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Review

A Review of Composting Process Models of Organic Solid Waste with a Focus on the Fates of C, N, P, and K

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Abstract: To foster a circular economy in line with compost quality assessment, a deep understanding of the fates of nutrients and carbon in the composting process is essential to achieve the co-benefits of value-added and environmentally friendly objectives. This paper is a review aiming to fill in the knowledge gap about the composting process. Firstly, a systematic screening search and a descriptive analysis were conducted on composting models involving the fates of Carbon (C), Nitrogen (N), Phosphorus (P) and Potassium (K) over the past decade, followed by the development of a checklist to define the gap between the existing models and target models. A review of 22 models in total led to the results that the mainstream models involved the fates of C and N, while only a few models involved P and K as target variables. Most of the models described the laboratory-scale composting process. Mechanism-derived models were relatively complex; however, the application of the fractionation of substrates could contribute to reducing the complexity. Alternatively, data-driven models can help us obtain more accurate predictions and involve the fates of more nutrients, depending on the data volume. Finally, the perspective of developing composting models for the fates of C, N, P, and K was proposed.

Keywords: composting; organic solid waste; models; nutrients; modeling scale; checklist

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1. Introduction

Organic solid waste (OSW), the solid waste containing organic matters (i.e., food waste, livestock manure, green waste), has been a critical issue for sustainable development due to its continuous increasement in amount and non-recycled treatment [1–3]. Till today, most OSW is still disposed of in unsustainable and conventional ways, such as landfilling and incineration [4], which result in the emission of greenhouse gases and leachate containing heavy metals [5], toxic gases such as sulfur dioxide, dust, heavy metal fumes, and incombustible hydrocarbons, and losses of valuable nutrients [4]. Therefore, the effective management strategies of OSW, including composting, are attached with more importance by relevant stakeholders and policy makers, with the aim of overcoming the challenge of environmental protection, promoting the circular economy and, hence, achieving sustainable development [6–8].

Compared with landfilling and incineration, composting is now one of the most popular technologies to recycle nutrients from organic waste [9], which can significantly shorten the processing cycle and more efficiently recover the nutrients from organic waste [4,10,11]. In China, about 76% of the poultry and livestock manure collected by intensive farming was processed through composting in 2015 [12], which can promote the organic fertilizer production industry and increase the circulation of regional nutrients [13]. Even

though fruitful results have been achieved in the research on composing, there remains a large challenge when microorganisms convert complex substrates into ultimately useful products in the composting process, in which some by-products, such as Ammonia (NH_3), Carbon dioxide (CO_2), Methane (CH_4), Nitrous oxide (N_2O), etc., are produced to burden the atmosphere [14,15]. The accumulation of P in surface soil can lead to the transfer of Phosphorus (P) to groundwater, which becomes an environmental concern during the compost application [16]. During the composting process, the Carbon (C) loss to the atmosphere ranges from 30% to 63% [17], and the Nitrogen (N) loss ranges from 19% to 42% mainly because of the vigorous NH_3 volatilizations, while the Phosphorus (P) loss is less than 2% mostly due to the runoff [18,19]. These data may be different due to the origin of various raw materials. The loss and dissipation of nutrients may not only lead to potential environmental risks, but also reduce the agronomic quality of the composted product [20]. Instead, applying more remaining C from composted fertilizer to the soil can reduce greenhouse gas emissions and sustainably mitigate climate change through storage or sequestration strategies [21]. It will also contribute to the efficiency of other fertilizers by altering soil properties, so as to bring environmental and agronomic co-benefits [22]. Therefore, for composting technology, it is significant to minimize both C and nutrient losses for the production of stable products with high quality.

Generally, the motivation of modeling is to develop mathematical tools to integrate the knowledge with the phenomena, determine the direction of experimental design, evaluate experimental results, test hypotheses, reveal relationships between variables, predict the system development, and design the process and management strategies [23]. Since 1976, mathematical models of composting technology have appeared in the literature [24]. In recent years, many models have been developed to contribute to predicting the distribution of temperature, humidity, solids, oxygen content, and carbon dioxide during the composting process [25–31]. However, from an environmental and agronomic point of view, the focus should be placed on regional C and nutrients for a better understanding of composting technology and assessment of the effectiveness of this sustainable solution [32]. Moreover, the methodology for regional assessments, such as life cycle assessment and material flow analysis, requires the accuracy of the model and a certain number of target variables to be simulated when it is used to simulate and evaluate composting technologies on a regional scale with high accuracy [33]. According to the research of Lauwers et al., the models can be grouped as mechanism-derived models that are established based on the biochemical reaction to reveal more mechanisms and data-driven models focusing more on the experimental data than the process of intermediate reaction [34]. According to the research results from the database of the *Web of Science Core Collection*, the number of papers on the composting process has shown an increase from 74 in 2011 to 114 in 2020. Initially, the focus of relevant research was mechanism-derived models [24], while in recent years, data-driven models based on various algorithms have gained more popularity [35].

Previous articles on the review of composting models usually focused on composting kinetics to discuss the process parameters, such as temperature, water content, pH, and carbon-to-nitrogen ratio (C/N). For instance, Mason reviewed and extensively analyzed composting models proposed in published papers before the end of 2003 [24]. He systematically described the establishment and improvement of the models on heat balance and mass balance during the composting process. Walling et al. conducted a comprehensive review on composting models published in the last 40 years to determine the trend of the composting models in terms of the goal and method, focusing on the research development of composting kinetics, heat balance, and mass (mainly water and oxygen) balance [35]. In recent years, more importance has been given to the simulation of the fates of C, N, P and Potassium (K) in the composting model. However, due to the complexity of the composting process, only a few papers have been published about the systematic review of the modeling of the fates of C and nutrients in the composting process. So, a further study with the application of models is necessary to delve into the fates of C, N, P and K

during the composting process. Therefore, the following two research questions are to be addressed with the aim of attaining a deeper understanding and new knowledge based on available studies through the systematic review:

1. What are the key features of existing composting models that involve the fates of C, N, P, and K? (RQ1);
2. How could the gaps between the existing model and the target model be well defined and presented? (RQ2).

The following parts of this paper are structured as follows: Section 2 presents the applied methods to show the process of a systematic review with a descriptive analysis; Section 3 includes the results; Section 4 proposes the guiding perspective of composting models involving the fates of C, N, P, and K, as well as the discussion on the implications of the study, and includes the explanation of how the fate of C, N, P and K in composting can be effectively described through modeling.

2. Methods

2.1. Literature Screening

A systematic screening search of relevant literature was conducted based on the core collection in the database of *Web of Science (https://www.webofknowledge.com)*, which is considered to cover papers of high quality and in sufficient quantity for a systematic review [36]. The time scope is defined as in the past ten years, from January 2011 to June 2020. The following search rule is used in the advanced search: "(TS = compost) AND (TS = model) AND ((TS = carbon) OR (TS = nitrogen) OR (TS = phosphorus) OR (TS = potassium))", where TS is defined as Topics.

A total of 722 related articles were collected, followed by a precise refining process based on the following three criteria, including: (1) the substrates for composting were OSW; (2) the target variables of modeling objectives involved at least one of C, N, P, and K; (3) the research modeled the process of composting technology. Specifically, the process of study selection and data extraction consists of three steps of results retrieval [37,38], as shown in Figure 1. First, search for articles based on a prioritized search strategy. Then, filter out irrelevant or unsuitable articles according to their titles and abstracts. Third, read the filtered articles in full text. Finally, a total of 22 models were selected for further studies, which are mainly from peer-reviewed journals or conferences such as *Bioresource Technology, Environmental Technology, and Waste Management*.

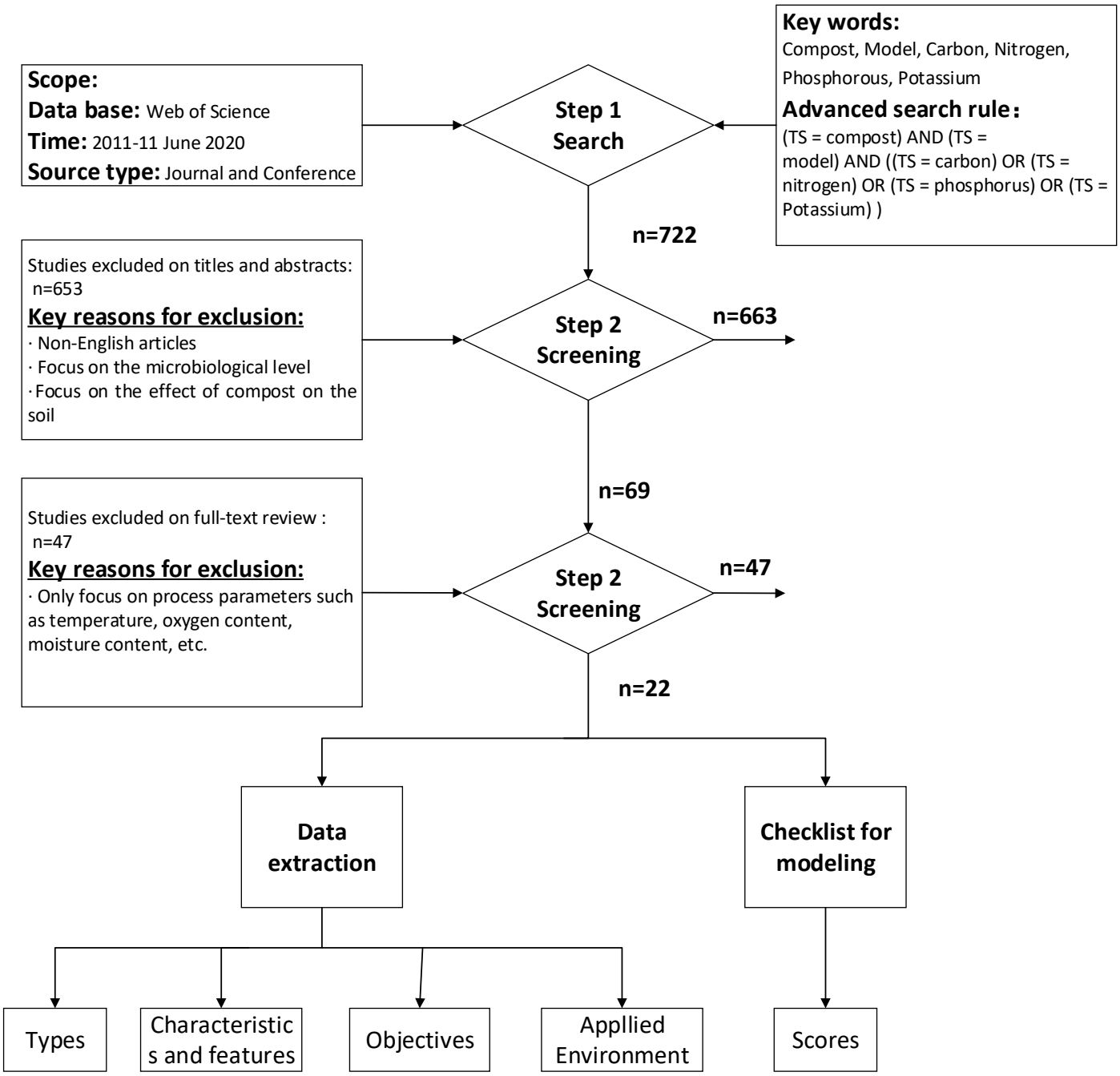

Figure 1. Process of study selection and data extraction.

2.2. Data Extraction

In order to further characterize the models, we developed code lists of target variables related to modeling objects, modeling approach types (mechanism-derived model types and data-driven model types), and applied environmental types as indicators to conduct data extraction as shown in S1, S2, S3, and S4. From these code lists, we then developed tables shown in S5 to describe and summarize the selected models.

2.3. Checklist for Model Assessment

A checklist approach was used to define the gap between the reviewed models and the target models. In this study, a checklist was designed according to the target models and the developing process of models. Given the fact that there is no consensus on the

best method of evaluating composting models, a brand-new checklist was finally developed and applied here to evaluate the models and help define the gaps of target models, while this method has been applied in other subject areas, such as ecology and medicine [39,40]. The most common questions in the checklists are whether the model clearly describes the objectives of modeling, whether the approach to modeling is reasonable, and whether the sensitivity and accuracy of the model are evaluated [39–41]. Developing a model follows six steps: analyze the problem, formulate a model, solve the model, verify and interpret the model's solution, report by the model, and maintain the model [42]. Furthermore, the emphases in the previous research on composting models, such as the composting substrates [43] and the model's reflection on the mechanism [44], have been combined in developing the checklist to determine three major categories: the start points of the model, the process of modeling, and the internal assessment of models. In addition, to be more in line with our review scope, the target variables of modeling were set on whether the fates of C, N, P and K are all involved as an indicator at the start point of the model. Moreover, since the nutrients' transformation mechanism plays an essential role in studying the balance of elements [44], we set the 7th item to explore the part of the data-driven model of revealing the mechanism in order to better identify the main factors influencing the composting process. The weight of each category is 5-point. As the modeling process of the mechanism-derived models is different from that of the data-driven models, in the second category, different questions were applied to evaluate the two types of models. If we assume the score for the most optimal model is 15, the gap between the model in the checklist and the most optimal one is reflected by 15 subtracting the score for the model. The specific checklist for the composting model is shown in Table 1.

Table 1. The checklist for composting models

Category	Items		References
Start points of models	Were the target variables of modeling clearly described? (1 point)		[39,40]
	Do the research objectives fit our review scope (C, N, P, and K)? (3 points) (1 point will be calculated for only one of C, N, P, and K involved in modeling; 2 points will be calculated for 2 or 3 of C, N, P, and K involved in modeling; 3 points will be calculated for all of C, N, P, and K involved in modeling. If partially involved in each related element only, such as CO_2 or C/N, 0.5 points will be calculated.)		
	Were the substrates of the study clearly described? (1 point)		[43,45]
Process of modeling	Mechanism-derived models	Data-driven models	
	Does the selection equation in the model clearly list the reference basis? (1 point)	Does the study identify the sources of the data and describe how the data were collected clearly? (1 point)	[39,41,42]
	Were the assumptions about the model clearly described? (1 point)	Was the modeling approach used clearly described? Does it include the reasons for adopting this approach (1 point)	[39,40,42]
	Was the basis for the selection of relevant parameters clearly described? (1 point)	Was the basis for the selection of variables clearly described? (1 point)	[24,40]

	How about the complexity of the models? (1 point, 0.5 points, or 0 will be calculated for Not complicated, Complicated, and Very complicated, respectively)	How well does the model reflect the composting process? (1 point, 0.5 points, or 0 will be calculated for Well reflect, Partly reflect, and Not reflect, respectively)	[42,44]
	Was the platform/software clearly described to solve/simulate the model? (1 point)		[42]
Internal assessment of models	Was the sensitivity analysis conducted? (1 point)		[40,46]
	Were experiments conducted to compare the models? (1 point)		[39]
	Was the accuracy evaluation method of the models clearly described? (1 point)		[34,42]
	How about the accuracy of the models? (2 points, 1 point, or 0 will be calculated for Very accurate, Relatively accurate, and Not accurate or not mentioned, respectively)		[42]

Out of the 12 questions, 9 were judged between yes or no, and the other three were scored based on the reality of the model. With reference to Wijewardhana et al. and Harris et al., we applied multiple reviewers to the checklist to ensure relative objectivity. All indicator questions were rated by three reviewers who have a research background in modeling or composting technology [39,40]. For yes/no questions, a discussion with the author would be proposed in case of a different judgment. For questions that needed to be scored according to circumstances, an average score was calculated. What is worth mentioning is that, in order to make the whole procedure as objective as possible, two rounds of review were conducted on the checklist and results, one internally by the authors and the other by an invited expert from the Institute of Soil Science, Chinese Academy of Sciences, an the external reviewer.

3. Results

3.1. Overview of Reviewed Models

The substrates, modeling approaches, and target variables of objectives for 22 referred models are shown in Figure 2. The 22 models were divided into two main categories based on the modeling approaches: 10 mechanism-derived models and 12 data-driven models. In particular, semi-empirical models fell in between [44], which are established based on mechanism-derived models but modified with experimental data. Since these three semi-empirical models were developed from a process perspective, they were also summarized in the mechanism-derived model in this section. The composting substrates of these models were mainly related to two categories including municipal solid waste (MSW) and agricultural waste. The target variables involved in the simulation, however, were mostly C and N, and to a lesser extent, P and K.

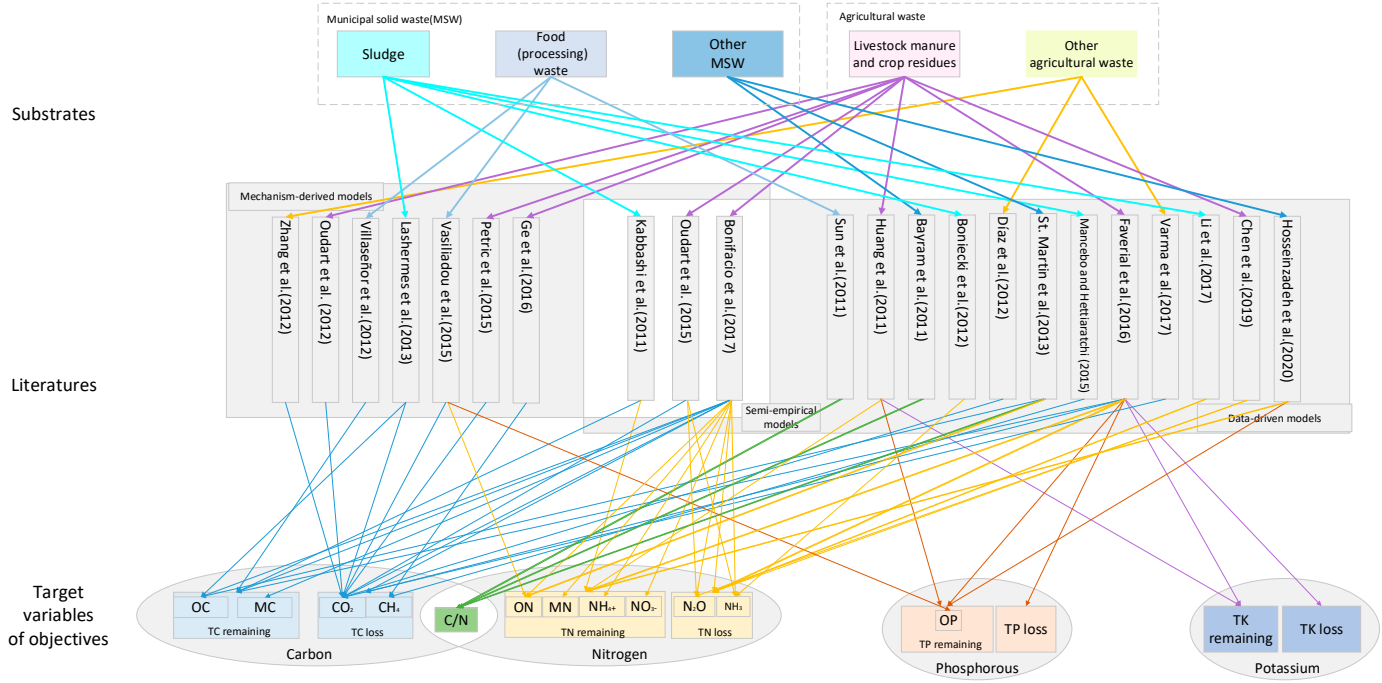

Figure 2. An overview of 22 reviewed models.

Notes: The abbreviations are defined as follows: **MSW** (municipal solid waste), **OC** (organic carbon), **MC** (microbial biomass carbon), **TC** (total carbon), **ON** (organic nitrogen), **C/N** (carbon-to-nitrogen ratio), **MN** (microbial nitrogen), **OP** (organic potassium), **TP** (total phosphorus), **TK** (total potassium).

3.2. Composting Substrates and Target Variables

The specific substrates of these models involved MSW and agricultural waste, as shown in Figure 3a. MSW mainly includes sludge (n = 5) and food waste or food processing waste (n = 3). In comparison, other types of municipal waste have been studied, including cardboard, boxwood leaves, and sawdust (n = 3). In these models, most of the simulation of agricultural waste concentrated on livestock manure and crop residues, such as pig manure, chicken manure, and cattle manure mixed with straws of rice, wheat, and corn (n = 8). In addition, other types of agricultural wastes include vegetable wastes and fruit leaves (n = 3).

To address the challenges posed by the complexity of the substrates for compost modeling, fractionation of the substrates was applied to separate the organic matter into multiple components. Simply put, the substrates are divided into three categories, namely, soluble, insoluble, and inert substrates [44,47–50]. Furthermore, a more detailed fractionation method was applied, in which the organic matters were divided into five compartments: the easily degradable and soluble; slowly degradable and soluble; hemicelluloses, cellulose, and lignin fractions [51,52]. With this method of fractionation, the degradation process of the organic matters can be described according to different degradation kinetics, thereby improving the accuracy of the model, and at the same time, providing a solution to the modeling of complex substrate composting.

Since the review scope of this paper was the fates of carbon and nutrients, only the target variables related to C, N, P, and K in modeling were included. There were two parts in each element: the remaining and the lost. It can be seen from Figure 3b that most models involved the simulation of C and N. Models involving carbon mainly included organic carbon (OC) (n = 3) and microbial carbon (MC) (n = 1). There was also research on the remaining of total carbon (TC) (n = 4). The simulation of carbon loss mainly involved CO_2 (n = 9) and CH_4 (n = 2). In terms of nitrogen, Bonifacio et al., St Martin et al. and Vasiliadou et al. developed models for organic nitrogen (ON) (n = 3) [33,49,53]. As for total nitrogen (TN) loss, Li et al. and Faverial et al. modeled this part as a whole variable (n = 2) [15,54];

others focused on the emissions of N_2O (n = 3) and NH_3 (n = 3). There were some models related to the C/N that are considered to play a key role in the composting process, and these models also involve the mass balance of C and N (n= 3). Vasiliadou et al., Faverial et al., and Huang et al. have developed models for the mass balance of total phosphorus (TP) (n = 3) [15,49,55]. The research by Faverial et al. and Huang et al. also involved the model of total potassium (TK) (n = 2) [15,55].

In addition, mechanism-derived models mainly simulated the relevant mass balance of C and N, and, to a lesser extent, the mass balance of P. In contrast, the data-driven models could cover a broader range of simulated objects and even involved K. However, there were no mechanism-derived models that included K in the selected research.

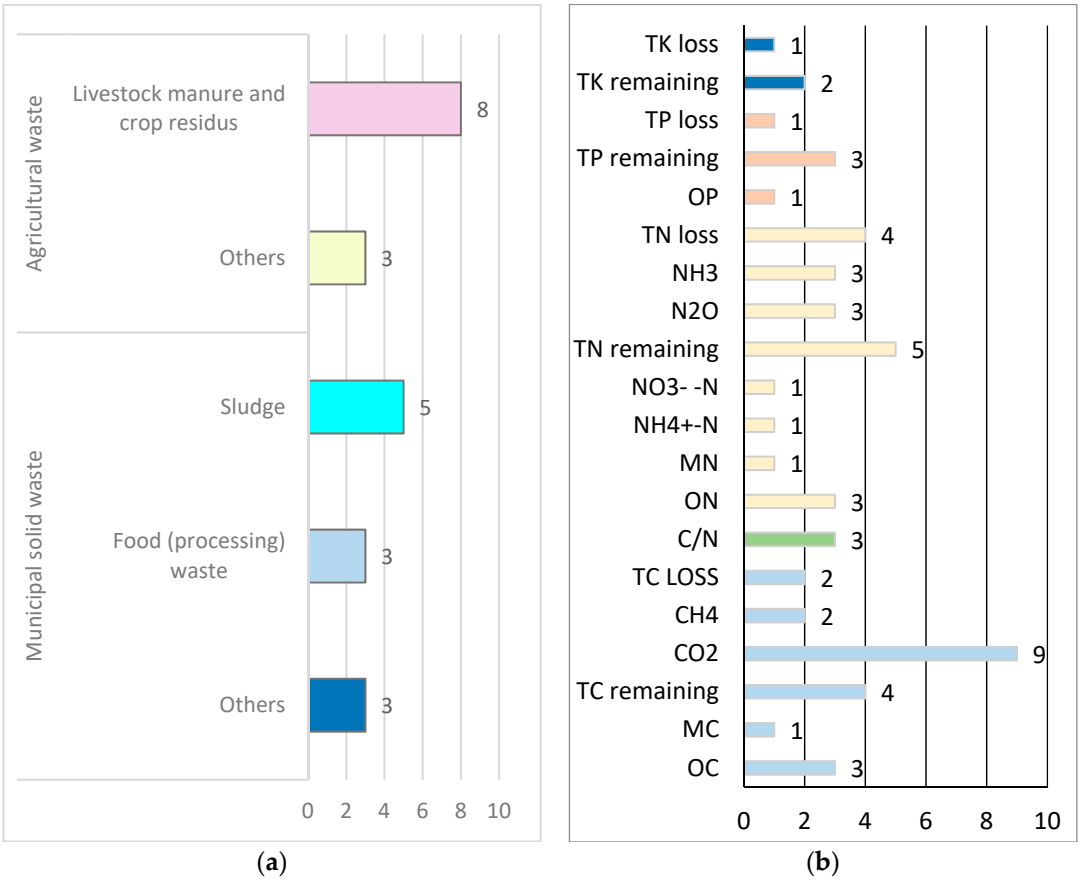

Figure 3. The specific situation regarding the (**a**) substrates and (**b**) the target variables of modeling objectives.

Notes: The abbreviations are defined as follows: **OC** (organic carbon); **MC** (microbial carbon); **TC** (total carbon); **ON** (organic nitrogen); **C/N** (carbon-to-nitrogen ratio); **MN** (microbial nitrogen); **OP** (organic potassium); **TP** (total phosphorus); **TK** (total potassium).

3.3. Modeling Approaches

3.3.1. Mechanism-Derived Models

The mechanism-derived models are generally based on mass balance, energy balance, and kinetics [56]. Composting kinetics describes methods of controlling the rate of waste degradation through environmental factors, such as temperature, oxygen utilization, and moisture. So far, various kinetics models for biomass degradation through composting have been developed based on the physical and biochemical characteristics of composting materials [57]. A summary of 10 mechanism-derived models and modeling objectives is shown in Table 2.

Table 2. Summary of 10 mechanism-derived models and modeling objectives.

No.	References	Mechanism-Derived Model Type Involved	Related Modeling Objectives
1	Zhang et al. 2012 [51]	Monod kinetics model	CO_2 corresponding to mineralization (% of initial total organic carbon)
2	Oudart et al. 2012 [47]	First-order kinetics model	CO_2 emission rate
3	Lashermes et al. 2013 [52]	Mass balance model	OC and CO_2 corresponding to mineralization (% of initial total OC)
4	Villaseñor et al. 2012 [50]	First-order kinetics model	C degradation (% of DM)
5	Vasiliadou et al. 2015 [49]	Monod kinetics model First-order kinetics model Mass balance model Heat (energy) balance model	Insoluble organic matter mass, insoluble N and P mass, and CO_2 emission volume
6	Petric and Mustafić 2015 [56]	Monod kinetic model Mass balance model Heat (energy) balance model	CO_2 mass
7	Ge et al.2016 [48]	First-order kinetics model Michaelis–Menten kinetics model Energy balance model Mass balance model	CH_4 emission rate
8	Kabbashi 2011 [58]	Semi-empirical model Multi-stage model	The remaining of TC and TN (% of DM)
9	Oudart et al. 2015 [44]	Semi-empirical model Process-based model	Production yield of CO_2, N_2O and NH_3
10	Bonifacio et al. 2017 [33,59]		OC, MC, ON, MN, NH_4^+, NO_3^- (% of DM), and emission rates of CO_2, N_2O and NH_3

OC (organic carbon); **TC** (total carbon); **TN** (total nitrogen); **MC** (microbial carbon); **ON** (organic nitrogen); **MN** (microbial nitrogen); **DM** (dry matter).

The common kinetics model is the first-order kinetics model (n = 6) related to the degradation of volatile solids or the utilization of oxygen. Hence, it has a close connection with the fate of C. The first-order kinetics model is based on temperature, oxygen, moisture, biodegradable volatile solids (BVS), and free space as parameters that affect the rate of degradation [60,61].

Another widely used kinetics model is the Monod kinetics model (n = 5), which was developed from the mechanical or deductive point of view by integrating the basic principles of physics, chemistry, and microbiology involved in the composting process [56,62,63].

The derivation of each kinetics model focuses on their mathematical formulas, which allows them to explain certain processes in composting. In the first-order kinetics model, the substrate concentration is used as the primary force determining the reaction rate, while the Monod kinetics model involves microbial activity, which makes the model more realistic.

Semi-empirical models are based on the mechanism with test data to modify and determine their model parameters. This approach is different from other mechanism-derived models, which requires a comprehensive understanding of the process. Unlike data-driven models that rely on large amounts of data, it is developed based on internal processes or stages. Oudart et al. simulated the interaction of nitrogen and carbon during

animal manure composting based on the main processes governing carbon and nitrogen transformations [44]. Then, models were analyzed and simulated according to the experimental data. Bonifacio et al. developed a process-based model for simulating cattle manure compost windrows [33,64]. In their research, the fate of C and N through processes affected by compost windrows was established. Combined with a large amount of empirical data, the parameters were determined to study the mass balance of C and N.

In order to describe more variables, more equations and parameters are required, leading to the complexity of models. In mechanistically derived models, the studies by Bonifacio et al. and Oudart et al. involved more related modeling objectives [33,44]. The former included 10 equations and 52 parameters, while the latter included more, with 26 equations and nearly 90 parameters. In addition to using mathematical models to simulate microbial growth, nitrification, denitrification and other biochemical process reactions, some physical processes were also described. For example, Bonifacio et al. incorporated the leaching and runoff of NO_3^-, as well as ammonia volatilization, into the model [33]. Oudart et al. also considered ammonia volatilization [44].

3.3.2. Data-Driven Models

Data-driven models are usually accompanied by experimental and empirical data collection to ensure the effective prediction of fundamental parameters [34], thereby establishing a reliable relationship between the model and the prediction of essential parameters or variables. A summary of 12 data-driven models and simulation objects is shown in Table 3.

Table 3. The summary of 12 data-driven models and simulation objects.

No.	References	Modeling Type	Input Variables	Target Variables Related to Modeling Objects
1	Sun et al. 2011 [65]	Genetic algorithm aided by the stepwise cluster analysis method	$NH_4^+ - N$ concentration, moisture content, ash content, mean temperature, and mesophilic bacteria biomass	C/N
2	Huang et al. 2011 [55]	Linear regression analysis	pH, EC, and DM content	The remaining TN, TP, and TK (% of DM)
3	Bayram et al. 2011 [66]	ANN model MLR model	Food and yard percentage, ash and scoria percentage, moisture content, fixed carbon content, the total proportion of organic matter, high, calorific value, and pH	C/N
4	Hosseinzadeh et al. 2020 [67]		pH, EC, C/N, NH_4^+/NO_3^-, water-soluble carbon, dehydrogenase enzyme, and total phosphorus	The remaining TN and TP (% of DM)
5	Boniecki et al. 2012 [59]	ANN model	Time, temperature, pH, EC, DM concentration, C/N, $NH_4^+ - N$ concentration	NH_3 emissions (% of air released from bioreactor chamber)
6	Díaz et al. 2012 [68]	An adaptive network-based fuzzy inference system	Aeration rate, moisture content, particle size, and time	CO_2 emission rate
7	St Martin et al. 2014 [53]	Critical exponential function	Composting formula, time and composting formula interacting through time	TOC and TKN (% of DM)

		Rectangular hyperbola function (Double) Fourier function MLR model		
8	Faverial et al. 2016 [15]	Bayesian network model	Total C, N, lignin, P and K contents, pH, and loss of mass	The remaining, and loss of, TN, TP, and TK (% of DM)
9	Mancebo and Hettiaratchi 2015 [69]	Regression model	Air-filled porosity, moisture content, and dissolved OC content	CH_4 emission rate
10	Li et al. 2017 [54]		Sucrose-adding ratio, adding time, sucrose concentration	The loss TN ration
11	Varma et al. 2017 [70]	RBF neural network model	Moisture content, pH, EC, TOC, TKN, soluble biochemical oxygen demand, $NH_4^+ - N$ concentration, available phosphorous, C/N, total phosphorous, oxygen uptake rate, Na, K, Ca	CO_2 emission rate
12	Chen et al. 2019 [71]	Backpropagation neural network model Linear regression model	Moisture content, C/N, aeration rate, and superphosphate content	Proportion of N_2O on TN

ANN (artificial neural network); **BP** (backpropagation); **RBF** (radial basis functional); **MLR** (multiple linear regression); **EC** (electrical conductivity); **DM** (dry matter); **C/N** (carbon-to-nitrogen ratio); **TN** (total nitrogen); **TP** (total phosphorus); **TK** (total potassium); **TOC** (total organic carbon); **TKN** (total Kjeldahl nitrogen).

Artificial neural network (ANN) is most widely used in data-driven models (n=6), which is designed to simulate the biological nervous system's response to real-world tasks [72]. In the reviewed articles, different types of neural networks have been studied, including multilayer perceptron (MLP) [59,67], backpropagation (BP) [71], and radial basis functional (RBF) [70]. BP is a systematic approach to training MLP. Bayram et al. (2011) used the MLP trained with the BP algorithm to develop models for simulating C/N of MSW composting [66].

Linear regression analysis of data is a monitoring technique used to model target values based on independent predictors [72]. The composting process can be modeled based on one variable (single regression) model or multiple variables (multiple linear regression (MLR)) model. St Martin et al. used different function models to simulate different parameters of the composting process, leading to the recognition that the composting temperature and OC are best described by the critical exponential function and the rectangular hyperbolic function, respectively [53]. ON, C/N, and pH are best described by double Fourier functions, while electrical conductivity (EC) is best described via Fourier functions. Huang et al. discussed the efficiency and feasibility of nutrient elements in chicken manure during composting with physical and chemical properties, such as pH, EC and DM [55]. It can be concluded that DM is a better predictor constructed as a single linear regression of nutrients, while DM and pH are more notable for MLR. Since MLR also involves multiple variables, it is usually compared with the ANN model in articles (n = 3). However, in terms of accuracy, the ANN model performed better in all three articles. Other models, such as Bayesian network models [15] and Genetic algorithms [65], are all used in data-driven models.

The selection of input is an important step in developing the data-driven model. As can be seen in Table 3, pH is the most commonly used input variable (n = 7), which has a

great influence on the decay, odor emission, nutrient conversion, and loss rate in the composting process [15,59]. Others, such as moisture content (n = 6), EC (n = 5), C/N (n = 4), and temperature (n = 3), are also commonly used as input variables.

3.4. Application Scales

Overall, as can be seen from Table 4, most of the mathematical models are still in the scope of the laboratory (n = 18). Bonifacio et al. and Oudart et al. developed semi-empirical models for the farm scale since the simulation and data collection were based on a farm over several years [33,44,64]. Huang et al. modeled based on data from composting plants in the perspective of a factory [55]. In addition, Vasiliadou et al. conducted a modeling study in the scale of the olive plant from the industrial plant scale [49]. According to the modeling approaches, both mechanism-derived and data-driven models could be studied at different scales. The research on the lab scale is more concerned with the composting reaction process itself through describing the target variables in detail. In contrast, research from the industrial plant scale and farm scale tends to account for more indicators.

Table 4. The numbers of reviewed models according to applied scales.

Applied Scales	Number of Reviewed Models	
	Mechanism-Derived Models	Data-Driven Models
Lab scale	7	11
Industrial plant scale	1	1
Farm scale	2	0

3.5. Sensitivity Analysis and Validation

Sensitivity analysis and model validation are the main approaches to evaluating models [42]. Since the mechanism-derived models have more parameters, sensitivity analysis on the model is often conducted to assess the uncertainty of model parameters (n = 6). It was noted in these studies that the maximum growth rate coefficient [49,51,56] and mortality constant have a more considerable influence on the composting process parameters [51,52]. For the data-driven model, in addition to the conventional sensitivity analysis (n = 7), there is the adopting analysis of variance (ANOVA), which can also be used to achieve the purpose of sensitivity analysis (n = 3) in terms of selected input variables. For instance, the ANOVA of St Martin et al. indicated that composting formula, time and composting formula interacting through time had a significant impact on the variables such as temperature, total organic carbon (TOC), total Kjeldahl nitrogen (TKN), C/N, pH, and EC [53]. Li et al. showed that the effect of addition ratio and addition time on nitrogen loss was statically significant at the 95% confidential level through ANOVA[54].

After obtaining a model, to verify the accuracy of the model, the determination coefficient (R^2) (n = 12) and root-mean-square error (RMSE) (n = 6) are the most commonly used methods to evaluate the quality of the fitting accuracy under the assumption that the parameters of the model are normally distributed. The calculation formulas are as follows [47]:

$$\mathrm{RMSE} = \frac{100}{E} \cdot \sqrt{\sum_{i=1}^{n} (S_i - E_i)^2 / n} \quad (1)$$

$$\mathrm{R}^2 = \frac{\sum_1^n (S_i - E)}{\sum_1^n (E_i - E)} \quad (2)$$

where E, S_i, E_i and n are referred to as the averages of experimental values, simulated values, experimental values, and the number of samples, respectively.

Others, such as Nash–Sutcliffe efficiency (NSE), a normalized statistic used to determine the relative size of the residual variance compared to the variation of the measured

data, is also used to evaluate a model's quality [51,52,70]. St Martin et al. adopted a parallel curve analysis to carry out variance accumulation analysis of the effect of compost type and time on physical and chemical parameter models [53].

3.6. Gaps with the Target Models Reflected by the Checklist

With the checklist, the scores of gaps ranged from 1.3 to 7.7, which can be seen in Figure 4. The model's scores were only obtained in the checklist that we created to show the gaps between the target models. The checklist could efficiently describe the fates of C, N, P, and K during composting. It was not aimed to completely distinguish the advantages and disadvantages of models, but largely focused on checking whether these models fit the scope and subject of the review, and how well they fitted the procedures modeled. It can be seen from Figure 4 that the research of Faverial et al. was more in line with the scope of the review, while the overall modeling was also in line with the specification, having an excellent performance in accuracy [15]. The paper of Chen et al., a conference paper with limited space, also attracted our attention, in which their scores were affected as some modeling procedures may not be described in details [71]. The starting points of the model involve the target variables of modeling objectives; however, there are many models that do not fully include C, N, P, and K. When the starting points of the model are excluded from checklist results, there are more models that also perform very well.

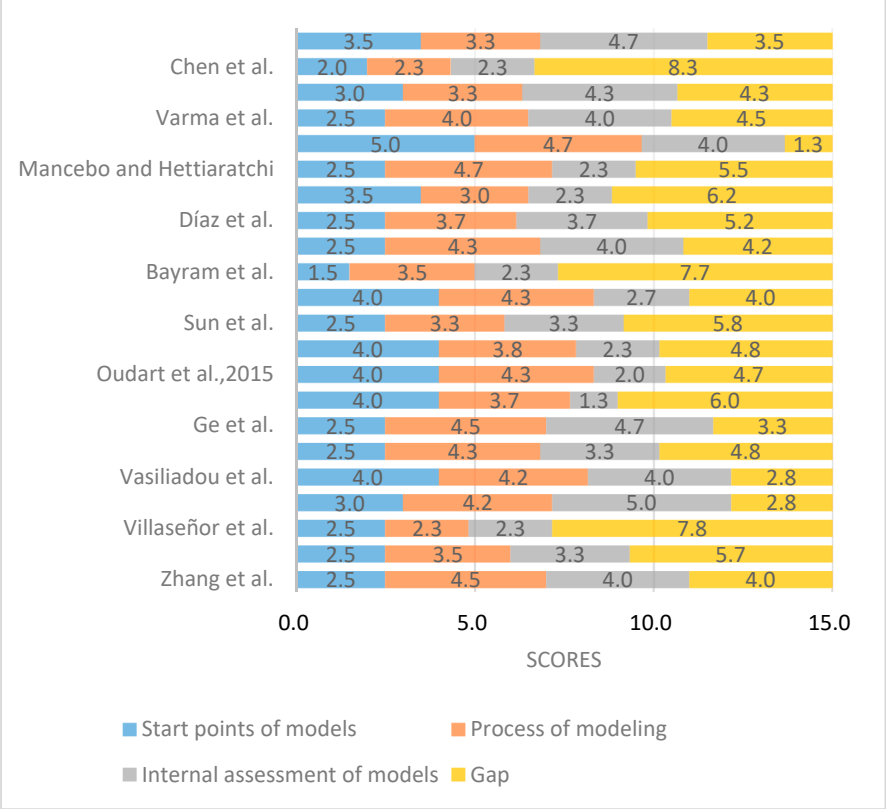

Figure 4. Results of the checklist for defining gaps.

4. Discussion

The purpose of developing models for the fates of C, N, P, and K is to improve process operations and, more importantly, deepen our understanding of the process, so as to improve the utilization of nutrients and reduce greenhouse gas emissions to achieve co-benefits for building the regional circular economy [73]. Therefore, the mechanics and the accuracy of the models are significant for the realization of the above purpose. Mechanism-derived models are ideal models for revealing mechanisms; however, a lot of effort is required due to the complexity of the models. Moreover, the composting process is a

biochemical reaction process that involves physical phenomena, such as volatilization and leaching [74], which are often ignored by most of the mechanism-derived models, resulting in compromised accuracy. With the study of microbial communities, more and more composition information about a data-rich microbial community will be gained to significantly improve the performance of the model. For example, further knowledge of microbial growth coefficients and mortality coefficients, etc., contributed a lot to the description of microbial activity in the composting process [34]. Additionally, in order to be able to simulate more nutrients, such as P and K, a focus on this part of the research would advance the development of mechanism-derived models of composting that involve more fates of nutrients. As Oudart et al. mentioned, black-box models such as data-driven models, due to the ignorance of complex reaction processes, often cause difficulty in explaining the differences between the results of simulation and observation [44]. The selection of input variables, sensitivity and uncertainty analysis is precisely the part that can react to the mechanism of the composting process. So, for data-driven models, this study will advance their role in revealing mechanisms. The issue of data reliability, however, has always been one of the top priorities for data-driven models. The application of advanced monitoring technology in the composting process will provide the model with certain intermediate process parameters, thereby reducing the possible errors.

At present, most of the models are at lab scale, which tend to focus on the fate of the C and nutrients in the process during composting. For the models on industrial plant or farm scales, more factors will be incorporated, such as N run off and leaching on the surface [33], as the data come from a wider perspective. In order to describe the modeling of composting in agricultural production activities on a regional scale, more indicators should be included, such as greenhouse gas emissions, nutrient losses, and proxies for ecosystem service that result from material exchanges among stakeholders [75].

Meanwhile, the development of open science will also promote the progress of the model. It is worth mentioning that among the 22 selected models, the model of Bonifacio et al. is based on the Integrated Farm System Model (IFSM) [33], which is a public integrated farm research tool for many physical and biological processes [76]. In addition, huge amounts of empirical data are included to provide support for the development of the model. In addition, it can be found that the researchers working on these models gradually began to pay attention to the significance of open science for scientific progress. For instance, Faverial et al. obtained the highest score in the checklist and their paper can be openly accessed [15]. Another treatment technology, anaerobic digestion (AD), a unified and open model of Anaerobic Digestion Model No. 1 (ADM1) was proposed as early as in 2002, which undoubtedly has played a positive role in the development of the AD models. Furthermore, some databases such as PHYLLIS 2 database are gradually being established, which provide a large amount of reliable, high-quality, and shared biomass processing data as strong support for the development of data-driven models.

Regarding this research, some limitations are also worth our attention: First, the research on latest models involving the fates of C, N, P, and K was conducted in the time scope of past decade, and only English-written papers from Web of Science were selected, which means less involved models were selected. Second, as we focused more on C and nutrients balance, the overview of composting modeling in our research is not as comprehensive as that in some other review papers regarding modeling of the composting process [35]. In fact, as was mentioned by Mason and Walling et al., heat balance, moisture content balance, and oxygen content balance have an essential impact on composting. Furthermore, there is inevitable subjectivity when the checklist is used to assess models [24,35]. These models and scientific articles are peer-reviewed and have a high level of creativity. However, data extraction through listing codes and the checklist evaluation method we applied are based on our review scope and more in line with the modeling procedure. Therefore, a degree of subjectivity may occur in our research of the checklist, mainly due to the professional background of the reviewers. More reviewers or multiple rounds of reviews would help to reduce the subjectivity. More importantly, our study

intends to provide guidance for future model development in the field of modeling on the fates of C, N, P, and K during composting process.

5. Conclusion

In this study, a systematic review was performed on the composting models involving C, N, P, and K. After reviewing the existing literature, 22 composting models were selected with the process of study selection. The application of a code-listing data extraction method could provide a framework for a better summary and cross-model comparisons. In addition, the characteristics and features of these 22 models were presented after data extraction. A checklist for composting models was created to define the gap between existing models and target models. The aim was to find the best fitting model for the composting of various types of substrates. According to the modeling approaches, 22 models were divided into two categories: the mechanism-derived models and the data-driven models. The results of the checklist showed that the score of the mechanism-driven models was slightly higher than that of the data-driven models. The main reason is that the description of the selection basis of variables is ignored in some data-driven models, resulting in a deficiency in highlighting the mechanism of the composting process.

The mechanism-derived model does not involve the simulation of the mass balance of K. Through the sensitivity analysis in these studies, it is found that maximum growth rate coefficients and mortality constants are the main factors for the kinetics parameters. Although the mechanism-derived model is complicated, adopting the method of substrates fractionation has reduced the complexity and improved the accuracy. At the same time, proposing a model framework such as ADM1 is also an approach to reducing the complexity of the model. With the development of artificial intelligence algorithms, data-driven models can cover more target variables involving more nutrients. However, how to reveal the mechanism of the composting process based on the selection of input variables and the establishment of a reliable database still needs some further research.

From the perspective of the model supporting the circular economy assessment at a regional scale, the focus should be on more indicators and high accuracy of models. On a larger scale, more indicators will be included in the modeling to allow for a more comprehensive assessment of circularity. At the same time, it is a scale-up process that requires a high level of accuracy for small scale models in order to ensure the accuracy of the regional model. These set requirements for the future development of composting models.

Abbreviations

AD	Anaerobic digestion
ADM1	Anaerobic Digestion Model No. 1
ANN	Artificial neural network
ANOVA	Adopting analysis of variance
BP	Backpropagation
BVS	Biodegradable volatile solids
C	Carbon
CH_4	Methane
CO_2	Carbon dioxide
C/N	Carbon-to-nitrogen ratio
DM	Dry matter
EC	Electrical conductivity
IFSM	Integrated Farm System Model
K	Potassium
MC	Microbial carbon
MLP	Multilayer perceptron
MLR	Multiple linear regression

MN	Microbial nitrogen
MSW	Municipal solid waste
N	Nitrogen
NH_3	Ammonia
N_2O	Nitrous oxide
NSE	Nash–Sutcliffe efficiency
OC	Organic carbon
ON	Organic nitrogen
P	Phosphorus
R^2	Determination coefficient
RBF	Radial basis functional
RMSE	Root-mean-square error
TC	Total carbon
TK	Total potassium
TKN	Total Kjeldahl nitrogen
TN	Total nitrogen
TOC	Total organic carbon
TP	Total phosphorus
VOC	Volatile organic compounds

Supplementary Materials: The following are available online at www.mdpi.com/2227-9717/9/3/473/s1, Table S1: Code list of target variables related to modeling objects, Table S2: Code list of mechanism-derived model types, Table S3: Code list of data-driven model types, Table S4: Code list of applied scale types, Table S5: Summary of 22 models.

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