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## Review

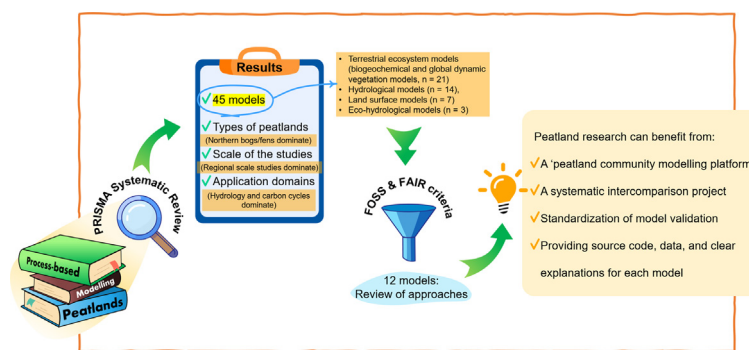
## Peatland dynamics: A review of process-based models and approaches

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## HIGHLIGHTS

- An extensive systematic search identified many process-based models being used for peatland dynamics.
- Only about a quarter of the models meet the FOSS and FAIR criteria for an open-source and active community.
- It is essential to standardize model calibration/validation and data sharing.
- No one-size-fits-all model exists, but the models overlap in scope and approach.
- A peatland community modelling platform can optimally exploit the strengths of existing models.

## GRAPHICAL ABSTRACT



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## ABSTRACT

Despite peatlands' important feedbacks on the climate and global biogeochemical cycles, predicting their dynamics involves many uncertainties and an overwhelming variety of available models. This paper reviews the most widely used process-based models for simulating peatlands' dynamics, i.e., the exchanges of energy and mass (water, carbon, and nitrogen). 'Peatlands' here refers to mires, fens, bogs, and peat swamps both intact and degraded. Using a systematic search (involving 4900 articles), 45 models were selected that appeared at least twice in the literature. The models were classified into four categories: terrestrial ecosystem models (biogeochemical and global dynamic vegetation models,  $n = 21$ ), hydrological models ( $n = 14$ ), land surface models ( $n = 7$ ), and eco-hydrological models ( $n = 3$ ), 18 of which featured "peatland-specific" modules. By analysing their corresponding publications ( $n = 231$ ), we identified their proven applicability domains (hydrology and carbon cycles dominated) for different peatland types and climate zones (northern bogs and fens dominated). The studies range in scale from small plots to global, and from single events to millennia. Following a FOSS (Free Open-Source Software) and FAIR (Findable, Accessible, Interoperable, Reusable) assessment, the number of models was reduced to 12. Then, we conducted a technical review of the approaches and associated challenges, as well as the basic aspects of each model, e.g., spatiotemporal resolution, input/output data format and modularity. Our review streamlines the process of model selection and highlights: (i) standardization and coordination are required for both data exchange and model calibration/validation to facilitate intercomparison

**Abbreviations:** FOSS, free and open-source software; FAIR, findable-accessible-interoperable-reusable; CO<sub>2</sub>, carbon dioxide; CH<sub>4</sub>, methane; N<sub>2</sub>O, nitrous oxide; NO<sub>3</sub><sup>-</sup>, nitrate; NO, nitric oxide; DOC, dissolved organic carbon; POC, particulate organic carbon; NH<sub>3</sub>, ammonia; NH<sub>4</sub><sup>+</sup>, ammonium; IPCC, inter-government panel on climate change; GHG, greenhouse gas; ESM, earth system model; LSM, land surface model; TEM, terrestrial ecosystem model; WoS, web of science; N/A, not available; I/O, input/output; CCA, common component architecture; CD, coefficient of determination; MSE, mean square error; RMSE, root mean square error; RRMSE, relative root mean square error; MAE, mean absolute error; MBE, mean bias error; PBIAS, percent bias; NSE, Nash Sutcliffe efficiency; KGE, Kling-Gupta efficiency; CN, curve number; LRM, linear reservoir model; GPP, gross primary production; NPP, net primary production; R<sub>A</sub>, autotrophic respiration; R<sub>H</sub>, heterotrophic respiration; GW, groundwater; SW, surface water; WTD, water table depth; SEB, surface energy balance; PFT, plant functional type.

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studies; and (ii) there are overlaps in the models' scopes and approaches, making it imperative to fully optimize the strengths of existing models rather than creating redundant ones. In this regard, we provide a futuristic outlook for a 'peatland community modelling platform' and suggest an international peatland modelling intercomparison project.

## Contents

1. Introduction . . . . .	2
2. Material and methods . . . . .	3
2.1. Review set-up . . . . .	3
2.2. Study selection . . . . .	3
3. Results and discussion . . . . .	3
3.1. FOSS and FAIR comparison of the models . . . . .	4
3.2. The FOSS-FAIR models: basic aspects . . . . .	5
3.3. The FOSS-FAIR models: modelling approaches . . . . .	8
3.3.1. Energy balance . . . . .	8
3.3.2. Water cycle components . . . . .	11
3.3.3. Carbon cycle . . . . .	12
3.3.4. Nitrogen cycle . . . . .	12
3.4. Potentials for a peatland community modelling platform . . . . .	13
4. Conclusions . . . . .	13
CRediT authorship contribution statement . . . . .	13
Data availability . . . . .	14
Declaration of competing interest . . . . .	14
Acknowledgments . . . . .	14
References . . . . .	14

## 1. Introduction

Peatlands are a specific type of wetland where waterlogged conditions slow the microbial decomposition of organic matter, resulting in peat accumulation, which supports plant production to form new peat layers (Clymo et al., 1998). Depending on the source of incoming water, active peat-forming peatlands (or mires) can range from bogs, which are rainwater fed (ombrotrophic), to fens, which are also supplied by groundwater (minerotrophic) (Wheeler and Proctor, 2000). The water sources of bogs and fens usually differ in mineral and nutrient contents, which in turn affects soil physio-chemical properties and the biotic-abiotic interactions (Rydin and Jeglum, 2013).

Peatlands cover an estimated 4.4 M km<sup>2</sup> of the Earth's surface, from southern America (Patagonia) peatlands (~0.04 M km<sup>2</sup>) to tropical (~0.37 M km<sup>2</sup>) and northern (subarctic/boreal, and temperate) peatlands (~4 M km<sup>2</sup>) (Yu et al., 2010). While occupying <3 % of the global land surface, they account for about one-third of the terrestrial store of soil organic carbon and provide significant freshwater resources (Xu et al., 2018a; Xu et al., 2018b). Moreover, peatland ecosystems are important for nature conservation since they are home to fragile flora and fauna species (Bonn et al., 2016; Hannigan and Kelly-Quinn, 2012; Renou-Wilson, 2018; Renou-Wilson et al., 2011).

Peatlands are 'complex adaptive systems' where internal (endogenic) and external (exogenic) processes determine their eco-hydrological interactions (Belyea and Baird, 2006). These interactions are driven by energy and mass (e.g., water, carbon, and nitrogen) exchanges within and between the soil-vegetation-atmosphere continuum, that may have connectivity (biological and hydrological) with the surrounding environment (Pringle, 2001). Their dynamics are nonlinear, meaning that any change can generate multiple responses and uncertain feedbacks (Belyea, 2009). In addition, climate change and other disturbances (natural and anthropogenic), such as wildfires or land-use changes, can adversely impact these ecosystems and further complicate their behaviour (Gallego-Sala et al., 2018). Although studies have qualitatively noted the feedbacks in peatlands (e.g., Limpens et al., 2008; Waddington et al., 2015), it remains difficult to gauge their extent and magnitude mainly due to (i) the inherent

complexity of the interactions; (ii) monitoring limitations; and (iii) the uncertainties associated with modelling the processes.

Several studies have raised concerns about the gaseous (e.g., carbon dioxide (CO<sub>2</sub>) and nitrous oxide (N<sub>2</sub>O)) and fluvial (e.g., dissolved organic carbon (DOC), particulate organic carbon (POC), and ammonia (NH<sub>3</sub>)) release from the decomposition of the organic matter when peatlands are managed (e.g., Kandel et al., 2018; O'Driscoll et al., 2016; Regan et al., 2019; Wilson et al., 2016). The United Nations Inter-Government Panel on Climate Change (IPCC) estimates that 5–14 % of total Greenhouse Gas (GHG) emissions are from land use and land-use change, including deforestation and peatland degradation (IPCC, 2019). Accordingly, a growing number of policies seek to improve the management of peatlands to restore degraded peatlands and achieve climate neutrality targets (e.g., European Commission, 2019; LIFE Peat Restore, 2021), which call for a holistic view of the behaviour of peatlands and reliable predictive tools.

The purpose of numerical models for peatland dynamics can be twofold: (i) as 'explanatory' tools to describe processes for which the model has been conceptualized/limited, i.e., how we expect peatland systems to behave in the real world under specified conditions; and (ii) as 'heuristic' tools that aid in discovering some features of the behaviour of peatland systems, where inferences can be drawn by manipulating, adapting, and evaluating the models (Jakeman et al., 2006; Pianosi et al., 2016). There may be aspects of the peatlands' behaviour (e.g., thresholds, nonlinearities, missing processes, influencing variables) that are not included in the conceptualisation, and thus, are not in the model (Lenton, 2013). In such a case, experimentation with the model alone will not provide knowledge of behaviour influenced by those missing elements. There is a role for the comparison of models with observations/data and a process in which models (i.e., their conceptualisations) are improved or even 'supported' by the comparison, although there are also limits to the information contained in any set of observations (Herrera et al., 2022; Jakeman et al., 2006; Oreskes et al., 1994). Depending on the purpose, the 'explanatory' function can be motivated by practical issues, whereas the 'heuristic' function can be driven by research concerns. In the past five decades, different mathematical approaches have been used to simulate an array of eco-hydrological processes in peatlands in an efficient, low-cost, and fast way (e.g., Baird et al., 2012;

Borcard et al., 1992; Clymo, 1984; Dooge, 1972; Keane and Dooge, 1972; Walter et al., 1996; Warncke, 1980). Advances in computational power have made it easier to develop numerical techniques and support more complex applications (e.g., Chen and MacQuarrie, 2004; Cobb et al., 2017; Hahti et al., 2014; McNevin and Barford, 1998; Reeve et al., 2001; Siegel et al., 1995; Thompson and Waddington, 2014).

Four classes of process-based (or equivalently physically based) models can be identified that simulate peatland dynamics: (i) climate models; (ii) Land Surface Models (LSMs); (iii) Terrestrial Ecosystem Models (TEMs); and (iv) (eco-) hydrological models. These classifications are supported by a comprehensive literature review, which is detailed in Section 3. Each model emphasises different aspects of the carbon, nutrient, energy, and water cycles within and between the biosphere and atmosphere. Since the models are increasingly overlapping, it is imperative to determine their primary focus to distinguish between them.

Climate models simulate regional or global atmospheric circulation patterns using equations for mass and energy transfer within fluids. The main inputs for climate models are energy, momentum, and water fluxes from the ocean surface and, to a lesser extent, from the ground (Bonan, 2019b). However, due to their high computational requirements, their domain of applicability is limited to relatively coarse spatiotemporal resolutions.

Earth System Models (ESMs) are a subset of climate models that are coupled to terrestrial components (e.g., LSMs and TEMs) to reflect both exogenous (e.g., climate) and endogenous drivers (e.g., land use and biogeochemical-physical fluxes) (Melton et al., 2017).

It is becoming increasingly common to refer to LSMs and TEMs interchangeably, as mixed models, or as 'terrestrial biosphere models' (Bonan, 2019b; Krinner et al., 2005; Melton et al., 2020). LSMs were initially developed as an integral part of climate models to provide the Earth's boundary condition for biogeophysical and hydrometeorological processes. With advances in their development and functioning as standalone models, LSMs analyse the coupled water, energy, momentum, and biogeochemical cycles at the land surface and their feedbacks to the atmosphere (Fisher and Koven, 2020). Compared to LSMs, TEMs place less emphasis on climate feedbacks. They include a wide range of models, such as biogeochemical and dynamic vegetation models, to simulate water, carbon, and nutrient pools, as well as biological activities within ecosystems (Bonan, 2019b). However, their representation of water movements is often simplified with semiempirical equations based on limited observed input data (e.g., water table depth (WTD)) (Frolking et al., 2002; Kurnianto et al., 2015; Metzger et al., 2015).

On the other hand, hydrological models can simulate the water cycle (primarily runoff generation and storage) more intricately (depending on the resolution), often coupled with energy exchanges, while paying less, or even no, attention to ecological processes (Xu et al., 2017). In response to growing interest in how ecological processes influence water dynamics, eco-hydrological models evolved from hydrological models (Rajaram et al., 2015). Having a hydrological sub-model as their primary component, they employ additional modules to specify how plant physiological processes, including carbon and nutrient pools and fluxes, affect the water cycle. In this regard, eco-hydrological models may adopt similar approaches to TEMs and LSMs when simulating ecological drivers, but their primary focus remains on the hydrologic cycle.

Choosing the appropriate model type is often subjective and requires a multidimensional consideration of the objectives, suitable scales, and resolution. This can prove challenging since: (i) the concept of 'scale' still has no universal definition in interdisciplinary research (e.g., ecology-hydrology) (Dooge, 1997; Gleeson and Paszkowski, 2014); (ii) data and computational resources are typically limited; (iii) there is no definitive 'best' approach, since various approaches differ in terms of data requirements and complexity levels (Clark et al., 2017); and (iv) according to the concept of 'equifinality', different model structures or parameter sets can produce similar outcomes and replicate observations fairly well, causing uncertainty in the modelling calibration, intercomparison studies, and interpretation of results (Beven and Freer, 2001).

A new model is supposed to show significant improvements over the prior model(s) (Jorgensen et al., 2006), e.g., in terms of conceptual structure or computer code efficiency (Alexandrov et al., 2011). However, in the quest to improve, a plethora of models has emerged that adopt the same common structures or approaches (e.g., Gong et al., 2014; Kettridge and Baird, 2010; Suryadi et al., 2021; Willeit and Ganopolski, 2016). This can lead to difficulty in identifying the uniqueness of each model and comparing their approaches, especially with respect to increasingly complex data implementations, resulting in a waste of community efforts and resources (Weiler and Beven, 2015).

This paper aims to (i) identify the widely used process-based models and approaches for simulating energy and mass (water, carbon, and nitrogen) exchanges in peatlands by highlighting their proven successful domain of applicability; and (ii) suggest a blueprint to minimize the 'duplication of effort' for future model developments. For this purpose, a comprehensive systematic review of literature on 'named' process-based models applied to peatlands was conducted, followed by a critical review of a subset of models and their approaches. Throughout our review, we highlight the main takeaways from the large number of models and corresponding research. It is strongly recommended that readers refer to each model's original documentation and the references provided in Data S1 for additional information. To our knowledge, this work is unique in its contribution to the field of peatland modelling that can assist in (i) model selection; (ii) maximizing the utility of successful modelling approaches; and (iii) optimizing future model development initiatives. We believe it is a timely endeavour given the rapid growth of using such models as decision support tools for climate mitigation and sustainable peatland management.

## 2. Material and methods

### 2.1. Review set-up

We conducted a systematic review of the literature using the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) method (Page et al., 2021). Scopus and Web of Science (WoS) databases were searched for process-based models that simulate peatland dynamics. These sources were used as they are the two main comprehensive scientific bibliographic databases relevant to our topic and provide access to a large number of papers worldwide (Pranckutė, 2021). The following search string was used to search within the title, abstract, and keywords of published works: ((peatland\* OR bog OR fen OR mire OR (peat swamp\*)) AND (model\* OR simulat\*)). Additional inclusion criteria were: journal articles; written in English; published between January 1st, 2000, and October 31st, 2022; that name a model in either title, abstract, or keywords; that the model employs process-based approaches for simulating energy, water, carbon, or nutrient exchanges in relation to peat. Non-peer-reviewed papers; grey literature (reports, policy documents, technical notes); inaccessible full-text papers; reports of pilot studies, surveys; studies with generalized linear or additive black-box models were not considered.

### 2.2. Study selection

The search (undertaken on 31/10/2022) in Scopus and WoS yielded a total of 4219 and 3722 entries, respectively. These were combined using the *bibliometrix* package (Aria and Cuccurullo, 2017) in R (R Core Team, 2021), and this removed 3041 duplicates, leaving 4900 unique records. After manually reviewing the title, abstract, and keywords, and applying the inclusion criteria, 4669 studies were removed. This resulted in a total of 231 publications and 45 different models satisfying the conditions for inclusion in this review.

## 3. Results and discussion

Information regarding model implementation (i.e., the principal use-cases, location, and type of peatlands) was extracted from each of the shortlisted studies (supplementary data; Data S1). Based on their original

documentation, each model was classified as either (i) a LSM, (ii) a TEM (including biogeochemical and dynamic global vegetation models), (iii) exclusively a hydrological model, or (iv) an eco-hydrological model. Fig. 1 shows the number of publications and named models by year and reveals that exclusively hydrological models have recently (from 2018 to 2022) overtaken TEMs as the dominant model type in the literature. Overall, the use of process-based models for peatland dynamics has increased over the last decade. Fig. 2 shows the global distribution of the plot to regional-scale studies conducted using these models, with the majority focusing on northern (temperate to Arctic) peatlands, while, at the time of the review, no studies were found for South America. Fig. 3 lists all selected models along with the number of papers on their use for peatland simulation published each year. There is a large variation in the reported use of each model since 2000. Models that have been repeatedly used over a longer period may have useful or valuable characteristics, such as a robust theoretical foundation, manageable input data requirements, flexible and modular structure, computation efficiency, detailed documentation, and community support.

The scales of the studies range spatially from plots to global and temporally from single events to millennia. Twenty studies were conducted at the global scale, fifteen at the continental scale (fourteen in the northern hemisphere, and only one in the tropical regions (Apers et al., 2022)), seven in lab-based or synthetic setups, and 189 involved regional/multiple and single peatland(s) scales (Fig. 4). The types of peatlands are listed in Table 1 (N/A denotes studies that did not mention a type; see Data S1 for more information). Among the bogs were the ORNL SPRUCE experimental site (Krassovski et al., 2015), as well as a cutover bog (Elliott and Price, 2020), where a portion of the peat mass has been extracted domestically (for burning). Our search string did not include ‘permafrost’, ignoring the studies that only use ‘permafrost’ in the context of peatland.

The principal application domains associated with each model were identified based on the primary modelling purpose. Fig. 5 links each model with its relevant application domain(s) (using R and the *circlize* package; Gu et al., 2014). The outer edge of each circle indicates the number of applications and published use of the model, with a larger border indicating a model has been used more frequently within its domain. If a model is applied to more than one application in one study, then the chord width is divided by that number, meaning thinner chords may reach each application domain. The chords in the figure are not color-coded.

The most common application domain was hydrology (40 %), followed by carbon dynamics (32 %), energy fluxes and soil temperature (11 %), peat accumulation (7 %), and nitrogen fluxes (3 %). TEMs are the most numerous ( $n = 21$ ) models, followed by hydrological models ( $n = 14$ ), LSMs

( $n = 7$ ), and there are only three eco-hydrological models. Of all the models, 18 feature ‘peatland-specific’ modules/structures that consider certain characteristics and processes unique to peatlands, e.g., microtopography, shallow water tables, and peat accumulation (‘bold brown’ names in Fig. 5). The rest are ‘non-peatland-specific’ models, which have been applied and calibrated solely based on peatland properties, e.g., soil and vegetation type. Water and carbon cycles in TEMs and LSMs are typically related to processes over larger scale areas (e.g., gross primary production, autotrophic and heterotrophic respiration).

### 3.1. FOSS and FAIR comparison of the models

To ensure transparency, replicability, and reproducibility of research software, it should be both open source and comply with the FAIR (Findable, Accessible, Interoperable, Reusable) principles (Hasselbring et al., 2020; Hut et al., 2022; Tucker et al., 2022). The FAIR principles provide guidance for managing scientific data (Wilkinson et al., 2016). According to FAIR, the data for all formal scholarly digital publishing, as well as the tools and algorithms generating the data (e.g., computer codes), should be made available globally. Several modifications have been suggested to FAIR to address the unique characteristics of research software (Hong et al., 2022; Lamprecht et al., 2020). However, the FAIR recommendations do not prescribe any standards or frameworks for assessing the FAIRness of research software, particularly in earth sciences (Agu.org, 2022). Therefore, to evaluate and compare the FAIRness of all 45 models found by our systematic search, we have put forth a set of criteria that may not cover all aspects of the models, as this would complicate the evaluation process. We additionally considered FOSS (Free and Open-Source Software) in our comparison as a complementary criterion for ensuring community reuse, with an open-source license for the model’s source code. Our FAIR criteria are detailed as follows:

- 1) ‘F’ (Findable): Using the general-purpose search engines (e.g., Google), the model and its metadata (e.g., the model’s version, authors, I/O type, and license) should be identified unambiguously on any web-based platform, such as open-access software registry or repository, domestic websites, public hosting systems for software development (e.g., GitHub (<https://github.com/>), and GitLab (<https://gitlab.com/>)), or any language-specific archives (e.g., CRAN; <https://cran.r-project.org/>).
- 2) ‘A’ (Accessible): The model should be retrievable using an open, free, and universally implementable protocol (HTTP/s).
- 3) ‘I’ (Interoperable): The model uses a formal, accessible, shared, and widely applicable programming language to exchange data with other

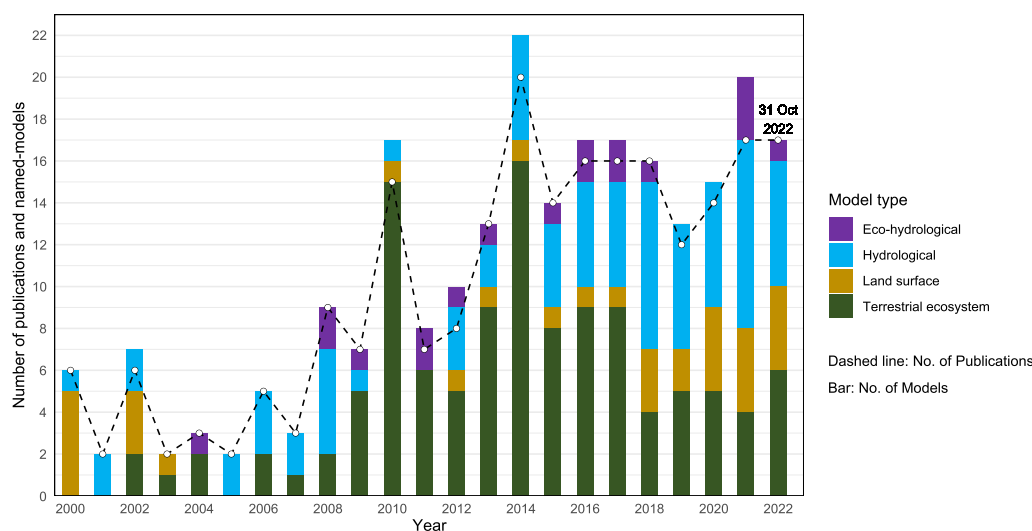


Fig. 1. Number of publications and proportion of different model categories by year. Note: some studies used multiple models; therefore, the number of models may exceed the number of studies.

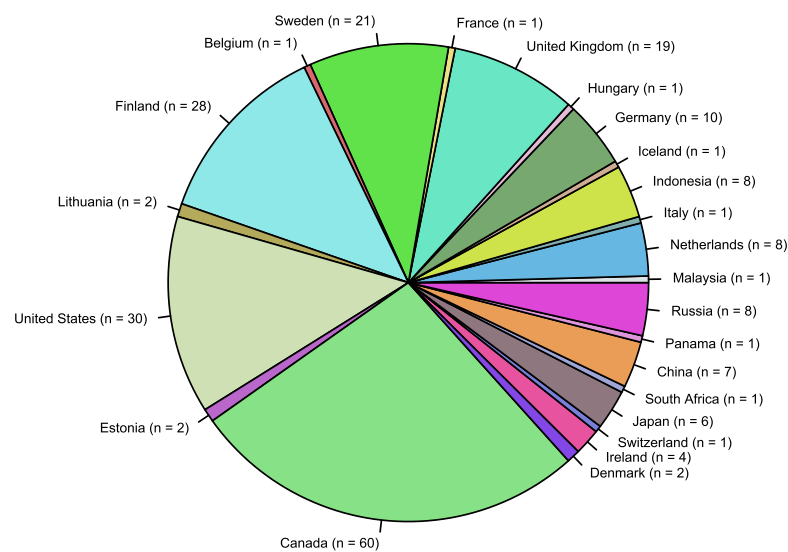
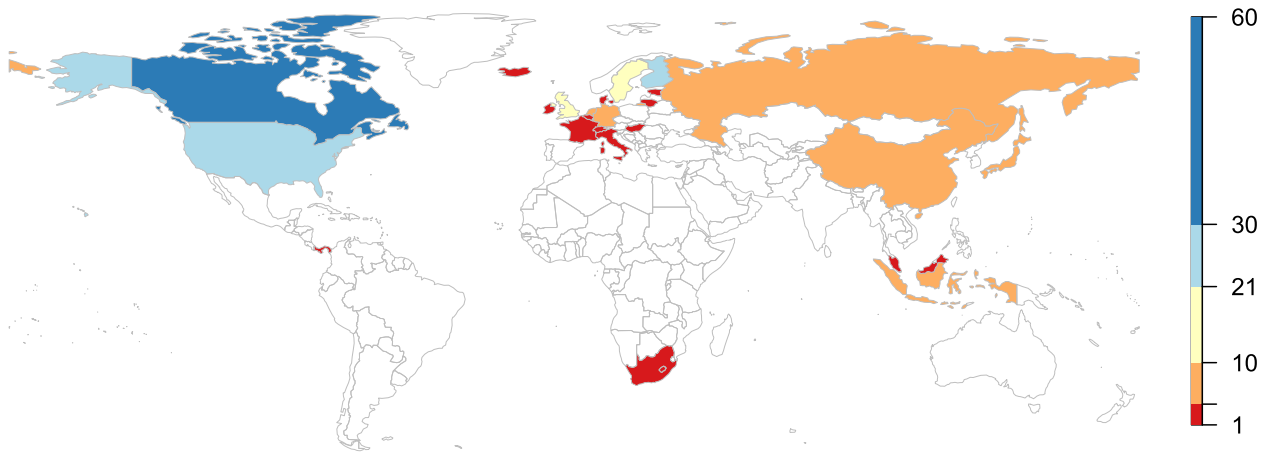


Fig. 2. The locations of plot to regional-scale peatland studies using process-based models.

software. This criterion was deemed satisfied only if the model's source code was written in a popular programming language, such as Fortran, C, Python, or R. The reason behind this is that several approaches have already been proposed to make such models interoperable, including the use of hub languages (e.g., Tucker et al., 2022), Common Component Architecture (CCA) and the babel transpiler (Epperly et al., 2012), and software containers (e.g., Hut et al., 2022).

- 4) 'R' (Reusable): The model should have (i) detailed documentation or user manual to ensure the attributes are well described; (ii) a clear and accessible usage license; and (iii) an active community with diverse users (this was considered to mean the model was repeatedly used three times or more and by different individuals outside of the core development team).

Table 2 shows the final list of models that met the FOSS and FAIR (FOSS-FAIR) criteria. Only 12 models meet these criteria, and these will be used for further comparative analysis and discussion. The full list of models and their detailed evaluation can be found in the supplementary data (Table S1).

For the shortlisted FOSS-FAIR models, we determined their key characteristics, including: (i) typical spatial and temporal resolutions; (ii) input/output data format; (iii) adaptability and flexibility (process-wise

modularity) (described in Table 3; Section 3.2); (iv) the model's scope; and (v) modelling approaches (described in Table 4; Section 3.3).

### 3.2. The FOSS-FAIR models: basic aspects

All the models in Table 3 have been developed for one or more specific purposes. Thus, each model may be 'fit for purpose' in one application domain, but not in another (Fig. 5; Sargent, 2010). Each focuses on particular scales (local to global), with resolution varying across time (minutes to annual) and space (meters to 1°; 110 km), making inter-scale implications uncertain (Wu et al., 2016) and comparisons difficult or even inappropriate. Based on their application to peatlands, Table 3 summarizes the typical spatial and temporal resolutions of each model's simulation output. These resolutions do not necessarily represent the highest or lowest resolution possible. The models can be run at any resolution for which forcing data is provided. However, for example, when a model is run at higher spatio-temporal resolutions for which (some) processes are not parameterized, not only does the model (in part) become physically meaningless, but can also be restricted by RAM, conflict with the required 'integration time step' (e.g., in GEOtop; Endrizzi et al., 2014), and may not guarantee a more accurate solution or even convergence (Wan et al., 2015). In this

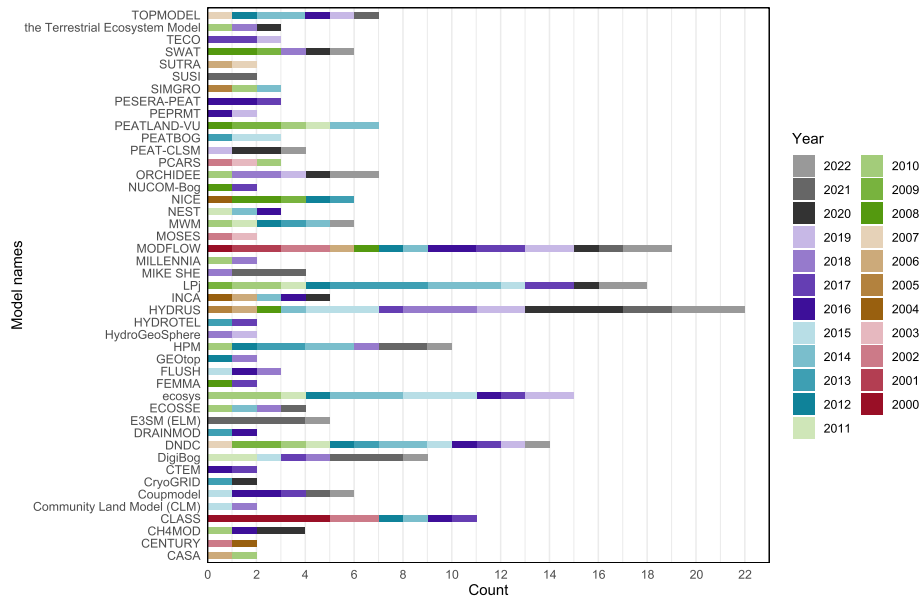


Fig. 3. Model names, along with the number of publications on their use for peatland simulation per year since 2000.

respect, practical resolutions can vary depending on the application or processes simulated.

The models all contain inherent uncertainties, primarily due to our limited understanding of the dominant mechanisms that drive processes across scales (i.e., epistemic uncertainty), and how these processes are represented

in the models (i.e., parametric uncertainty). As we move towards larger or global scales, it can become more challenging as key processes must be considered holistically. There is no single model that can fully represent all known processes (Blair et al., 2019); small-scale models are more able to capture tiny local variations and heterogeneities and are more sensitive to

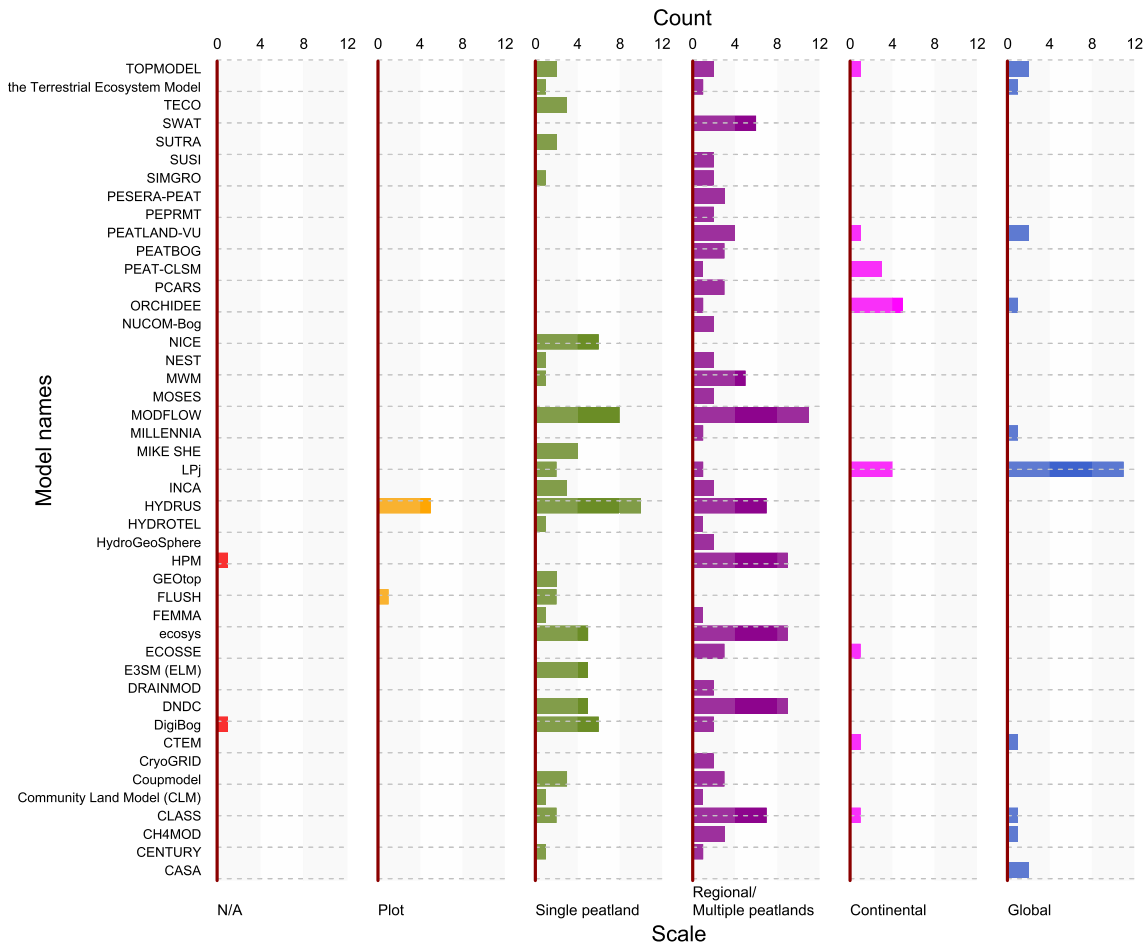


Fig. 4. Model names, along with their successful scale of application for peatland simulation.

**Table 1**  
Types of peatlands studied using process-based models worldwide.

Type of peatland	Number of studies
Bog	56
Fen	41
Mixed fen-bog	29
Permafrost (mixed with bogs, fens, or peat swamps)	20
Blanket bog	12
Tropical peatlands	9
N/A	43

disturbances. In contrast, large scale models are more comprehensive and describe average properties (e.g., fire in LSMs; Lawrence et al., 2019), requiring datasets with different spatiotemporal resolution. However, in certain cases and for comparable spatial scales, a climate or land surface model can overlap with a hydrological model, e.g., in the use of empirically derived functions for continental runoff modelling (Graham and Bergström, 2000). Several attempts, not specifically in peatland research, have been made to bridge the scaling gaps between the models, mostly based on: (i) statistical up- and down-scaling and (dis-) aggregation methods (e.g., Gao et al., 2015; Zhang et al., 2013); (ii) model integration (e.g., Guillaumot et al., 2022; Tucker et al., 2022); and (iii) the concept of ‘models of everywhere’ (Blair et al., 2019).

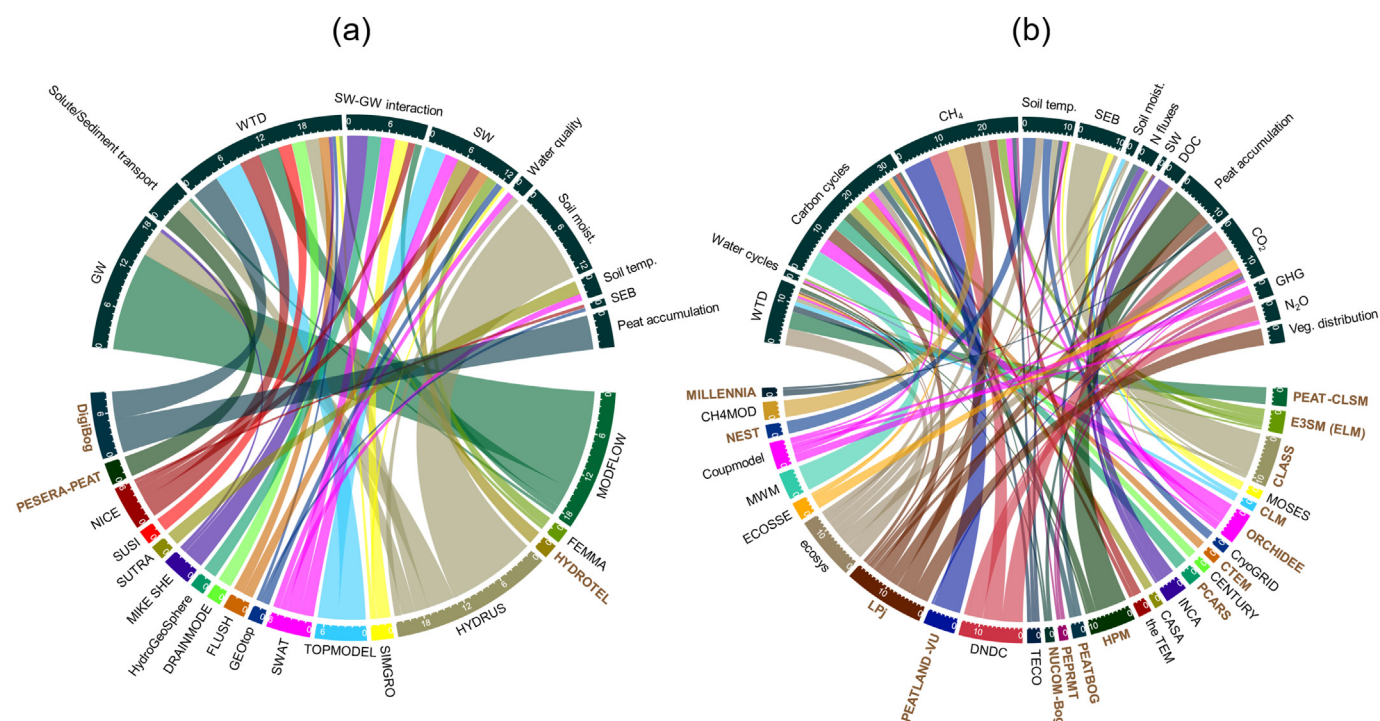
Developing a physically based model involves making key decisions regarding the representation of spatial variability (e.g., (micro-) topography, soil, and vegetation properties) and lateral fluxes (Clark et al., 2015). In accordance with Todini (1988), the models selected here can be classified spatially as distributed ‘integral’ or ‘differential’ models. Distributed integral models consist of one-dimensional (1D) column models spatially arranged in (ir-) regular grids, matched with boundary conditions and sink/source terms, but without simulating lateral fluxes dynamically. Among the models of this type are LSMs/TEMs in Table 3. These models can be applied to any area, from a single grid point to the global domain. To represent land surface variability at sub-grid scales, they can be coupled to other high-resolution models (e.g., a runoff/river routing model; Li et al., 2013) or configured to run using the (i) ‘mosaic/tiling’ approach, which

divides each grid cell into a set number of patches with varying properties; or (ii) ‘composite’/‘statistical dynamical’ approach, which aggregates the properties of each tile into a single grid cell. Thus, we considered the dimension of ‘1D + spatial sub-grid variability’ for these models (Table 3). The remaining models are distributed differential models, in which all subsystems are represented by coupled differential equations discretized in time and space. Using their mutual boundary conditions, they can simulate lateral fluxes within their individual elements. While some of these models can use different numbers of spatial dimensions, this can result in quite different simulation outcomes (e.g., 1D versus 3D), even when the governing equations and modelling approaches build on the same physical principles (Glock et al., 2019). Therefore, care is needed when comparing them appropriately to draw meaningful conclusions.

Input data may be a limiting factor since their quality and availability are variable (Faticchi et al., 2016). Some models require large amounts of forcing data (e.g., SWAT; Bieger et al., 2017), and sometimes data must be combined from multiple data sources with different and even sparse resolutions, complicating model calibration and validation. To improve the accessibility of model results, several initiatives are working to make models more interoperable (e.g., Unidata UCAR, 2020). Agreement on the standardization of data formats is essential for this. For instance, NetCDF is a binary, self-describing (contains metadata), and platform-independent data format that can be read and written by different operating systems and is widely used in some domains. Peatland research and input-output data analysis can benefit from shared databases and standardizations (both for data and metadata). The PeatDataHub initiative, for example, focuses on the efficient monitoring and linking of existing peatland databases worldwide (PeatDataHub, 2022). However, its database is currently limited to peat bogs and small-sedge fens, with most of the data related to WTD, peat conditions, and vegetation composition.

‘Modularity’ is another important feature that can make the models versatile and reliable and is reported in Table 3.

Although we list here some of the basic features of the models, it is essential to evaluate each model carefully to determine its ‘relevance’, ‘legitimacy’, and ‘credibility’ for a particular application (Bellocchi et al., 2010). Our analysis of the 231 studies that simulate peatland dynamics



**Fig. 5.** a) Hydrological and eco-hydrological models, b) TEMs and LSMs. Models are at the bottom of the circles, and use cases are at the top. Models with ‘bold brown’ names feature ‘peatland specific’ modules.

**Table 2**

A summary of the FOSS-FAIR evaluation for the shortlisted models. 'Bold' models feature 'peatland-specific' modules.

Model	Criteria					
	FOSS	'F'	'A'	'I'	'R'	FAIR
MODFLOW	✓	✓ <a href="https://www.usgs.gov/">https://www.usgs.gov/</a>	✓	✓ Fortran/ Python	✓	✓ Detailed user manual + Active community (+ GitHub)
TOPMODEL	✓	✓ <a href="https://cran.r-project.org/">https://cran.r-project.org/</a>	✓	✓ R (based on the 1995 FORTRAN version)	✓	✓ Detailed user manual + Active community (+ GitHub)
SWAT	✓	✓ <a href="https://swat.tamu.edu/">https://swat.tamu.edu/</a>	✓	✓ Fortran	✓	✓ Detailed user manual + Active community (+ Bitbucket/GitHub)
GEOtop	✓	✓ <a href="https://github.com/">https://github.com/</a>	✓	✓ C++	✓	✓ Detailed user manual + Active community (+ GitHub)
SUTRA	✓	✓ <a href="https://www.usgs.gov/">https://www.usgs.gov/</a>	✓	✓ Fortran	✓	✓ Detailed user manual + Active community
DigiBog	✓	✓ <a href="https://github.com/">https://github.com/</a>	✓	✓ Fortran	✓	✓ Active community Detailed user manual (considered original publications)
E3SM (ELM)	✓	✓ <a href="https://github.com/">https://github.com/</a>	✓	✓ Fortran	✓	✓ Detailed user manual + Active community (+ GitHub)
CLASS-CTEM (CLASSIC)	✓	✓ <a href="https://gitlab.com/">https://gitlab.com/</a>	✓	✓ Fortran	✓	✓ Detailed user manual + Active community (+ GitLab)
Community Land Model (CLM) 5	✓	✓ <a href="https://github.com/">https://github.com/</a>	✓	✓ Fortran	✓	✓ Detailed user manual + Active community (+ GitHub)
ORCHIDEE	✓	✓ <a href="https://forge.ipsl.jussieu.fr/">https://forge.ipsl.jussieu.fr/</a>	✓	✓ Fortran	✓	✓ Detailed user manual + Active community
LPJml	✓	✓ <a href="https://github.com/">https://github.com/</a>	✓	✓ C	✓	✓
PEAT-CLSM	✓	✓ <a href="https://github.com/GEOS-ESM/GEOSldas">https://github.com/GEOS-ESM/GEOSldas</a>	✓	✓ Fortran	✓	✓ Detailed user manual + Active community (+ GitHub)

shows no generally accepted framework for either developing or validating the models. Despite many published recommendations for the systematic and proper use of models (e.g., Alexandrov et al., 2011; Hamilton et al., 2019), a wide range of different statistical measures and visualization techniques have been applied across the studies, making it difficult to compare the models' performance. Fig. 6 presents a Venn diagram of the most used goodness-of-fit (GOF) measures for verifying the models used in the studies.

There are two main groups of GOF measures: (i) Association-based methods: e.g., correlation coefficient (Pearson (r) and Spearman) and R-squared ( $R^2$ , also known as the Coefficient of Determination (CD)); and (ii) Residual based methods: e.g., Mean Square Error (MSE), Root MSE (RMSE), Relative RMSE (RRMSE), Mean Absolute Error (MAE), Mean Bias Error (MBE), standard deviation, coefficient of variance, Percent bias (PBIAS), as well as modelling efficiencies, including Nash Sutcliffe efficiency (NSE; Nash and Sutcliffe, 1970), Willmott's index of agreement (Willmott, 1981), Kling-Gupta Efficiency (KGE; Gupta et al., 2009). Using multiple evaluation techniques can provide a more holistic view of a model's performance (N. Moriasi et al., 2007). However, few studies provided multiple measures to calibrate and verify their models (e.g., Bechtold et al., 2019; Elliott and Price, 2020; Wu et al., 2012), and some relied solely on graphs that may not adequately depict discrepancies (e.g., in peak values or timing) (e.g., Kasimir et al., 2018; Nakayama and Watanabe, 2004). Depending on what is being modelled, opinions differ on what is 'acceptable' or 'satisfactory' performance (Ritter and Muñoz-Carpena, 2013). For example, N. Moriasi et al. (2015) state an NSE coefficient of over 0.5 would normally be considered 'satisfactory' for daily mean flows, but above 0.45 for sediment concentrations or loads.

### 3.3. The FOSS-FAIR models: modelling approaches

The size of a model's scope, or 'granularity' (Tucker et al., 2022), indicates the range of processes it can simulate. Table 4 shows which models simulate the main processes shown in Fig. 5, and their approaches, categorized under energy balance, water, carbon, and nitrogen cycles. There are different levels of empiricism among approaches: (i) Purely physics-based: where the equations describing the system behaviour are governed

by physical laws and employ first principals (e.g., conservation of mass and momentum); (ii) Conceptual-based: where the system processes are simplified representations of the physical mechanisms (e.g., Darcy law; Darcy, 1856); and (iii) Empirical-based: where empirical linkages are sought for the behaviour through observations and statistical tools (e.g., correlations, interpolations and optimizations of generic equations), without consideration of internal processes (e.g., van Genuchten equation; van Genuchten, 1980). Although the empirically derived equations may contain some variables with direct physical interpretations (semi-empirical), their coefficients are mostly of limited physical significance (Refsgaard and Knudsen, 1996).

A detailed discussion of individual modelling approaches can be found elsewhere (e.g., Bonan, 2019a; Maskey, 2022) and is not the focus of this paper. Here, we focus on their commonalities and, if possible, the challenges and opportunities associated with the approaches for the study of peatland dynamics. Our discussion does not address the implementation-specific details but concentrates on the broader consideration of their components.

#### 3.3.1. Energy balance

Some of the models (Table 4) simulate a subsurface or surface energy balance. The surface energy balance describes how incoming solar energy splits into absorbed and radiant fluxes at the earth's surface. It is linked with subsurface heat transfers and determines the surface temperature. A key component is the latent heat flux, which describes the amount of surface energy lost through evapotranspiration. The latent heat flux can be calculated using an energy conservation or a water budget approach. Due to the difficulty of simulating surface energy components, most (eco-) hydrological models (e.g., SWAT) rely on a simple energy budget combined with mass transfer equations, such as the Priestley-Taylor and Penman-Monteith methods (Drexler et al., 2004). According to Admiral and Lafleur (2007), modelling the surface energy balance in bogs poses particular challenges due to their: (i) co-dominant vascular and non-vascular (i.e., moss) species surface cover, allowing significant ground surface involvement in the energy balance; (ii) hummocks and hollows' microscale heterogeneous moisture, differentiating them from flatter surfaces (lawns); and (iii) water

**Table 3**  
Basic aspects of shortlisted FOSS-FAIR models: Typical spatiotemporal resolution (peatland applications), Grid structure, I/O data format, Modularity. 'Bold' models feature 'peatland-specific' modules.

Model	Spatial dimension	Typical spatial res.	Typical temporal res.	Grid structure	Input format	Output format	Modularity	Reference
MODEFLOW 6	3D	0.4 - 200 m	D - M	✓ Runs with regular/irregular grid/mesh structure	ASCII, Binary	ASCII, Binary	✓	Hughes et al., 2017; Langevin et al., 2017
TOPMODEL (in R)	2D	20 m - 1' (in LSMs)	6 min - M (in LSMs)	✓ Runs with regular grid structure (grid size <= 50 m is recommended)	ASCII, Binary	ASCII, Binary	✗	Beven and Kirkby, 1979; Buytaert, 2018
SWAT +	2D	HRU	D	○ Sub-unit structure, but can be run on grid	ASCII, GIS vector	ASCII	✓	Bieger et al., 2017
GEOtop	1D, 3D	8 - 25 m	Hr - M	✓ Runs with regular grid structure	ASCII	ASCII	✓	Endrizzi et al., 2014; Rigon et al., 2006
SUTRA	2D, 3D	1 cm - 1 m	15 min - Hr	✓ Runs with regular/irregular grid (and mesh) structure	ASCII, Binary	ASCII	✓	Provost and Voss, 2019
DigitBog PDM	1D, 2D (& 3D)	1 m - 1'	Min - Annual	✓ Runs with square grid structure	ASCII	ASCII	✗	Baird et al., 2012
ESSM (ELM)	1D + spatial sub-grid variability	Single point - 1km	30 min - M	✓ Runs with regular/irregular grid (sub-grid: tile) structure	netCDF-4, HDF5, DAP	netCDF, ASCII, Binary	✓	Golaz et al., 2019; Ricciuto et al., 2021
<b>CLASSIC (CLASS-CTEM)</b>	1D + spatial sub-grid variability	Single point - 0.22°, some processes not tuned for <10 km	D (CTEM), <0.5 Hr (CLASS)	✓ Runs with regular grid (sub-grid: tile/mosaic + composite) structure	netCDF-4	netCDF, csv	✓	Melton et al., 2020; Seiler et al., 2021
Community Land Model (CLM) 5 (CLM-SPRUCED)	1D + spatial sub-grid variability	0.25°-2.5°	6 Hr - D	✓ Runs with regular grid (sub-grid: tile/mosaic) structure	netCDF, csv	netCDF	✓	Lawrence et al., 2019; Shi et al., 2015
ORCHIDEE (ORCHIDEE-PEAT)	1D + spatial sub-grid variability	0.5°-2°	30 Min - M	✓ Runs with regular grid (sub-grid: tile) structure	netCDF	netCDF	✓	Krinner et al., 2005; Qiu et al., 2018
LPJml (LPJ-WhYme)	1D + spatial sub-grid variability	0.5°-3.75°	D - Annual	✓ Runs with regular grid (sub-grid: mosaic) structure	netCDF, Binary	netCDF, Binary	✓	von Bloh et al., 2018; Wania et al., 2010
CLSM (PEAT-CLSM)	1D + spatial sub-grid variability	1 and 9 km-0.25°	1 and 3 Hr - D	✓ Runs with regular grid (sub-grid: tile/mosaic) structure	netCDF	netCDF	✓	Bechtold et al., 2019; Koster et al., 2000

✓: Fulfilled.

✗: Not fulfilled.

○: Fulfilled to some extent.

D: Dimensional.

Min: Minute.

Hr: Hourly.

D: Daily.

M: Monthly.

HRU: Hydrological Response Unit.

**Table 4**  
Process representation in the FOSS-FAIR models. 'Bold' models feature 'peatland-specific' modules.

Model	Energy balance		Water cycle		Surface runoff		GPP	Carbon cycle		Nitrogen cycle	
			Subsurface		Infiltration			CO <sub>2</sub> (R <sub>A</sub> and R <sub>H</sub> )		CH <sub>4</sub> (Methanogenesis)	
	2D Groundwater flow										
MODFLOW 6	X	✓ #∞ Darcy	✓ Richards, K(θ): Brooks-Corey	✓ f(GW/stream depth)	X	X	X	X	X	X	X
TOPMODEL (in R)	X	X	✓ Green-Ampt	✓ f(topographic index)	X	X	✓ SWAT-MKT: f (MKT)	✓ f (biomass volume)/ SWAT-MKT: f(MKT)	X	X	✓ Exp. rate Coef./ SWAT-MKT: f(MKT)
SWAT+	X	✓ #2 LRM	✓ Green-Ampt	✓ CN	✓ Sat. excess/ Infiltr. excess/ f (GW)	X	X	X	X	X	X
GEOtop	✓ Surface/Subsurface	✓ #∞ Richards	✓ Richards, K(θ): van Genuchten-Mualem	✓ Sat. excess/ Infiltr. excess/ f (GW)	X	X	X	X	X	X	X
SUTRA	✓ Subsurface	✓ #∞ Darcy	✓ Richards, K(θ): van Genuchten	X	X	X	X	X	X	X	X
DiBiBog PDM	X	✓ #∞ Darcy (Dupuit-Boussinesq)	X	X	X	X	X	X	X	X	X
E3SM (ELM) (ELM-SPRUCE)	✓ Surface/Subsurface	✓ #1 Darcy	✓ Richards, K(θ): van Genuchten-Mualem	✓ Sat. excess/ f(topographic index)/VIC/ **ELM-SPRUCE	✓ Farquhar/ (**ELM-SPRUCE)	✓ R <sub>A</sub> (Rubisco), R <sub>H</sub> : f(T <sub>soil</sub> , θ, O <sub>2</sub> )	✓ (ELM-SPRUCE)	✓ Century N model	✓ Century N model	✓ Century N model	✓ Century N model
CLASSIC (CLASS-CTEM) Community Land Model (CLM) 5 (CLM-SPRUCE)	✓ Surface/Subsurface	X	✓ Green-Ampt	✓ Infiltr. excess/ f(soil)	✓ Farquhar	✓ R <sub>A</sub> : (Rubisco), R <sub>H</sub> : f(T <sub>soil</sub> , θ, C <sub>SOM</sub> )	✓ f(T <sub>soil</sub> , θ, sand content) ✓ f	✓ f(T <sub>soil</sub> , NH <sub>4</sub> <sup>+</sup> )	✓ f(T <sub>soil</sub> , θ, NO <sub>3</sub> )	✓ Century N model	✓ Century N model
ORCHIDEE (ORCHIDEE-PEAT)	✓ Surface/Subsurface	X	✓ Richards, K(θ): van Genuchten-Mualem	✓ Infiltr. excess / f(soil/ topographic index)	✓ f(PFT, Farquhar)	✓ f(PFT)	(decomposition rate)	✓ Century N model	✓ Century N model	✓ Century N model	
LPJml (LPJ-WHyMe)	X	X	✓ #1 f(θ) or Green-Ampt	✓ Sat. excess/ f(soil)	✓ Farquhar	✓ R <sub>H</sub> : f(T, θ)/similar to Century	✓ ORCHIDEE-PEAT	✓ O-CN/ Century model	✓ f(T, θ, pH)	✓ f(T, θ)	
CLSM (PEAT-CLSM)	✓ Surface/Subsurface	X	✓ Richards/TOPMODEL combination/ **PEAT-CLSM	✓ Sat. / infiltr. excess f(topographic index)/ **PEAT-CLSM	X	X	X	X	X	X	

✓: Included.

X: Not included.

VIC: Variable Infiltration Capacity.

R: Respiration.

MKT: Microbial Kinetics and Thermodynamics.

LRM: Linear Reservoir Model.

#n: indicates number of layers (∞: no limit).

R<sub>A</sub>: Autotrophic Respiration.

Exp.: Exponential.

PFT: Plant Functional Type.

CN: Curve Number approach.

R<sub>H</sub>: Heterotrophic Respiration.

Coef.: Coefficient.

BC: Boundary Condition.

T: Temperature.

C<sub>SOM</sub>: Soil C mass.

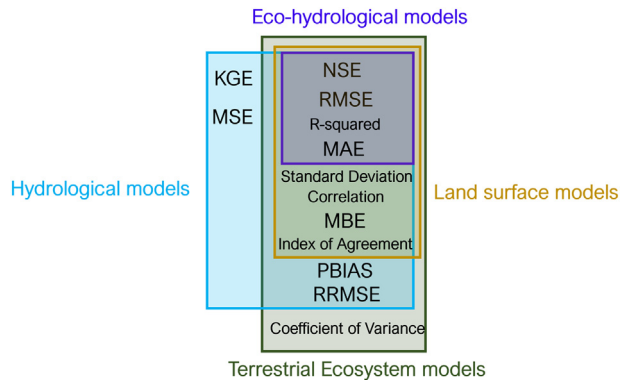
GPP: Gross Primary Production.

GW: Groundwater.

K(θ): Unsaturated hydraulic conductivity.

θ: Soil moisture.

\*\* Peatland-specific module adopts a different approach when simulating the process. See the text and references for more information.



**Fig. 6.** Venn diagram of the most commonly used goodness-of-fit (GOF) measures for verifying the models (See Section 3.2 for explanation of abbreviations).

transfer mechanisms and latent heat exchanges on moss carpet, distinguishing them from mineral soil and vascular plant surfaces.

For models that only estimate the subsurface energy balance, surface boundary conditions can be derived empirically to account for atmospheric forcing and surface thermal hydrology (Jan and Painter, 2020). For instance, GEOTop simulates freezing-thawing using the Dall'Amico et al. (2011) model for variably saturated soils coupled with Richards' equation (Richards, 1931). The model links (liquid or solid) water content with soil temperature and saturation degree but ignores their impact on ground surface temperature. Although widely used, this approach can be computationally demanding, since it solves coupled subsurface water-energy balances with snow and water-ice phase change processes (Nagare et al., 2021). Its data-intensive nature may also limit its use for large-scale arctic peatlands, where groundwater monitoring and data are scarce (Krogh and Pomeroy, 2021; Lamontagne-Hallé et al., 2020).

### 3.3.2. Water cycle components

**3.3.2.1. Surface runoff.** The models typically simulate surface runoff directly or via a regional water balance equation. The direct method includes empirical Curve Number (CN; USDA, 1972) and topographic index (TOPMODEL; Beven and Kirkby, 1979), which are both popular and not computationally demanding, but have several shortcomings for applications in peatlands. For instance, CN considers only total rainfall, ignoring intensity and duration, which control hydrograph shape. It can also be problematic to use soil-defined CN tables (typically for urban and agricultural watersheds) to model peatlands with waterlogged, highly heterogeneous, and site-specific conditions (Menberu Meseret et al., 2015). On the other hand, the TOPMODEL approach does not have an explicit spatially distributed component for overland flow. Therefore, it cannot model the effects of land surface changes (e.g., vegetation distribution) on surface runoff, especially for deep peatlands with gentle slopes. This issue was explored by Gao et al. (2015) for blanket peatlands (i.e., bogs with relatively shallow peat depths) by introducing a spatially distributed structure and an overland flow module to the model. Some global-scale models (e.g., CLSM (Koster et al., 2000), ORCHIDEE (Krinner et al., 2005), and CLM5 (Lawrence et al., 2019)) also use the topographic index approach. However, (i) its scale-dependent sub-grid parameterization remains a challenge (Zhang et al., 2016); and (ii) it may not be appropriate for bogs (and to some extent for fens), since wide areas of lowland bogs are rainfed and receive water from surrounding bogs or large watersheds rather than groundwater (Bechtold et al., 2019).

Simulating surface runoff using the regional water balance equation accounts for water storage changes at the surface. Some models apply this approach and simulate overland flow either as (i) an infiltration excess (Hortonian flow; Horton, 1933), when rainfall intensity exceeds the soil infiltration capacity; or (ii) a saturation-excess (Dunne mechanism; Dunne and Black, 1970), when surface water comes from (or mixes with) water

returning from saturated soil. Holden and Burt (2003) found that shallow water tables cause saturation-excess overland flow and near-surface throughflow to dominate flashy flow regimes in blanket peat catchments. Their measurements indicate that macropores and pipe flow pathways, surface cover, and topography are controlling factors in blanket peat runoff and infiltration.

**3.3.2.2. Infiltration.** The models simulate infiltration using Green-Ampt (Heber Green and Ampt, 1911) or Richards methods. The former is oversimplified and relatively fast, while the latter is more complex and has greater physical realism. According to the classical Green-Ampt model (i) infiltration occurs in a homogeneous column of soil with evenly distributed antecedent moisture content; (ii) instead of a realistic sigmoid distribution of water content, it generates a sharp wetting front of saturated soil moving downward at a constant velocity; and (iii) the soil is always ponded, and the rainfall intensity always exceeds the infiltration capacity, which equals the actual infiltration rate. These assumptions may not hold true early in a storm if the soil has a high infiltration capacity (Almedej and Esen, 2014), or for peatlands with heterogeneous layers. Richards' equation, on the other hand, combines the continuity principle with Darcy's law to simulate infiltration as unsaturated flow. It requires calculating the water content (or capillary capacity if a non-conservative form is used) and unsaturated hydraulic conductivity of the material/soil. For this purpose, most of the models include the Mualem hydraulic conductivity function (Mualem, 1976) and the van Genuchten water retention function, and only MODFLOW applies the Brooks-Corey equation (Brooks and Corey, 1966; Langevin et al., 2017). Richards' equation, however, assumes the infiltration occurs in a rigid and isotropic porous medium under isothermal conditions (Assouline, 2013), which is not necessarily the case in peat soils. Moreover, the equation is highly nonlinear elliptic (for saturated conditions) and parabolic. Hence, its use in large watersheds with high resolution is limited by the computational cost and potential non-convergence of the numerical solution (Ogden et al., 2015). ORCHIDEE also provides an alternative method to describe vertical water diffusion in soil by using the Fokker-Planck equation and van Genuchten-Mualem parameters. Compared with other soil types, further research is needed to show if the approaches can adequately simulate infiltration in peatlands, particularly when considering (i) water repellency (hydrophobicity), which can be extremely high in dry conditions (Moore et al., 2017), making the traditional approaches problematic (Wang and Wallach, 2021); and (ii) macropore flow, as Baird (1997) points out, the classic Richards' equation will not suffice alone, and there may be a need to partition flow between Richards-type and macropore flows. In addition, Rezanezhad et al. (2012) and Rezanezhad et al. (2016) demonstrate that peat soils exhibit a 'dual-porosity' structure, in which the active (open and connected) macropores coexist with inactive (dead-end) pores, which significantly complicates water flow and solute transport.

**3.3.2.3. Groundwater flow and water table depth.** For groundwater flow (i.e., flow in the saturated zone), most models use a physics-based approach based on the continuity equation (conservation of mass) and Darcy's law, commonly referred to as the 'groundwater flow equation'. Only one model (SWAT) relies on the conceptual-based Linear Reservoir Model (LRM; Dooge, 1973). However, the LRM approach is problematic as it assumes a linear relationship between groundwater storage and base flow, which is not always the case, particularly in heterogeneous aquifers, where (i) preferential flow paths exist; and (ii) the storage varies nonlinearly with depth (Wang et al., 2019; Yoo et al., 2020). Alternatively, Darcy's law has been widely adapted to groundwater applications, in which flow is assumed to be (i) from high to low hydraulic head; and (ii) linearly proportional to hydraulic gradient. In peatlands, the Darcian flow has been argued to be fairly valid, despite possible deviations caused by: (i) high elastic storativity of peat; (ii) variations in hydraulic conductivity; (iii) preferential pathways (e.g., macropores, piping, root channels, and animal burrows); and (iv) trapped biogenic gases in peat, which occlude pores and reduce hydraulic conductivity (Glaser et al., 2021; Grover and

Baldock, 2013; Hemond and Goldman, 1985; Nijp et al., 2017; Reeve et al., 2000; Winde, 2011). Models may implement the groundwater flow equation differently. Among the large-scale LSMs, only CLM 4.5 (Zeng et al., 2018) and ELMv1 (the land component of the Energy Exascale Earth System Model (E3SM); Bisht et al., 2018) found to simulate 2D lateral groundwater.

Some models can include more than one groundwater store or soil layer, each with a separate mass-balance, to deal with aquifer vertical heterogeneity, and shallow/deep groundwater (Table 4). In peatlands, shallow groundwater can contribute the most to runoff through base flow, especially during prolonged dry periods (e.g., Flynn et al., 2021). Gibson et al. (2000) studied a hypermaritime forest-bog and found that 85 % of runoff from a mid-summer rainfall event came from shallow groundwater, 12 % from new water, and 3 % from the bog and deep hillslope groundwater.

Water table elevation in an unconfined aquifer can be modelled using the groundwater flow equation with a fixed boundary (e.g., SUTRA; Provost and Voss, 2019) or, more rigorously, with a moving free surface boundary condition (e.g., MODFLOW6), which involves complex implicit solutions. The boundary can be specified either at points with atmospheric (zero) pressure head (e.g., in DigiBog; Baird et al., 2012) or, more generally, with zero flux.

Some models do not calculate the WTD based on the groundwater flow equation, but rather estimate it based on soil moisture content and other factors. However, their complexity, in terms of the inclusion of soil layers, lateral flow, and effects of microtopography, can vary. In SWAT, the WTD is simply assumed to be linearly proportional to the steady state groundwater flow. Some LSMs (Table 4) can apply (i) the variable infiltration capacity (VIC) model (Liang et al., 1994), which calculates WTD as a function of soil moisture and texture; or (ii) the topographic index concept (with slight variations), which estimates the hydraulic gradient of the water table almost parallel to the slope of the land surface. Using the latter method, WTD can be determined either by (i) calculating the soil's 'saturation deficit', which indicates the depth of the saturated zone; or (ii) integrating throughflow flux with Darcy's law. Although widely used in global scale studies, peatland-specific modules reject this in favor of a more optimal approach. For example, PEAT-CLSM incorporates a surface water storage variable for microtopography and revised parameterizations for macropore flow, surface/subsurface runoff, soil moisture, evapotranspiration, and plant waterlogging stress based on literature data from natural northern and natural/drained tropical peatlands (Apers et al., 2022; Bechtold et al., 2019). Unlike PEAT-CLSM, other peatland-specific LSMs are solely parameterized using northern peatlands data. Both CLM-SPRUCE (Shi et al., 2015) and its successor, ELM-SPRUCE (Ricciuto et al., 2021), are developed based on data from the ORNL SPRUCE experimental bog forest site in northern Minnesota. These models incorporate revised hydrological parameters, microtopography, and lateral flows, and calculate the WTD using a water balance equation. In other peatland-specific LSMs, microtopography is not taken into account. For example, CLASS (now referred to as the physics submodule of CLASSIC; Melton et al., 2020) converts soil moisture into WTD by using specific yield and specific retention based on peat hydraulic properties for three layers of soil (Letts et al., 2000) and one layer of moss (Wu et al., 2016). In another method, LPJ-WhyMe uses a modified parameterization for lateral subsurface discharge to convert total water volume stored in soil to WTD (only within the upper 0.3 m of soil or 'acrotelm'; Wania et al., 2009). In ORCHIDEE-PEAT, WTD in a grid cell is calculated using the surface runoff input from non-peatland fractions and the relative water content within 11 layers of soil (Qiu et al., 2018).

A general problem associated with modelling shallow water tables in peatlands is the high spatial variability caused by (i) microtopography, which determines ponding in hollows and the thickness of unsaturated zones, making it difficult to estimate air-filled pore space for water storage (Dettmann and Bechtold, 2016), and can significantly vary between drained, restored, and intact peatlands (Holden et al., 2011); and (ii) dramatic changes in hydraulic conductivity and porosity within a few centimetres of the surface, resulting in pronounced variations in flow velocity (Quinton et al., 2008).

### 3.3.3. Carbon cycle

In an ecosystem, the total photosynthetic carbon gain, or Gross Primary Production (GPP), is partly lost to autotrophic respiration,  $R_A$  (emitting  $CO_2$ ), leaving the remainder as Net Primary Production (NPP). Besides disturbances such as fire, a portion of NPP is lost through microbial decay of litter and soil organic matter to heterotrophic respiration,  $R_H$  (emitting  $CO_2$  and  $CH_4$ ), and methanogenesis/anaerobic respiration (emitting  $CH_4$ ). In general, these carbon cycle components can be conceptualized in two ways: (i) as a function of plant community composition, which accounts for species, population structure, size, and age of individual plants; and (ii) through a conceptualization of ecosystems as pools of carbon and their flows. Models following the first method, e.g., LPJml (von Bloh et al., 2018), and ORCHIDEE, integrate sophisticated representations of vegetation dynamics, whereas models following the second approach, e.g., ELM, CLASSIC, and CLM5, rely solely on simple biogeochemical representations. For both methods, patches of plant functional types (PFTs) should be defined, with each having individual vegetation properties, but relying on similar environmental forcings and soil properties. They implicitly assume that (i) mass conservation governs the interconnected pools; and (ii) flow from donor to receiver pool is controlled by the size and chemical composition of the donor pool. As a result, a set of first-order linear differential equations can be derived to represent the pools and fluxes. These equations can provide some mechanistic insight; however, they are all semi-empirical and have been modified continually to account for observations.

For instance, GPP calculations have been widely conducted using the Farquhar biochemical approach (Farquhar et al., 1980). GPP is dependent on numerous factors, including nutrients, sunlight, relative humidity, temperature, atmospheric  $CO_2$  concentrations, and carboxylation rates, depending on Rubisco's maximum rate. To partition NPP into different components, these equations require allocation parameters, which can either be fixed or variable as a function of light availability, soil temperature, soil moisture, and nutrients. Typically,  $R_H$  is calculated using empirical coefficients along with WTD, temperature, and soil C mass.

Methane production can be modelled using emission factors based on the substrate available to methanogens. Temperature, pH, microbial biomass, microbial growth efficiency, and oxygen availability are generally assumed to affect  $CH_4$  production, parameterized as a fraction of the heterotrophic respiration. Xu et al. (2015), for example, developed a  $CH_4$  module based on a microbial functional group, which has been integrated into the CLM 4.5 model and is being adopted for the E3SM land model (ELM; Yuan et al., 2021). The inundated fraction (or WTD) of the peatland surface is a critical consideration when calculating  $CH_4$  emissions. LPJ-WhyMe (Wania et al., 2009) and ORCHIDEE-PEAT (Qiu et al., 2018; Salmon et al., 2022) both model inundation stress and have been used to estimate  $CH_4$  emissions.

There are two major challenges facing studies of the integration of peatlands into global carbon cycling models: (i) peatland-specific PFTs, especially those involving Sphagnum or other mosses in northern peatlands; and (ii) the dynamics of microtopography and the interaction between hummocks and hollows (Largeron et al., 2018; Qiu et al., 2020; Shi et al., 2021; Wania et al., 2010; Wu et al., 2016). The peatland-specific models (i.e., CLASSIC, CLM\_SPRUCE, ELM\_SPRUCE, ORCHIDEE\_PEAAT, LPJml) include the main peatland's PFTs and have been applied globally or at specific sites.

### 3.3.4. Nitrogen cycle

Nitrogen and carbon together form the coupled C—N biogeochemical cycle. Several nitrogen compounds present in the atmosphere, e.g., NO and  $N_2O$ , are by-products of nitrification and denitrification, which are aerobic and anaerobic processes, respectively. Models that simulate these processes rely on either (i) simple fractional representations of N mineralization or soil mineral N concentration; or (ii) variations of the CENTURY (Parton et al., 1993; and its daily time-step version, DayCent; Parton et al., 1998) model or the DNDC model (Gillespy et al., 2014; Li

et al., 1992) parameterisations, that incorporate site-specific parameters (Bonan, 2019a).

The CENTURY model parameterizes nitrification and denitrification using experimental data (from laboratory incubations or field studies) rather than explicit biogeochemical processes. The amount of nitrogen lost to nitrification is influenced by several factors, including soil moisture, temperature, pH, N mineralization, as well as the concentration of  $\text{NH}_4^+$  in the soil. Denitrification, on the other hand, is determined by the labile carbon,  $\text{NO}_3^-$  concentration, and oxygen levels in the soil. Heterotrophic respiration ( $\text{CO}_2$ ) and the moisture content of the soil provide proxies for labile carbon and oxygen, respectively. The more anoxic the soil, the more  $\text{N}_2\text{O}$  is reduced to  $\text{N}_2$  during denitrification. CLM5 and ELM (ELMv1-ECA; Zhu et al., 2019) share the same CENTURY N model (Koven et al., 2013), but with independent modifications. A similar N cycle model has recently been implemented in CLASSIC, which represents both nitrification and denitrification (Asaadi and Arora, 2021).

In contrast to the CENTURY model, which applies its empirical assumptions globally without post-hoc analysis (Nevison et al., 2022), the DNDC model provides a more detailed representation of the processes involved in nitrification and denitrification. The DNDC describes the biogeochemical processes based on the kinetics of chemical reactions and diffusion in soil, e.g., when  $\text{NH}_4^+$  is dependent on organic matter decomposition in soil. O-CN is a modified version of ORCHIDEE that incorporates some concepts from both the CENTURY and DNDC models (Zachle and Friend, 2010). Using a similar mechanistic approach, SWAT has recently been coupled with the Microbial Kinetics and Thermodynamics (MKT) model, which simulates the coupled C—N processes in soil organic matter decomposition (Bhanja et al., 2019a; Bhanja et al., 2019b). Despite this, the original SWAT has been widely used for nitrogen processes (not for peatland research), including  $\text{NO}_3^-$  leaching, due to its reliable simplifications derived empirically from accumulated expertise in agricultural systems.

### 3.4. Potentials for a peatland community modelling platform

Our review of current models and approaches for peatland dynamics may reveal directions for future model development. In this respect, one potential way to reduce the proliferation of duplicative and redundant models is through a ‘community modelling platform’ (Slingerland and Syvitski, 2013). This approach provides modelling communities with the opportunity to collaborate more efficiently and consolidate knowledge gleaned from various models. Community models have proved successful in the areas of climate modelling (e.g., CESM; Hurrell et al., 2013), land surface modelling (e.g., CLM (Lawrence et al., 2011) and CSDMS (Tucker et al., 2022)), and has gained attention in other fields (e.g., in hydrology: Hut et al., 2022; Hydroshare, 2022; Weiler and Beven, 2015). Nonetheless, the applicability of a community modelling platform for peatlands has not been well investigated. Despite peatlands being widely simulated with ‘non-peatland-specific’, and in some cases community-based (e.g., CLM), process-based models, some studies suggest special algorithms and components are required in peatland modelling (e.g., Apers et al., 2022; Baird et al., 2012; Bechtold et al., 2019; Frolking et al., 2009; Jutras et al., 2009; Salmon et al., 2022; Shi et al., 2021; Shi et al., 2015; Wu et al., 2011; Wu et al., 2016). This is due to the unique characteristics of peatlands, including their (i) shallow water table; (ii) vegetation types (e.g., mosses); (iii) high organic matter; (iv) high heterogeneity in microtopography; and (v) slow decomposition rates. A multi-disciplinary approach to the study of peatlands has already been identified as a necessity (e.g., Jurasinski et al., 2020); hence, a community modelling platform for peatlands may be useful, where the community can jointly test hypotheses specific to these ecosystems. Developers and users would benefit from the platform by (i) updating theoretical frameworks simultaneously to address increasingly complex and interconnected modelling questions; (ii) receiving feedback on unique applications where specific approaches may fail; and (iii) sharing advances in numerical techniques, justified simplifications, and parameterizations to enhance computing efficiency (Clark et al., 2017).

An envisioned platform for the community could be an exclusive stand-alone or a subdivision (branch) of a broader FOSS-FAIR generic (and community) agreed modelling framework to be maintained and distributed by the community. It is noteworthy that scientific communities and models come from different backgrounds and a flexible, modular, modelling platform may be the most useful outcome. There are several reasons why this is preferable to the objective of a single model, including (i) a lack of agreement on relevant concepts, parameterizations, scales, and resolutions (Weiler and Beven, 2015); (ii) an unknown level of uncertainty due to increased complexity and inter-dependency of processes (Alexandrov et al., 2011; Baartman et al., 2020); (iii) reluctance of scientists to investigate processes outside of their research area (Fisher and Koven, 2020); (iv) cumbersomeness of linked sub-models (Baird et al., 2012); and (v) difficulties in transferring/integrating model results from one platform to another (Yates et al., 2018). On the other hand, some of these problems may be addressed by (i) unifying multiple modelling approaches (e.g., SUMMA; Clark et al., 2015) into a modular framework that can implement alternative modelling options, spatial discretization, and parameterizations; (ii) advancing computational capabilities to facilitate data acquisition, storage, and processing (Blair et al., 2019); and (iii) standardizing data formats and metadata to make data sharing more effective (Wilkinson et al., 2016). It is worth noting that implementation and long-term sustainability of the solutions rely heavily on the support of funding schemes (national and international) that prioritize flexible approaches and promote cross-disciplinary collaborations.

## 4. Conclusions

Process-based models have increasingly been applied to study peatland dynamics. However, the plethora of models and the expansion of interrelated research and management questions pose a challenge in identifying the ‘fit-for-purpose’ models. In this study, a thorough systematic search was performed to identify existing process-based models used for predicting peatland dynamics. We evaluated all models based on their (i) applicability to different types of peatlands and climate zones; and (ii) ability to meet our FOSS-FAIR criteria, which require open-source code, detailed documentation, and an active user community. After shortlisting FOSS-FAIR models, we reviewed and compared their key features and approaches (for energy, water, carbon, and nitrogen cycles) to summarize available modelling options and their shortcomings.

We conclude that there is currently no widely accepted one-size-fits-all model or approach, given the compromises between the complexity and the limited availability of data or computing resources. The shortlisted models described here, however, overlap in their scopes and approaches, and their similarities may extend to other aspects, e.g., code structure, which were not examined in our study. In this regard, we argue that a ‘community modelling platform’ for peatlands may enhance the ability to leverage the diversity of models and engage more scientists in cooperative research for a solid peatland modelling framework.

Finally, as our analysis is subjective and qualitative in nature, a systematic quantitative evaluation of each model/approach’s performance for specific applications remains to be carried out. An international intercomparison project is needed, as has been done with climate models, flood forecasting and wetland models. This will require a universal framework for data exchange and model calibration/validation, which our study showed is currently lacking. We anticipate that the findings of this study will serve as a useful guide for future model selections/development and stimulate the suggested international intercomparison project.

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## CRedit authorship contribution statement

**Behzad Mozafari:** Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Validation, Visualization, Writing – original draft, Writing – review & editing. **Michael Bruen:** Conceptualization,

Writing – review & editing, Funding acquisition, Supervision. **Shane Donohue**: Conceptualization, Writing – review & editing, Funding acquisition, Supervision. **Florence Renou-Wilson**: Writing – review & editing, Funding acquisition. **Fiachra O'Loughlin**: Conceptualization, Methodology, Writing – review & editing, Funding acquisition, Validation, Supervision.

#### Data availability

Data related to the review are attached as supplementary files.

#### Declaration of competing interest

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

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