too responsive to climate drivers. Nitrogen immobilization or mineralization depends on the C/N ratio of the plant residues. The C/N ratio generally tends to decrease as the organic matter becomes more decomposed. Erroneous C/N parametrization can easily lead to errors in C and N cycle related outputs. For instance, Li et al. (2015) observed for the DSSAT model that differences between the modelled and measured soil C/N ratio led to SOC overestimation.

Finally, climate conditions influence the C and N outputs in several studies analysed. Some issues were related to how the climate data have been used. For instance, in APSIM, Thorburn et al. (2010) found discrepancies in N emissions (i.e. underestimation of denitrification and N_2O peaks) due to the application of spatially averaged rainfall data instead of the use of specific test-site rainfall data. In other cases, the main issues were due to the sensitivity of the models subroutines. For instance, Wattenbach et al. (2010) observed overestimation in NEE peaks in southern European regions due to issues in coupling water and C-fluxes. These issues were probably caused by the fact the model was developed for Northern regions. Again, Lawton et al. (2006) reported overestimation of NEE because of the oversensitivity of PaSim to initial conditions/winter conditions. Most of the issues related to general discrepancies in simulated C and N cycles, however, were related to precipitation only (Stehfest and Muller, 2004, Jarecki et al., 2008, De Gyrze et al., 2010, Ludwig et al., 2011, Lehuger et al., 2014). Precipitation and the resulting soil water dynamics strongly influence N cycling in terrestrial ecosystems since it affects both physical transport and N biological transformations by soil microorganisms (Brooks et al., 1999, Corre et al., 2002, Aranibar et al., 2004).

4.2. Model structure and management

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

In the models, fertilization, which influences soil C and N transformations (e.g. acidification following fertilization) and trace gas emissions, was often not well represented (Tab. 7). For DayCent, Fitton et al. (2014a, b) indicated an underestimation of N_2O emissions due to the low sensitivity of the model at low N application rates. In DNDC, Congreves et al. (2016) found that NH_3 emissions were underestimated due to a simple modelled cascade water flow, which may have limited the ability of the model to simulate slurry infiltration rates. Also, Causarano et al. (2007) observed general discrepancies in C-dynamics (i.e. overestimation of microbial biomass C and total organic C, underestimation of particulate organic C), due to inadequate representation of the effects of tillage and manure in the EPIC model. Another issue related to fertilization was the inability of many models to replicate the effect of specific types of fertilizer. For instance, using DayCent Stehfest and Muller (2004) found overestimation of N_2O emissions under urine application, where N was concentrated in small hotspots. For the same model, Ryals et al. (2014 and 2015) underestimated CO_2 emissions since no soil water benefits were provided by adding compost. This condition was likely due to the lack of increased modelled decomposition because the model was not able to increase soil water contents when compost was added. Gu et al. (2014) overestimated N_2O emissions, soil nitrate and ammonia concentrations due to the inability of DNDC to include canopy interception and foliar N uptake when spraying liquid fertilizer.

Finally, residue management was one of the main weaknesses related to N management (Cavero et al., 1996, Sleutel et al., 2006, Rampazzo Todorovic et al., 2010, Wang et al., 2013). The amount of N applied with residues depends on the quantity of residues and their N concentration. These two factors affect the mineralization-immobilization turnover, whilst their net balance varies with environmental conditions (mainly soil moisture and temperature) and the characteristics of the OM (i.e. C:N and the decomposition rate). Since residues directly influence soil C and N processes, residue management in the models resulted in consistent modelling weaknesses. For instance, Justes et al. (2009) underestimated the N mineralization in STICS due to inappropriate parametrization of the model (i.e. default values of the decomposition module were used). In a similar way, Liu et al. (2009) overestimated the SOC content when stubble (wheat and lupine) was applied due to the use of the conventional setting of the stubble retention factor in RothC. Using DayCent and DNDC, Smith et al. (2012) underestimated SOC due to a slight overestimation of residue removal impact. However, the authors indicated that this could have been partly due to the inherent variability in SOC measurements. Smith et al. (2012) also found that DNDC tended to underestimate the rate of SOC change as affected by residue removal at some sites. Using DSSAT, Hartkamp et al. (2004) overestimated SOC in the crop rotations with N fertilization. This overestimation was due to inaccurate initial SOC (i.e. overestimated SOC values) which was related to an overestimation of the biomass incorporated into the soil. Similarly, Wang et al. (2005) underestimated the SOC content using the EPIC model due to a structural error in underestimating the return of corn residues. He et al. (2006) found general discrepancies in C and N dynamics due to underestimation of the soil capacity to transform crop residue in SOC.

Tillage is one of the agricultural practices most commonly simulated by the models and an issue in most modelling applications. The use of tillage or reduced tillage can greatly affect soil properties, and since the models don’t adjust some soil properties overtime (such as bulk density) which results in inaccuracies in simulations. Also, the use of tillage or no/reduced tillage may lead to increasing rather than decreasing emissions (e.g. due to higher density and WFPS, more SOM near the soil surface thus higher denitrification potential, tendency to acidification and thus lower reduction of N_2O to N_2, etc.). Identifying mechanisms which help understand simulate emissions with no tillage is thus a key issue. In our analysis management effects (i.e. tillage) which influences topsoil erosion emerged as a point of weakness. This is because many models do not take into account adequately C-losses due to erosion. For instance, Nieto et al. (2010, 2013) overestimated SOC content using RothC, whilst Billen et al. (2009) observed general discrepancies in SOC content with EPIC.

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

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

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

4.3. Time-scale

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

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

Concerning time-scale weaknesses, Xing et al. (2011) underestimated N_2O emissions at the daily time step using APSIM, while the use of the hourly time step may have likely improved the estimate of predicted total daily emissions. This is because, in the APSIM model, as in most models, N_2O emissions were released immediately to the atmosphere without delay upon change in environmental conditions whereas the observations indicated that there was a 1-10 hour lag between peaks of soil moisture and gaseous emissions. Similarly, Lehuger et al. (2011) using CERES-EGC indicated an overestimation in N_2O emissions, probably due to a possible time lag between the production of gaseous N_2O in the soil and its emission to the atmosphere. Also, several studies carried out using DayCent (Parton et al., 2001, Del Grosso et al., 2005, 2010) observed some discrepancies in simulated N emissions due to time-lag. This was found to agree with Li et al. (2005), which indicated that DayCent often has a 1 day lag before emissions occur. In all these cases, the use of hourly time step may result in better predictions especially in conjunction with the addition of a description of gas diffusion into soil which could result in a delay between N_2O production and emission.

Concerning spatial-scale weaknesses, Gabrielle et al. (2006) found discrepancies in N_2O emission peaks using CERES-EGC. This was probably due to soil property parametrization (i.e. soil water retention properties and bulk density) which may have led to differences in N outputs from test sites to the regional scale. Using EPIC, general discrepancies in C-fluxes (i.e. overestimation of microbial biomass C and total organic C, underestimation of particulate organic C) were likely caused by spatial differences in C fraction due to differing soil landscapes (Calanca et al., 2007). Schnebelen et al. (2004) overestimated soil N absorption with the STICS model. This was probably due to propagation of errors for continuous simulations compared to single-year simulations. More specifically, the underestimation of some parameters in the previous year may have led to errors in the following years.

5. New developments/future perspectives

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

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

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

Another important aspect regarding SOM turnover is the effect of N shortage on SOM decomposition. Soil microorganisms are characterised by a narrow range of variation in their C to N ratio (Cleveland and Liptzin, 2007, Xu et al., 2013); thus, they can be approximately considered homeostatic (i.e. they do not change markedly their C to N ratio according to substrate C to N ratio). Mechanisms of adaptation to stoichiometric imbalances between substrates and SMB were reviewed in detail by Mooshammer et al. (2014a). One postulated mechanism of adaptation regards the variation of microbial C use efficiency (CUE, defined as the ratio between newly-formed biomass C and decomposed C) and of N use efficiency (NUE, defined similarly to CUE) to accommodate for excess or deficit of C or N (Manzoni et al., 2012, Sinsabaugh et al., 2013, Mooshammer et al., 2014b). According to this hypothesis, when decomposition is N-limited, excess C is lost through overflow metabolism (Russel and Cook, 1995), either with the synthesis of extracellular C compounds (as polysaccharides) (Hadas et al., 1998, Cavalli et al., 2016), or as CO_2 (Schimel and Weintraub, 2003, Neill and Gignoux, 2006). Conversely, when N is in excess (decomposition is limited by C availability), net N mineralisation occurs. Models usually implement N deficit effects on SOM decomposition with the N inhibition hypothesis (Manzoni and Porporato, 2009), that is, SOM turnover is reduced according to N availability, and thus CUE does not change. Alternatively, other models (Izaurralde et al., 2006, Withmore, 2007) allow SMB to vary its C to N ratio according to stoichiometric imbalances, and thus they consider SMB as non-homeostatic.

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

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

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

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

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

6. Summary and concluding remarks

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

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

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

The major limitations of model structure related to C-cycles were observed under management practices (43.4%), whilst for the scale of application the major weaknesses were due to different pedo-climatic conditions (11.8%). 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%).

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

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. Although different avenues could be considered to improve models (e.g. Coucheney et al., 2015), mainly depending on the purpose of modelling, to overcome the reported limitations and account for the effect of multiple disturbances (i.e. pedo-climatic conditions, management practices, scale of analysis) affecting basic processes, as well as to simplify the decision of which model to choose to understand mechanistically specific study-contexts and to make detailed predictions in a large diversity of situations, some innovative aspects should be considered in the modelling work. Among these, we target the representation of SOM turnover driven by SMB, the effect of N shortage on SOM decomposition, improvement related to the production and consumption of gases (O_2, CO_2, CH_4, N_2O, and N_2), adequate simulations of gas transport in soil, the use of a 3D soil structure in order to achieve a more realistic representation of environmental effects (soil temperature and moisture), especially in the context of climate change.

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

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Table
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Tables

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. European Journal of Agronomy 18, 267-288. ; Holzworth DP, Huth NI, et al. (2014) APSIM – Evolution towards a new generation of agricultural systems simulation. Environmental Modelling & Software 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. Soil Science Society Of America Journal 59, 1402-1411; Gabrielle et al., 1996. Analysis and field evaluation of the CERES models' soil components: Nitrogen transfer and transformations. Soil Science Society of America Journal 60, 142-149; Gabrielle et al., 1998. Development and evaluation of a CERES-type model for winter oilseed rape. Field Crops Research 57, 95-111; Gabrielle et al., 1998. A model of leaf area development and senescence for winter oilseed rape. Field Crops Research 57, 209-222; Hénault et al., 2005. Predicting in situ soil N_2O emissions using NOE algorithm and soil data base. Global Change Biology 11, 115-127, 2005
DayCent	DaycCent 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: Quantitative modeling of soil forming processes, SSSA Spec. Public. No. 39. Madison, WI, USA; Parton et al., 2001. Generalized model for NO_x and N_2O emissions from soils. Journal of Geophysical Research 106(D15), 17403-17419. doi:10.1029/2001JD900101. Del Grosso et al., 2000. General model for N_2O and N_2 gas emissions from soils due to denitrification. Global Biogeochemical Cycles 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. Environmental Pollution 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. Nutrient Cycling in Agroecosystems 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. Nutrient Cycling in Agroecosystems 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. European Journal of Agronomy 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. Computers and Electronics In Agriculture 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. Field Crops Research 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.), Computer Models of Watershed Hydrology, 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. Environmental Modelling & Software 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) Evaluation of soil organic matter models using existing, long-term datasets. 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. Geoderma 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. Agronomie 18, 311–346; Brisson et al., 2003. An overview of the crop model STICS. European Journal of Agronomy 18, 309–332; Brisson et al., 2009. Conceptual basis, formalizations and parameterization of the STICS crop model, ed. Quae, 297 pp.; Coucheney 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. Environmental Modelling & Software 64, 177–190. doi:10.1016/j.envsoft.2014.11.024

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

General Classes (Lev.1)		**% of models able to simulate at least 1 Main process contained within each General Class**		
Name of Class	*N° of Main Processes contained within each General Class*	*Able (%)*	*Not able (%)*	*N.A **
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	- - -

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

Main Processes (Lev.2)		% of models able to simulate at least 1 methods, options or components contained within each Main Processes		
Name of the Main Processes	*N° of methods, options or components contained within each Main Processes*	*Able (%)*	*Not able (%)*	*N.A **
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	- - -

Table 3 – Level 2 of compositional sub-systems: the main processes identified within each general class, the number of methods, options or components contained within each main processes and the percentage of models able to simulate at least 1 methods, options or components contained within each main processes. * No information is available. Numbers in brackets represents specific information 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_2O 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_2O 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

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

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

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

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

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

	France	Arable	C-N	O	*Justes et al. (2009)*
	France	Arable	N	O	*Jego et al. (2012)*
	France	Arable	N	O	*Constantin et al. (2012)*

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

			N° of weaknesses per each model				% of weaknesses per each model			
			C-Cycle		N-Cycle		C-Cycle		N-Cycle	
Model	N° of Ref.	Factor of weaknesses	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	*Snow et al. (1999)*	Pedo-climatic	**0**	**0**	**1**	**0**	Underestimation of soil N supply	Soil properties (C)	Modelling HUM decomposition too slow
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Thorburn et al. (2010)	Pedo-climatic	**0**	**0**	**1**	**0**	General discrepancies (Underestimation of Denitrification, Unpredicted N_2O 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**	- - - -	- - - -	- - - -
	Sharp et al. (2011)	Pedo-climatic	**0**	**0**	**1**	**0**	Overestimation of annual leaching	Soil properties (N)	Overestimation of soil solution nitrate concentration
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Xing et al. (2011)	Pedo-climatic	**0**	**0**	**1**	**1**	Underestimation of N_2O 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**	- - - -	- - - -	- - - -
	Luo et al. (2011)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		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.
	Giltrap et al. (2015)	Pedo-climatic	**0**	**0**	**1**	**0**	Under/Overestimation of N_2O emissions	Soil properties (general) - Climate	Average field soil properties used for running the model rather than specific values
		Management	**0**	**0**	**1**	**0**		Management (Fertilization)	Fertilization type: urine patches is much more extreme than typical fertilization as NH_4^+
CERES-EGC	*Gabrielle et al. (2006)*	Pedo-climatic	**0**	**0**	**0**	**1**	Under/Overestimation of N_2O 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
	Lamboni et al. (2009)	Pedo-climatic	**0**	**0**	**1**	**0**	General discrepancies (N_2O emissions)	Soil properties (N)	Sensitivity of N_2O emissions: Denitrification, Potential denitrification rate, Fraction of denitrified N.
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Wattenbach et al. (2010)	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
	Drouet et al. (2011)	Pedo-climatic	**0**	**0**	**1**	**0**	General discrepancies (N_2O emissions)	Soil properties (N - BD)	Sensitivity of N_2O emissions: N_2O emissions from denitrification; Max. rate of nitrification, Soil Bulk Density
		Management	**0**	**0**	**1**	**0**		Management (Crop type)	Sensitivity of N_2O emissions: Cropland area (crop variety and management)
	Lehuger et al. (2011)	Pedo-climatic	**0**	**0**	**1**	**1**	Overestimation of N_2O emissions	Soil properties (N)	N_2O emission peak was produced in response of the high ammonium content in topsoil - Possible time lag in N_2O emissions
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Goglio et al. (2013)	Pedo-climatic	**0**	**0**	**1**	**0**	Underestimation of N_2O emissions peaks	Climate	Inter-annual variability
		Management	**0**	**0**	**1**	**0**		Management (Fertilization - water conservation)	Legumes incorporation and mulching
	Lehuger et al. (2014)	Pedo-climatic	**0**	**0**	**1**	**0**	General discrepancies (N_2O emissions)	Climate (Rainfall)	Rainfall
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Noirot-Cosson (2016)	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	*Parton et al. (2001)*	Pedo-climatic	**0**	**0**	**1**	**1**	General discrepancies (N_2O 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
	Stehfest and Muller (2004)	Pedo-climatic	**0**	**0**	**1**	**0**	Overestimation of N_2O 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
	Del Grosso et al. (2005)	Pedo-climatic	**0**	**0**	**1**	**1**	General discrepancies (N_2O emissions)	Soil properties (general) - Climate	Soil properties
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Li et al. (2005)	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**	- - - -	- - - -	- - - -
	Smith et al. (2008)	Pedo-climatic	**0**	**0**	**1**	**1**	Underestimation of N_2O emissions	Soil properties (N - SWD)	Under prediction of Mineralization and soil properties (SWC, soil N and soil ammonium)
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Jarecki et al. (2008)	Pedo-climatic	**0**	**0**	**1**	**0**	Underestimation of N_2O emissions	Soil properties (N - SWD) - Climate	Soil properties (inorganic N, soil moisture) - Rainfall
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Del Grosso et al. (2008)	Pedo-climatic	**0**	**0**	**1**	**1**	Overestimation of N_2O emissions	Soil properties (N)	Nitrification rates too high, NO_3 too low, N_2O too high.
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	David et al. (2009)	Pedo-climatic	**0**	**0**	**1**	**1**	Overestimation of N_2O emissions	Soil properties (general)	Crop evapotranspiration and the impact of tile drainage
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Li et al. (2010)	Pedo-climatic	**1**	**0**	**1**	**0**	General discrepancies (CO_2, N mineralization and Nitrification)	Soil properties (SWD)	Soil moisture
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Abdalla et al. (2010)	Pedo-climatic	**0**	**0**	**1**	**0**	General discrepancies (Overestimation N_2O emissions, underestimation N_2O 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.
	Del Grosso et al. (2010)	Pedo-climatic	**0**	**0**	**1**	**1**	Overestimation of N_2O 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
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	De Gyrze et al. (2010)	Pedo-climatic	**1**	**0**	**1**	**0**	General discrepancies (SOC; underestimation N_2O 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
	Xing et al. (2011)	Pedo-climatic	**1**	**0**	**0**	**0**	General discrepancies (CO_2 emissions)	Soil properties (SWD - WFPS)	Soil moisture variations, high sensitivity to WFPS
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Smith et al. (2012)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		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
	Scheer et al. (2014)	Pedo-climatic	**0**	**0**	**1**	**1**	General discrepancies (Overestimation N_2O emissions and soil NH_4; Underestimation NO_3 emissions)	Climate	Drying out periods
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Fitton et al. (2014a,b)	Pedo-climatic	**0**	**0**	**1**	**0**	Underestimation of N_2O 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
		Management	**0**	**0**	**1**	**0**		Management (Fertilization)	Model sensitive at low N application rates
	Ryals et al. (2014, 2015)	Pedo-climatic	**1**	**0**	**0**	**0**	Underestimation of CO_2 emissions	Soil properties (N - WFPS)	N mineralization rates may be off, underestimated WFPS
		Management	**1**	**0**	**0**	**0**		Management (Fertilization)	No soil water benefits provided by adding of compost
DNDC	*Smith et al. (2002)*	Pedo-climatic	**0**	**0**	**1**	**1**	Overestimation of N_2O emissions	Soil properties (general)	Overestimation N_2O emissions from shoulder position (upper landscape). Inability to characterize differences in soil properties and water/nutrient flow for 3-D landscape
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Cai et al. (2003)	Pedo-climatic	**1**	**0**	**1**	**0**	General discrepancies (CH_4, N_2O 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
	Pathak et al. (2003)	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
	Saggar et al. (2004)	Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		Pedo-climatic	**0**	**0**	**1**	**1**	Underestimation of N_2O emissions	Soil properties (T - SWD)	Under prediction of Temperature effect and moisture after rainfall (size and timing)
	Pathak et al. (2005)	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
	Babu et al. (2006)	Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		Pedo-climatic	**1**	**1**	**0**	**1**	General discrepancies (CH_4 and N_2O peaks)	Soil properties (SWD)	Soil shrinking and swelling - daily timescale
		Management	**1**	**0**	**0**	**1**		Management (Crop type)	CH_4 and N_2O peaks not well captured at the beginning and end of growing season. Type of cultivar (crop parameters)
	Sleutel et al. (2006)	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
	Liu et al. (2006)	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
	Tonitto et al. (2007)	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**	- - - -	- - - -	- - - -
	Smith et al. (2008)	Pedo-climatic	**0**	**0**	**1**	**1**	General discrepancies (timing of N_2O emissions).	Soil properties (N - SWD)	Soil water content and soil N underestimated. Too few chamber measurements of N_2O emissions available for detailed temporal testing.
		Management	**0**	**0**	**1**	**1**	Underestimation of N_2O emissions	Management (Fertilization)	Error in plant N uptake equation. Highest slurry rate
	Fumoto et al. (2008)	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
	Abdalla et al. (2010)	Pedo-climatic	**0**	**0**	**1**	**0**	Overestimation of N_2O emissions	Soil properties (C - WFPS)	Overestimation WFPS and SOC content
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Li et al. (2010)	Pedo-climatic	**0**	**0**	**1**	**0**	Underestimation of N_2O emissions	Soil properties (SWD)	Impact of soil freezing and thawing
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Wattenbach et al. (2010)	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
	Ludwig et al. (2011)	Pedo-climatic	**0**	**0**	**1**	**0**	Under/Overestimation of N_2O emissions	Soil properties (general) - Climate	Soil properties - Rainfall
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Leip et al. (2011)	Pedo-climatic	**0**	**0**	**1**	**1**	Under/Overestimation of N_2O emissions	Soil properties (general) - Climate	Soil properties - Rainfall
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Smith et al. (2012)	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
	Yu et al. (2015)	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
	Uzoma et al. (2015)	Pedo-climatic	**0**	**0**	**1**	**0**	Under/Overestimation of N_2O emissions	Soil properties (SWD) - Climate	Inability of cascade flow hydrology model to effectively simulate water content above field capacity - N_2O 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
	Zhang et al. (2015)	Pedo-climatic	**0**	**0**	**1**	**0**	General discrepancies (timing of daily N_2O and NO emissions)	Soil properties (SWD)	Soil water content was not well simulated
		Management	**0**	**0**	**1**	**0**	Overestimation of N_2O and NO emissions	Management (Fertilization)	High fertilizer treatments: Need to better simulate the limitation of dissolved organic carbon on denitrification
	Gu et al. (2014)	Pedo-climatic	**0**	**0**	**1**	**0**	Overestimation of N_2O 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.
	Congreves et al. (2016)	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.
	Gagnon et al. (2016)	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	*Gijsman et al. (2002)*	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**	- - - -	- - - -	- - - -
	Liu et al. (2011)	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
	Hartkamp et al. (2004)	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.
	De Sanctis et al. (2012)	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**	- - - -	- - - -	- - - -
	Li et al. (2015)	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
	Li et al. (2015)	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**	- - - -	- - - -	- - - -
	Prasad et al. (2015)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		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	*Jackson et al. (1994)*	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.
	Cavero et al. (1996)	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)
	Ramanarayanan et al. (1998)	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
	Roloff et al. (1998)	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**	- - - -	- - - -	- - - -
	Cavero et al. (1999)	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
	Chung et al. (2002)	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**	- - - -	- - - -	- - - -
	Potter et al. (2004)	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)
	Wang et al. (2005)	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.
	He et al. (2006)	Pedo-climatic	**1**	**0**	**1**	**0**	General discrepancies (soil C, Overestimation of N mineralization)	Soil properties (C)	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.
		Management	**1**	**0**	**1**	**0**		Management (Fertilization)	Underestimation of the soil capacity to transform crop residue in SOC
	Causarano et al. (2007)	Pedo-climatic	**0**	**1**	**0**	**0**	General discrepancies (Overestimation of microbial biomass C and total organic C, Underestimation particulate organic C)	Soil properties (C)	Spatial differences in C fraction due to differing soil landscapes
		Management	**1**	**0**	**0**	**0**		Management (Fertilization - Tillage)	Tillage and manure effects not adequately simulated by the model
	Apezteguıa et al. (2009)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		Management	**1**	**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.
	Billen et al. (2009)	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
	Zhang et al. (2015)	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	*Schmid et al. (2001)*	Pedo-climatic	**0**	**0**	**1**	**0**	Underestimation of N_2O emission peaks	Climate	Wet conditions
		Management	**0**	**0**	**1**	**0**		Phenology	Overestimation transpiration and N uptake by plants;
	Riedo et al. (2002)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		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
	Lawton et al. (2006)	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.
		Management	**0**	**0**	**0**	**0**		Management	Type of management (intensive vs extensive)
	Calanca et al. (2007)	Pedo-climatic	**1**	**1**	**1**	**0**	General discrepancies (Under/Overestimation of GPP, Reco and N_2O emissions; daily CO_2 emissions)	Soil properties (C - SWD)	Inappropriate setting of initial parameters, SOM stock initialization, over emphatization of water stress effect on assimilation
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Vuichard et al. (2007a)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		Management	**1**	**0**	**0**	**0**	Under/Overestimation of NEE	Management	Grazing effect
	Ma et al. (2015)	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**		Management	Type of management (intensive vs extensive)
	Sandor et al. (2016)	Pedo-climatic	**1**	**1**	**0**	**0**	General discrepancies (NEE)	Soil properties (T - SWD)	Improper representation of soil water content and soil temperature
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
RothC	*Skjemstad et al. (2004)*	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
		Management	**1**	**0**	**0**	**0**	General discrepancies (C)	Management	Disturbances (i.e. clearing and burning of pulled vegetation)
	Shirato and Yokazawa (2005)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		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)
	Zimmermann et al. (2007)	Pedo-climatic	**1**	**0**	**0**	**0**	General discrepancies (SOC)	Soil properties (general) - Climate	Soil properties - Air temperature
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Liu et al. (2009)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		Management	**1**	**0**	**0**	**0**	Overestimation of SOC content	Management (Fertilization)	Stubble (i.e. using the conventional setting of stubble retention factor)
	Rampazzo Todorovic et al. (2010)	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
	Nieto et al. (2010)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		Management	**1**	**0**	**0**	**0**	Overestimation of SOC content	Management (Tillage)	C losses due to soil erosion
	Xu et al. (2011)	Pedo-climatic	**1**	**0**	**0**	**0**	General discrepancies (SOC content)	Soil properties (general) - Climate	Soil properties
		Management	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
	Gonzalez-Molina et al. (2011)	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.
	Nieto et al. (2013)	Pedo-climatic	**0**	**0**	**0**	**0**	- - - -	- - - -	- - - -
		Management	**1**	**0**	**0**	**0**	Overestimation of SOC content	Management (Tillage)	Tillage (erosion)
	Wang et al. (2013)	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
	Farina et al. (2013)	Pedo-climatic	**1**	**0**	**0**	**0**	Under/Overestimation of GPP and Reco	Climate	Dry condition
		Management	**1**	**0**	**0**	**0**		Management (general)	Rotation with fallow
STICS	*Schnebelen et al. (2004)*	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.)
	Justes et al. (2009)	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).
	Constantin et al. (2012)	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
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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).

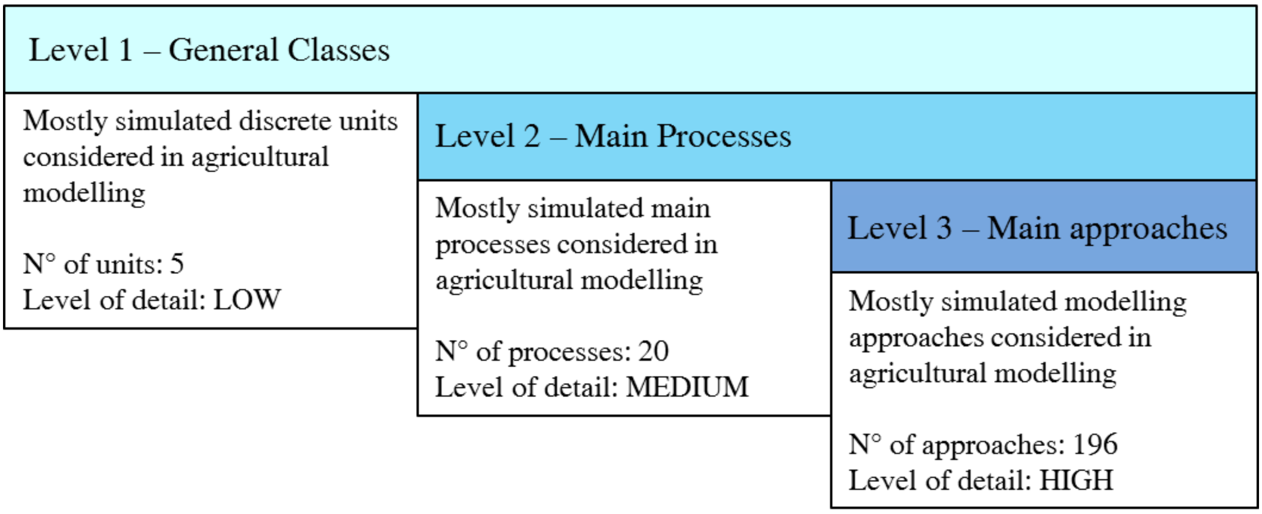
Level 1 – General Classes
Mostly simulated discrete units considered in agricultural modelling
N° of units: 5
Level of detail: LOW
Level 2 – Main Processes
Mostly simulated main processes considered in agricultural modelling
N° of processes: 20
Level of detail: MEDIUM
Level 3 – Main approaches
Mostly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

Fig. 1

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