Composting modelling: Towards a better understanding of the fundamentals, applications for enhanced nutrient recycling, greenhouse gas reduction, and improved decision-making

Thèse

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Résumé

Cette thèse de doctorat vise à consolider, développer et appliquer nos connaissances sur la modélisation du compostage, dans le but de fournir des informations, des outils et des perspectives accessibles et utilisables pour les chercheurs et les décideurs. L'espoir est que les travaux développés tout au long de cette thèse puissent aider à optimiser les procédés de compostage, notamment en réduisant les émissions de gaz à effet de serre (GES) et en améliorant le recyclage des nutriments. A ce titre, la thèse est divisée en trois phases : (1) la phase 1 est une consolidation et un développement des notions fondamentales de la modélisation du compostage, (2) suivie de la phase 2, où la modélisation de la perte de nutriments et des émissions de GES est étudiée, (3) avec la phase 3 qui est axée sur la manière d'assurer que ce travail puisse être utilisé par les décideurs et acteurs dans le milieu de compostage.

Dans la première phase, une revue complète et systématique de l'ensemble de la littérature sur la modélisation du compostage a été entreprise (chapitre 2), cherchant à fournir une meilleure compréhension du travail qui a été fait et sur la direction des travaux futurs. Ceci a été suivi d'une étudie détaillée des approches de modélisation cinétique actuelles, notamment par rapport aux facteurs de corrections cinétiques appliqués à travers le domaine (chapitre 3). La phase 2 s'est ensuite focalisée sur les notions spécifiques relatives aux émissions de GES et aux pertes de nutriments lors du compostage, et à la modélisation de ces phénomènes. Cette thèse présente les réacteurs expérimentaux et le plan conçu pour suivre et évaluer le processus de compostage (chapitre 4), ainsi que le modèle de compostage compréhensif développé pour prédire avec précision les émissions et la transformation des nutriments pendant le compostage (chapitre 5). Enfin, la phase 3 visait à rendre ces informations facilement et largement utilisables. Cela a commencé par une évaluation des meilleures pratiques pour développer des modèles et des systèmes d'aide à la décision pour la prise de décision environnementale (chapitre 6), suivi par le développement de nouvelles approches de modélisation cinétique simples (chapitre 7), culminant avec le développement, l'ajustement paramétrique et la validation d'un modèle de compostage parcimonieux (chapitre 8).

Grâce à ce travail, une base consolidée de l'état actuel de la modélisation du compostage a été développée, suivie par l'exploration et le développement de connaissances et d'outils à la fois fondamentaux et applicables.

Abstract

This PhD thesis aims consolidating, developing, and applying our knowledge on composting modelling, with the goal of providing accessible and usable information, tools, and perspectives for researchers and decision-makers alike. The hope is that the work developed throughout this dissertation can help in optimizing composting, notably by reducing greenhouse gas (GHG) emissions and improving nutrient recycling. As such, the thesis is divided into three phases: (1) phase 1 is a consolidation and development of the fundamentals of composting modelling, (2) followed by phase 2, where the modelling of nutrient loss and GHG emissions is investigated, (3) with phase 3 focusing on how to ensure that this work can be used by decision-makers.

In the first phase, a comprehensive and systematic review of the entirety of the literature on composting modelling was undertaken (chapter 2), seeking to provide a better understanding on the work that has been done and guidance on where future work should focus and how it should be approached. This review then raised some interesting questions regarding modelling approaches, notably regarding modelling of composting kinetics, which was studied in detail through the evaluation of current modelling approaches (chapter 3). Phase 2 then focused on the specific notions relating to GHG emissions and nutrient loss during composting, and how to model these phenomena. This section starts with a presentation of the experimental reactors and plan designed to monitor and evaluate the composting process (chapter 4), followed by the comprehensive composting model developed to accurately predict emissions and nutrient transformation during composting (chapter 5). Finally, phase 3 aimed to make this information easily and widely usable, especially for decision-makers. This started with a review on the best practices to develop models and decision support systems for environmental decision-making (chapter 6), followed by the development of novel simple kinetic modelling approaches (chapter 7), culminating with the development, calibration, and validation of a parsimonious composting model (chapter 8).

Through this work, a consolidated basis of the current state on composting modelling has been developed, followed-up by the exploration and development of both fundamental and applicable knowledge and tools.

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List of abbreviations

Abbreviation	**Description**
AHP	Analytical hierarchy process
AOB	Ammonia oxidizing bacteria
ASM	Activated sludge model
BA	Bulking agent
BOD	Biochemical oxygen demand
BOM	Biodegradable organic matter
C	Carbon
CBA	Cost benefit analysis
CF	Correction function
C/N	Carbon to nitrogen
COD	Chemical oxygen demand
CSTR	Continuous stirred-tank reactor
CTD	Controlled temperature difference
DM	Dry matter
DSS	Decision support system
EC	Electrical conductivity
EDSS	Environmental decision support system
ELECTRE	Elimination et choice translating reality
EPA	United States Environmental Protection Agency
EU	European Union
FA	Free ammonia
FAO	Food and Agriculture Organization of the United Nations
FAS	Free air space
FNA	Free nitrous acid
FTIR	Fourier-transform infrared spectroscopy
GC	Gas chromatography
GHG	Greenhouse gas
GI	Germination index
GIS	Geographic information system
K	Potassium
LCA	Life cycle assessment
LOI	Loss-on-ignition
MADM	Mult-attribute decision-making
MAUT	Multi-attribute utility theory
MC	Moisture content
MCDM	Multi-criteria decision-making
MODM	Multi-objective decision-making
N	Nitrogen
NOB	Nitric oxidizing bacteria
NRMSE	Normalized root mean squared error
ODE	Ordinary differential equation
OM	Organic matter
P	Phosphorus
PAO	Polyphosphate accumulating organism
PCM	Parsimonious composting model
PFR	Plug flow reactor
pH	Potential of hydrogen
PROMETHEE	Preference ranking organization method for enrichment evaluation

PSM	Phosphate solubilizing microorganisms
R^2	R-squared
RGB	Red, green, blue
RMSE	Root mean squared error
SA	Surface area
SA:V	Surface area to volume ratio
SOC	Soil organic carbon
T	Temperature
TC	Total carbon
TIC	Total inorganic carbon
TKN	Total Kjeldahl nitrogen
TN	Total nitrogen
TOC	Total organic carbon
TOPSIS	Technique for order preference by similarity to ideal solution
UN	United Nations

List of symbols

Symbols used throughout the thesis

Symbol	Description	Units
A	Pre-exponential factor (Arrhenius equation)	s^{-1}
a	Area	m^2
b_i	Microbial death rate	s^{-1}
BOM	Biodegradable organic matter	kg
c	Heat capacity	kJ kg^{-1} $°C^{-1}$
c_{T_i}	Temperature correction coefficient (cst.)	-
c_{MC_i}	Moisture correction coefficient (cst.)	-
$c_{O_{2i}}$	Oxygen correction coefficient (cst.)	-
c_{C/N_i}	C/N correction coefficient (cst.)	-
c_i	Combined correction coefficient (cst.)	-
$CO_{2,yield}$	Stoichiometric yield of CO_2 from carbon	kg CO_2 kg C^{-1}
$CH_{4,yield}$	Stoichiometric yield of CH_4 from carbon	kg CH_4 kg C^{-1}
ΔH_s	Biological heat generation coefficient	kJ kg^{-1}
E_a	Activation energy (Arrhenius equation)	kJ mol^{-1}
ε	Porosity	-
f_i	Correction function for i	-
f_{deg}	Biodegradable fraction of organic matter	-
G	Airflow	kg s^{-1}
GI	Germination index	%
$H_{A,i}$	Absolute humidity	kg H_2O kg air^{-1}
H_i	Enthalpy (inlet)	kJ kg^{-1}
H_o	Enthalpy (outlet)	kJ kg^{-1}
$H_{R,i}$	Relative humidity	-
H_2O_s	Water in substrate	kg H_2O kg S^{-1}
k_i	Rate of hydrolysis (1st order)	s^{-1}
$K_{s,i}$	Half-velocity constant	kg m^{-3}
$K_{M,i}$	Michaelis constant	kg m^{-3}
m	Mass	kg
$\dot{m}$	Mass flow rate	kg/d
MC	Moisture content	-
OM	Organic matter	%
ρ_a	Density of air	kg m^{-3}
ρ	Bulk/apparent density	kg m^{-3}
P	Ambient pressure	Pa
P_S	Saturated pressure	Pa
Q	Heat	kJ
Q_{bio}	Biological heat generation	kJ $m\text{-}^3$
R_i	Rate	kg s^{-1}
R	Universal gas constant	m^3 Pa $°C^{-1}$ mol^{-1}
S	Substrate concentration	kg m^{-3}
T	Temperature	°C
t	Time	s
T_a	Ambient temperature	°C
T_{max}	Maximum temperature (Rosso equation)	°C
T_{min}	Minimum temperature (Rosso equation)	°C
T_{opt}	Optimal temperature (Rosso equation)	°C
TIC	Total inorganic carbon	%

TOC	Total organic carbon	%
U	Global heat transfer coefficient	kW m^{-2} °C^{-1}
μ_i	Specific growth rate	s^{-1}
$\mu_{max,i}$	Maximum growth rate	s^{-1}
$\dot{v}$	Volumetric flow rate	m^3 d^{-1}
V	Volume	m^3
V_{FeSO4}	Volume of $FeSO_4$	mL
X_{deg}	Degradable fraction of organic matter	kg d^{-1}
$X_{non-deg}$	Non-degradable fraction of organic matter	kg d^{-1}
X_i	Biomass concentration	kg biomass m^{-3}
Y_{H2O}	Metabolic production of water	kg H_2O kg S^{-1}
Y_{O2}	Oxygen consumption	kg O_2 kg S^{-1}
$Y_{S,i}$	Yield coefficient	kg kg^{-1}
y_{exp}	Experimental result	variable
y_{model}	Model result	variable

Symbols used specifically in chapter 5 (comprehensive model)

Symbol	Description	Units
A	Area (contributing to conduction)	m^2
b_{BH}	Decay rate of heterotrophic bacteria	d^{-1}
b_{FH}	Decay rate of heterotrophic fungi	d^{-1}
b_{AOB}	Decay rate of AOB	d^{-1}
b_{NOB}	Decay rate of NOB	d^{-1}
c	Heat capacity of the substrate	kJ (kg °$C)^{-1}$
ΔH_s	Biological heat generation coefficient	kJ kg O_2^{-1}
ε	Porosity of the bed	-
f_p	Fraction of biomass going to inert products	-
G	Dry airflow	kg dry air/s
H_i	Inlet enthalpy	kJ/kg of air
H_o	Outlet enthalpy	kJ/kg of air
H_S	Saturated humidity of air	kg H_2O/kg dry air
η_y	Anoxic yield factor	-
η_{NO_3}	Difference in growth on NO_3	-
η_{NO_2}	Difference in growth on NO_2	-
η_{NO}	Difference in growth on NO	-
η_{N_2O}	Difference in growth on N_2O	-
η_H	Anoxic hydrolysis discount	-
η_{AOB}	AOB adjustment	-
i_{XB}	Nitrogen content of active biomass	g N/g cell TOC
i_{XP}	Nitrogen content of biomass debris	g N/g debris TOC
K_{15NO_3}	HSC for NO_3 for reaction 15	g N/m^3
K_{16NO_2}	HSC for NO_2 for reaction 16	g N/m^3
k_{aHB}	Ammonification rate of bacteria	m^3/(g biomass TOC.day)
k_{aHF}	Ammonification rate of fungi	m^3/(g biomass TOC.day)
K_{FA}	HSC for free ammonia	g N/m^3
K_{FNA}	HSC for free nitrous acid	g N/m^3
K_{PC}^{H}	Henry constant	atm L mol^{-1}

$k_{h,HB}$	Hydrolysis rate of bacteria	g TOC /(g biomass TOC.day)
$k_{h,HF}$	Hydrolysis rate of fungi	g TOC /(g biomass TOC.day)
K_{I11FA}	Free ammonia inhibition for reaction 11	g N/m^3
K_{I14FA}	Free ammonia inhibition for reaction 14	g N/m^3
K_{I11FNA}	Free nitrous acid inhibition for reaction 11	g N/m^3
K_{I14FNA}	Free nitrous acid inhibition for reaction 14	g N/m^3
K_{I3NO}	Nitric oxide inhibition for reactions 3 and 8	g N/m^3
K_{I4NO}	Nitric oxide inhibition for reactions 4 and 9	g N/m^3
K_{I5NO}	Nitric oxide inhibition for reactions 5 and 10	g N/m^3
K_{I15NO_2}	Nitrite inhibition for reaction 15	g N/m^3
K_{INH}	Ammonium inhibition	g N/m^3
K_{OA}	Half-saturation coefficient (HSC) for O_2 for AOB	g O_2/m^3
K_{OH}	HSC for oxygen	g O_2/m^3
K_{ON}	HSC for O_2 for NOB	g O_2/m^3
K_{N_2O}	HSC for N_2O	g N/m^3
K_{NO}	HSC for NO	g N/m^3
K_{NO_2}	HSC for NO_2	g N/m^3
K_{NO_3}	HSC for NO_3	g N/m^3
K_S	HSC for substrate (COD)	g TOC/m^3
K_{S5}	HSC for substrate for reactions 5 and 10	g TOC /m^3
K_X	HSC for hydrolysis	g slowly degradable TOC /g cell TOC
m	Mass of substrate	kg
μ_{BH}	Maximum growth rate for heterotrophic bacteria	d^{-1}
μ_{FH}	Maximum growth rate for heterotrophic fungi	d^{-1}
μ_{AOB}	Maximum growth rate for AOB	d^{-1}
μ_{NOB}	Maximum growth rate for NOB	d^{-1}
pH	Potential of hydrogen	-
P_{XH}	Phosphorus content of particulate matter	g P/g TOC
P_{XH}	Phosphorus content of biomass	g P/g cell TOC
ρ_a	Density of air	kg/m^3
ρ_{DM}	Dry bulk density of the substrate	kg/m^3
R	Gas constant	L Pa mol^{-1} K^{-1}
S_{alk}	Alkalinity	g HCO_3^-/m^3
S_I	Soluble inert organic matter	g TOC/m^3
S_{N2}	Dinitrogen-nitrogen	g N/m^3
S_{N2O}	Nitrous oxide-nitrogen	g N/m^3
S_{ND}	Soluble biodegradable organic nitrogen	g N/m^3
S_{NH}	Ammonia-nitrogen	g N/m^3
S_{NO}	Nitric oxide-nitrogen	g N/m^3
S_{NO2}	Nitrite-nitrogen	g N/m^3
S_{NO3}	Nitrate-nitrogen	g N/m^3
S_O	Oxygen (O_2)	g O_2/m^3
S_S	Soluble biodegradable substrate	g TOC/m^3
T	Temperature	°C
t	Time	s
T_a	Ambient temperature	°C
T_{max}	Maximum temperature (Rosso equation)	°C
T_{min}	Minimum temperature (Rosso equation)	°C
T_{opt}	Optimal temperature (Rosso equation)	°C
U	Global heat transfer coefficient	kW (m^2 °C)$^{-1}$

A	Area (contributing to conduction)	m^2
X_{AOB}	Autotrophic ammonia oxidizing biomass	g TOC/m^3
X_{DP}	Particulate decay products	g TOC/m^3
X_{HB}	Active heterotrophic bacteria biomass	g TOC/m^3
X_{HF}	Active heterotrophic fungi biomass	g TOC/m^3
X_{ND}	Particulate biodegradable organic nitrogen	g N/m^3
X_{NOB}	Autotrophic nitric oxidizing biomass	g TOC/m^3
X_I	Particulate inert organic matter	g TOC/m^3
X_S	Particulate biodegradable substrate	g TOC/m^3
Y_{AOB}	Yield coefficient AOB	g cell TOC formed/g N oxidized
Y_{CO_2}	CO_2 yield coefficient	kg CO_2/kg O_2
y_{H_2O}	Metabolic yield of water	kg H_2O produced/kg O_2 consumed
Y_{HB}	Yield coefficient heterotrophic bacteria	g cell TOC formed/g TOC oxidized
Y_{HF}	Yield coefficient heterotrophic fungi	g cell TOC formed/g TOC oxidized
Y_{NOB}	Yield coefficient NOB	g cell TOC formed/g N oxidized

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To **Lina Belia**, I am extremely grateful for your co-supervision. You were always available and willing to impart your knowledge unto me and have been one of the most significant factors in my development as a scientist and modeller. Your ability to get a project on track and to find a focused and realizable outcome by blocking out the noise (usually from an idealistic and slightly hyperactive graduate student) that can be so common in research, all while being kind and understanding, is something that I admire and aspire to as I continue to grow and develop in the field. I highly doubt that without your interventions, especially at the beginning of my studies, things would have gone so smoothly. I look very forward to what I am sure are inevitable future collaborations with one-another!

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Foreword

All of the work presented in this dissertation was undertaken at Laval University (Quebec, Canada) under the supervision of Prof. Céline Vaneeckhaute, Canada Research Chair in Resource Recovery and Bioproducts Engineering, between September 2018 and September 2021. Financing for this project stemmed from i) the Fond de Recherche de Québec sur la Nature et les Technologies (FRQNT) through a doctoral scholarship award to Eric Walling (138536) and ii) the Natural Sciences and Engineering Research Council of Canada (NSERC) through the award of an NSERC Discovery Grant (RGPIN-2017-04838) awarded to Céline Vaneeckhaute. Supplemental funding was awarded to Eric Walling by the following organisms throughout the course of his graduate studies: the Hydro-Quebec Institute for environment, development, and society (Institut EDS), Canadian National, Les Offices Jeunesse Internationaux du Québec (LOJIQ), the Saint-Lawrence Economic Development Council (Sodes), and CentrEau.

This dissertation has been undertaken by publication. All papers have been edited in order to ensure a flowing narrative and logical fit within this dissertation, as well as to avoid unnecessary repetition. The extent of this editing is restricted to removing and/or rewording the first few paragraphs of the introductions in some cases, as well as ensuring consistent spelling. In every case, the articles were envisioned, planned, researched, and written in totality by Eric Walling, with support, guidance, and revisions provided by the co-authors. The chapters of this work are made up of the following peer-reviewed papers, with a complete list of communications undertaken during the course of this PhD provided at the end of this dissertation, in Appendix G:

1. Introduction: The introduction has been written using a combination of original material and content from introductions of published and submitted works. These include:

- Walling E.[a,b], Trémier A.[c], Vaneeckhaute C.[a,b] (2020). A review of mathematical models for composting. Waste Management, 113, 379-394.
- Walling E.[a,b], Vaneeckhaute C.[a,b] (2020). Greenhouse gas emissions from inorganic and organic fertilizer production and use: A review of emission factors and their sources of variability. Journal of Environmental Management, 276, 111211.

- Walling E.[a,b], Vaneeckhaute C.[a,b] (under review). Modelling composting kinetics: An evaluation of functions used to correct for temperature, moisture, and oxygen.
- Walling E.[a,b], Vaneeckhaute C.[a,b] (2021). Nitrogen fertilizers and the environment. In Tsadilas C (ed.) Nitrate Handbook: Environmental, Agricultural, and Health Effects. CRC Press Taylor and Francis.

2. Chapter 2: Walling E.[a,b], Trémier A.[c], Vaneeckhaute C.[a,b] (2020). A review of mathematical models for composting. Waste Management, 113, 379-394.

3. Chapter 3: Walling E.[a,b], Vaneeckhaute C.[a,b] (under review). Modelling composting kinetics: An evaluation of functions used to correct for temperature, moisture, and oxygen.

4. Chapter 6: Walling E.[a,b], Vaneeckhaute C.[a,b] (2020). Developing successful environmental decision support systems: Challenges and best practices. Journal of Environmental Management, 264, 110513.

5. Chapter 7: Walling E.[a,b], Vaneeckhaute C.[a,b] (2021). Novel simple approaches to modelling composting kinetics. Journal of Environmental Chemical Engineering, 9:3, 105243.

6. Chapter 8: Walling E.[a,b], Vaneeckhaute C.[a,b] (under review). PCM, a parsimonious composting model for decision-making and optimization.

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Impact of the COVID-19 pandemic

Halfway through this PhD project, in early 2020, the world was struck by a pandemic caused by SARS-CoV-2, leading to widespread lockdowns across the globe and forcing a complete reimagining of our daily lives. Aside from the large-scale losses and societal shifts due to the pandemic, its impact was felt on a much smaller and less significant scale: the scope and course of this PhD.

The initial plan for this thesis was to develop a mathematical composting model that could accurately predict greenhouse gas emissions, nutrient transformation and loss, and pH during composting. As such, experimental composting reactors were designed and experiments using these reactors were planned to begin in May of 2020. However, the province of Quebec entered a full lockdown, with all non-essential businesses (including universities and research laboratories) closing on March 23rd, 2020. Access to our laboratories was only partially reinstated as of the end of May 2020, operating at a significantly reduced (25%) capacity for the rest of the year. In addition to this, administrative delays led to significant processing times for funding, orders, and shipping. Further restriction on the availability of materials and supply line delays meant that the experimental work planned for May of 2020 only commenced in July of 2021.

This delay greatly impacted the course of the PhD, given that the model had already been created and programmed by the time of the lockdown, only requiring calibration and validation with experimental results. To continue working on the advancement of knowledge during this time, the author decided to delve deeper into the fundamentals on composting modelling, leading to three chapters that had not originally been planned. Ultimately, given the delays, the knowledge gained during this time, and the necessary time to undertake the desired experiments, the difficult decision was taken to base model calibration and validation on data sourced from the literature and to leave a new graduate student take over the prepared experimental work. Nevertheless, the author firmly believes that, in the end, this benefited the quality of the final models and thesis, forcing their calibration and validation over a much larger set of data than what had initially been planned.

In addition to my prior acknowledgement, I want to take the opportunity to thank the essential workers, especially the medical personnel, who spent months working around the clock and fighting this virus, all the while physically and mentally exhausted. Your dedication and sacrifice are amazing.

Introduction

Over the course of the past century, the human population has nearly quintupled from about 1.6 billion people in 1900 to nearly 7.6 billion in 2017 (United Nations, 2017). This explosion in world population has resulted in a drastically increased demand for food and has put the agricultural sector under heavy stress to provide the necessary sustenance. Though the rapid growth in population has likely plateaued, the population is still expected to surpass 11 billion by the end of the century (United Nations, 2017). Because of this continued expansion (predominantly from developing countries in Africa) and of the increase in affluence in developing nations, we will continue to demand more from our resource-limited planet. Current estimates predict an increase in agricultural production of about 1.5% per year, totalling in a growth of about 15% over the next ten years (OECD, 2018) and 50 to 100% by 2050 (Baulcombe et al., 2009; Tilman et al., 2011).

To confront this threat, the initiatives undertaken during the “Green Revolution” of the 1950s and 1960s led to rapid developments in high-intensity agriculture. These innovative practices resulted in a threefold increase in cereal yields between 1950 and 1990, with similar outcomes in parts of Asia from 1960 to 1985 (Fageria et al., 2008; Smith et al., 2014). One of the driving factors behind these incredible results was, and still is, the use of mineral fertilizers.

Alongside these increasing crop yields, we also find an equally impressive 200-300% increase in fertilizer use between 1970 and 2010 (FAOSTAT, 2013; Smith et al., 2014), while China increased its nitrogen (N) fertilizer production by a factor of 39 between 1963 and 2015 (Luo et al., 2018). It is believed that, during this ground-breaking period in agriculture, at least 30-50% of the crop yield was attributed to the use of fertilizers (Baligar et al., 2001; Stewart et al., 2005). Consequently, it has been estimated that nearly 50% of the world’s population is dependent on nitrogen fertilizers for their sustenance (Erisman et al., 2008; Smil, 2002). Furthermore, this propensity towards fertilizer use does not seem to be waning, as the International Fertilizer Association (IFA) reported a 46% increase in urea production between 2003 and 2013 (Heffer and Prud’homme, 2016) and the Food and Agriculture Organization of the United Nations (FAO) predicted an annual increase in fertilizer nutrient demand of 1.5%, 2.2% and 2.4% for nitrogen, phosphorus (P) and potassium (K) between 2016 and 2020 (FAOSTAT, 2017).

However, though fertilizers have allowed us to keep up with the growing demand for agricultural products, their historical overuse (Byrareddy et al., 2019; Kurdi et al., 2020; Lu and Tian, 2017; Sun et al., 2019b; Withers et al., 2015; Zulfiqar and Thapa, 2017) has introduced an environmental crisis in many parts of the world. Indeed, improper use of fertilizers can have a detrimental effect on terrestrial, marine, and freshwater ecosystems by causing soil nutrient depletion (through unbalanced fertilization), soil acidification, eutrophication, nutrient run-off, reduced biological diversity, and greatly increased greenhouse gas emissions from agricultural practices (Horrigan et al., 2002; Sutton et al., 2013; Vitousek et al., 1997; Walling and Vaneeckhaute, 2021a).

Therefore, in the aim of maintaining our agricultural abilities while lessening the environmental and ecological impact of our current practices, a variety of alternative fertilization treatments have been explored. These, notably, include the growing use of waste-derived fertilizers and amendments that can present a solution to two of the major issues we face as a society. Indeed, concurrently to the environmental crisis of nutrient contamination, many areas around the world are also facing or dealing with a waste management crisis, particularly concerning organic waste. Organic waste represents about 50% of the total waste generated on the global scale and is composed of organic matter originating from sources such as food residue, human and animal waste, and garden and wood products (Hoornweg and Bhada-Tata, 2012). Currently, this organic matter is primarily dealt with by elimination through landfilling (Chen et al., 2020a). However, landfilling is an environmentally unsustainable method for waste treatment, resulting in a variety of undesirable and severe environmental impacts, coupled with a loss in potential recovery of valuable compounds. These consequences include contamination of the surrounding land and groundwater, large amounts of greenhouse gas emissions, and important spatial requirements (El-Fadel et al., 1997; Lou and Nair, 2009).

One of the leading tides to deal with this organic waste is by shifting the paradigm from disposal and elimination to recovery and reuse, especially given the valuable nutrients found in organic waste. Indeed, multiple biomass conversion technologies have been developed to address this issue (Walling et al., 2019), while many legislative frameworks have been and are being implemented to push for a transition towards these valorization processes (CCME, 2014; EU, 1999; Kjær, 2013). Many of these technologies, such as anaerobic digestion, composting, and pyrolysis, allow for the conversion of organic waste into value-added products, notably organic fertilizers (digestates, compost and biochars).

Of these various alternatives, composting has been amongst the most prominent over the past decades to divert organic waste from landfills and valorize the nutrients and organic matter within it (Chen et al., 2020a). Composting is the biological process through which organic matter is aerobically decomposed by bacteria, fungi, and macrofauna into compost. The process allows for the reduction of the weight and volume of the residual matter, while simultaneously killing off pathogens and organisms and leading to a value-added product (Hay and Kuchenrither, 1990). The resulting product, i.e., compost, is a humus-like substance that is rich in carbon and nutrients, thus promoting its use as an organic fertilizer or as a soil amendment. As such, compost has been demonstrated to increase the nutrient supply, increase crop yield, decrease soil erosion, and increase soil workability, all the while sequestering carbon and acting as a pesticide against certain insects (Lairon, 2010; Lazcano et al., 2014). There are also the added benefits derived from avoiding landfilling, such as reducing GHG emissions and decreasing soil and groundwater contamination. Furthermore, compost is a generally accepted product by the general population, in contrast to products of other biomass conversion processes, such as the digestate from anaerobic digestion and biochar from pyrolysis and gasification which, for the time being, require work to establish themselves in the eyes of the consumers (Al Seadi and Lukehurst, 2012; Dahlin et al., 2015; Dahlin et al., 2017; Riding et al., 2015; Torrijos, 2016).

Though organic fertilizers such as compost cannot replace the use of mineral fertilizers due to their significantly lower nutrient content, they do offer an important tool for farmers to properly balance their soil needs. However, despite the benefits derived from the composting process, the process still grapples with some important issues, notably related to nutrient loss during the process. Indeed, nitrogen loss can be significant during composting, either through ammonia (NH_3) volatilization, or denitrification into products such as nitrous oxide (N_2O) and dinitrogen (N_2). Indeed, some studies have reported N loss of up to 90% of initial nitrogen, with losses in the area of 20 to 70% being a common finding (Eghball et al., 1997; Li et al., 2017; Lim et al., 2017; Martins and Dewes, 1992; Ogunwande et al., 2008; Steiner et al., 2010; Witter and Lopez-Real, 1988). This not only represents an important loss in a valuable compound, but also an added environmental burden due to the significant greenhouse potential of N_2O. Similarly, phosphorus losses due to leaching of up to around 30% have also been reported in some works (Parkinson et al., 2004; Tiquia et al., 2002), presenting another economic and environmental burden.

Though some researchers have sought to shed a light on the state of nutrients and their recovery during composting through a variety of interesting and innovative experimental methods, the inherent complexity and variability encountered in the composting process can limit the generalization of this information. Indeed, many factors influence the composting process and to experimentally account for this variability over a large range of conditions (waste types, bulking agents, aeration rates, temperature, and moisture ranges, etc.) would require a massive investment in time and resources. This is where mathematical process modelling can play an important role. Instead of having to pass through extensive and repetitive experimental work, we can instead design a mechanistic model, i.e., a mathematical model based on theory, to represent physical and biochemical behaviour in the system that can allow us to simulate and optimize the composting environment. Having the ability to optimize the composting process to favor nutrient, notably nitrogen and phosphorus, recycling, ensure adequate degradation, and limit greenhouse gas emissions, can be an all-around boon, favoring the environmental, ecological, and economic benefits of the process.

Problem statement, objectives, and impact

The overall objective and expected impact of this project is to support the transition towards more sustainable and circular economies, while reducing the environmental impact of waste management treatment trains, notably regarding composting. This is achieved by providing decision-makers and experts with the targeted tools necessary to plan and optimize waste valorization and nutrient recovery trains. By increasing nutrient recovery and decreasing GHG emissions from composting, the overall environmental footprint of the process can be greatly decreased, and economic benefits can be increased. Future research should also be stimulated due to the work undertaken in this dissertation, notably through our efforts to provide easy access to knowledge on the field of composting modelling and the development of fundamental knowledge, while the models can be used to explore various new alternatives for process optimization that can then be validated experimentally.

The specific objectives of this PhD are pursued through the following problem statements and research questions, divided into three phases:

Phase 1: Consolidation and development of the fundamentals of composting modelling

- Problem statement/Research question 1: Composting modelling has been around for nearly 40 years, with a plethora of diverse modelling approaches being applied. Despite this continued growth in the field, there is very little knowledge on the current state-of-the-art. The only review on mathematical composting modelling dates to 2006 and, as such, presents a very limited picture of the progress in this area. Therefore, the first research question for phase 1 can be expressed as follows: What is the current state of knowledge in the field of composting modelling?
- Problem statement/Research question 2: Furthermore, despite decades of work on the subject, many areas in the field are still very contentious, such as the selection of kinetic expressions and the application of correction functions to best model the biodegradation process. Therefore, the second research question we address in phase 1 is: What correction functions (if any) are most appropriate to model composting kinetics?
- Objective of phase 1: To create a consolidated base of information on the fundamentals of composting modelling through a systematic review of existing composting models and modelling assessments of some of the "basic" but understudied areas of composting modelling. The aim of this phase is to create a strong knowledge base for the subsequent work undertaken during this PhD, while also providing a state-of-the art compendium to guide future modelling work in this field.
- Impact of phase 1: Through this consolidation and development of knowledge, it is expected that future modelling initiatives will have a clear guideline on how to approach composting modelling and easier access to information, hopefully favoring the development of high-quality models and guiding future research initiatives. Through this, practical and applicable model development should be promoted, leading to better outcomes for composting processes.
- Originality of phase 1: The current state of knowledge on composting is very spread out and unconsolidated, presenting an important roadblock to model development by limiting access to the field and knowledge transfer between

developers. As stated, the most recent review on composting modelling dates to 2006. Furthermore, certain knowledge, such as the use of correction functions which are fundamental to composting modelling (discussed in chapters 2 and 3), is greatly lacking, with limited and dated guidance provided to modellers. The work of phase 1 explores both these areas in great detail.

Phase 2: Experimental and modelling investigation of nutrient loss and GHG emissions during composting

- Problem statement/Research question 3: As highlighted during the introduction, despite the general advantages of the composting process, it still has many issues that could benefit from optimization. This is notably true for the loss of nutrients, thus decreasing compost quality, and the important emissions of potent GHGs. Given the great variability and impact of various operating parameters and variables on the process, undertaking this work experimentally would require extensive laboratory work that would likely suffer in generalizability and usability. Mathematical modelling provides a powerful tool to circumvent this issue by providing a generalizable framework to represent the composting system. However, current composting models do not consider the full breadth of GHG emission sources and nitrogen transformation pathways, presenting an important gap in knowledge. Therefore, the primary research question of phase 2 is: How can we mathematically model emissions of GHGs and nutrient loss during composting in a mechanistic fashion (and how do we apply such a model)?
- Objective of phase 2: To develop a dynamic comprehensive mechanistic mathematical composting model to predict GHG emissions and nutrient loss during the composting process. The aim of this model is to facilitate process optimization, allowing users to investigate the impact of various operating conditions on organic matter degradation, composting time, nutrient loss, GHG emissions, etc.
- Impact of phase 2: The development of a comprehensive model should allow for process evaluation and optimization, permitting users to reduce costs, decrease nutrient loss, and reduce environmental impacts from composting, particularly on a case-by case basis. Furthermore, such a model can be a valuable tool to research, validate, and understand the fundamentals of composting, allowing users to simulate and explore the various pathways for biodegradation, heat transfer, and nutrient transformation.

- Originality of phase 2: The originality of phase 2 stems from the development of the novel comprehensive model. Indeed, despite many experimental works following GHG emissions and a limited number following nutrient transformation and loss, modelling in these area remains nearly non-existent. The inclusion of the full nitrogen transformation pathway into a composting model has never been done. Furthermore, consideration of phosphorus and methane emissions is also a rarity.

Phase 3: Facilitating the use of models for successful environmental decision support

- Problem statement/Research question 4: Mathematical modelling is taking a more prominent place in environmental decision-making by providing decision-makers with a key tool to plan and predict for various alternatives and outcomes. In the context of composting, this can involve, for example, optimizing substrate selection to favor degradation, optimizing process volume or duration, or favoring factors such as nutrient recovery and GHG emissions reduction. This is most notably achieved through the ever-expanding field of environmental decision support systems, where stakeholders, experts, modelling, and decision sciences come together to aid in facilitating the decision process. However, despite significant work and guidance in these individual fields, the integration of these concepts together during the development of decision support systems remains understudied. This therefore raises the following research question: What practices, notably regarding mathematical modelling, should be implemented to favor successful environmental decision-making and system design?
- Problem statement/Research question 5: Based on the findings of research question 4, how can we develop a composting model that can best be suited for decision-making? One important notion for model usability by a wide range of users/stakeholders is that the model be simple enough to promote understanding and flexibility. Despite the existence of many simple composting models, the inherent complexity and dynamic nature of the process can still make these models relatively complex, depending either on data for many operating variables (temperature, moisture content, oxygen), all of which are highly variable, or using empirically derived expressions or parameters that are usually ungeneralizable, limiting the applicability. Therefore, the second research

question of phase 3 is: How can we model the composting process in both a simple and generalizable fashion?

- Objective of phase 3: To develop our knowledge on the practical and successful use of mathematical models in a decision-making context, with a notable focus on their practical use in decision support systems. From here, we can then create a novel model or library of models that can be best suited for use in this kind of application, notably through parsimonious (i.e., a model capable of explaining/predicting with minimal parameters and/or variables) and generalizable mathematical models.
- Impact of phase 3: Firstly, as in the case of phase 1, we hope that the consolidation of information on model use in decision-making can support the development of more usable and higher-quality models, favoring their use and implementation. Secondly, through the development of simple modelling approaches and a parsimonious model, the potential user-base of the work undertaken in this thesis will be greatly expanded, allowing for the benefits of phase 2 (economical, technical, and environmental optimization) to be at the hands of users other than experts, such as industries, municipalities, and operators.
- Originality of phase 3: As is the case for phase 1, there exists no guideline for environmental model development. Though the work presented in this thesis (chapter 6) is not a full development guide, it presents an important and lacking steppingstone towards achieving this guideline. The second primary point of originality is in the development of the parsimonious model, which resulted in the development of new empirical equations relating various variables/operating conditions to composting outcomes (emissions and nutrient loss), as well as the model itself.

The three phases of this project therefore address the above highlighted knowledge gaps by providing a consolidated base of knowledge about the state-of-the-art on composting modelling, developing our knowledge of composting kinetics modelling, creating a novel mechanistic mathematical composting model to predict GHG emissions and nutrient loss, exploring the integration of mathematical models into decision-making and how to best promote successful outcomes through decision support systems, and the development of a novel model library of simple composting models aimed at decision-makers.

Dissertation layout

The plan of the dissertation is as follows, with a visual representation of the phases of the project and the layout provided in Figure 1: the first chapter begins with a general overview of the composting process, with a focus on the mechanisms of biodegradation and nutrient transformation, as well as a brief section on the impact of operating parameters on nutrient loss and GHG emissions. It aims to provide the information necessary to both understand and validate the choices made throughout the experimental and modelling work undertaken in this project. Chapter 2 then goes on to provide a systematic literature review of the past 40 years of mathematical composting modelling, identifying trends in modelling approaches, the fundamental kinetics, heat and mass balances used to model the process, as well as exploring areas requiring research, and thus providing further justification to the interest and originality of this dissertation.

Following chapters 1 and 2, the dissertation transitions from a fundamental and theoretical framework to practical experiments and model development. Chapter 3 presents an assessment of correction functions used in composting modelling based on experimental results to further guide model development. Chapter 4 presents the experimental planning and reactor design, which was undertaken to assess nutrient transformation and loss, as well as GHG emissions, during the composting process. Chapter 5 presents the culmination of the prior work into the development and validation of the mechanistic composting model to predict nutrient transformation and GHG emissions. Chapter 6 explores the role of mathematical models in environmental decision support, highlighting important design considerations to facilitate the use of these models by a wider audience. Based on the results and discussion presented in chapter 6, chapter 7 presents novel simple modelling approaches are developed to simulate the composting process. Finally, chapter 8 contains the development, calibration, and validation of a parsimonious composting model, designed to follow nutrients and GHGs during composting, while being as simple to use as possible. This is followed by perspectives and concluding remarks in the final section of this thesis.

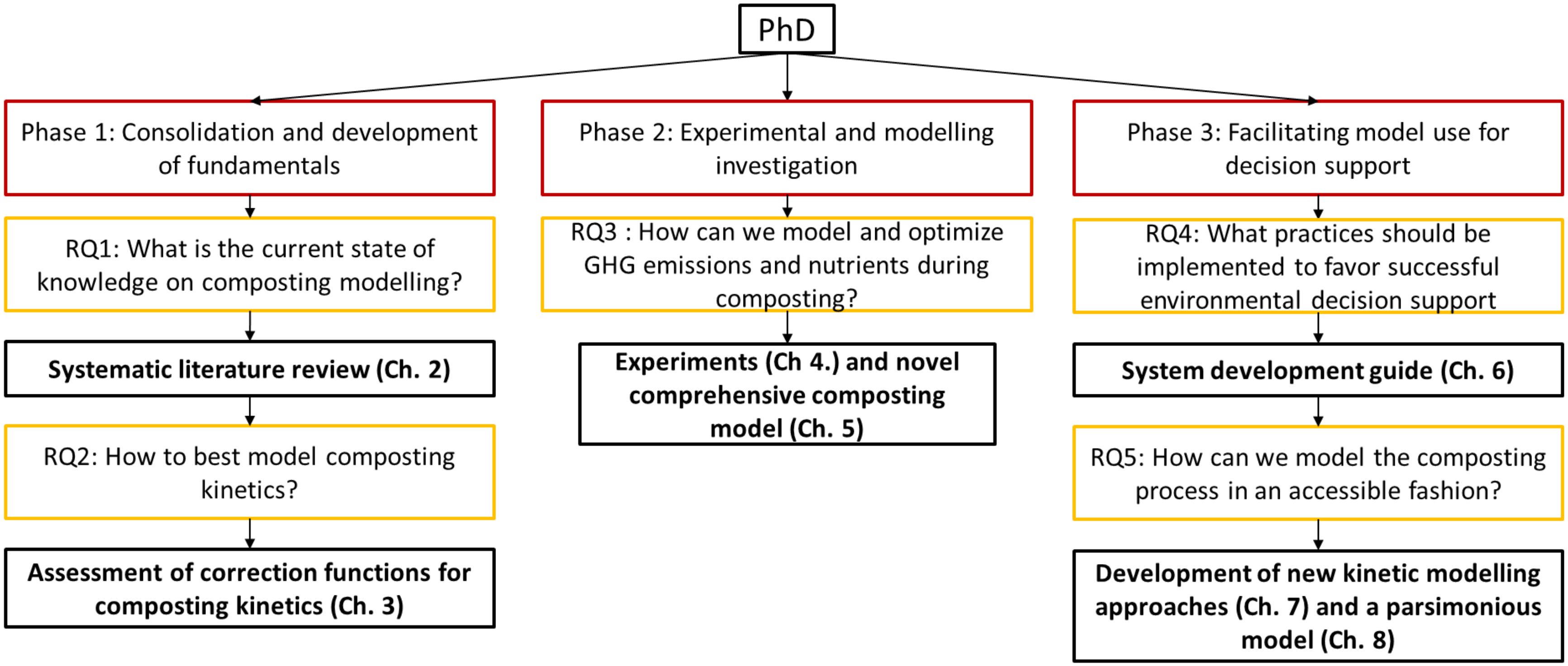
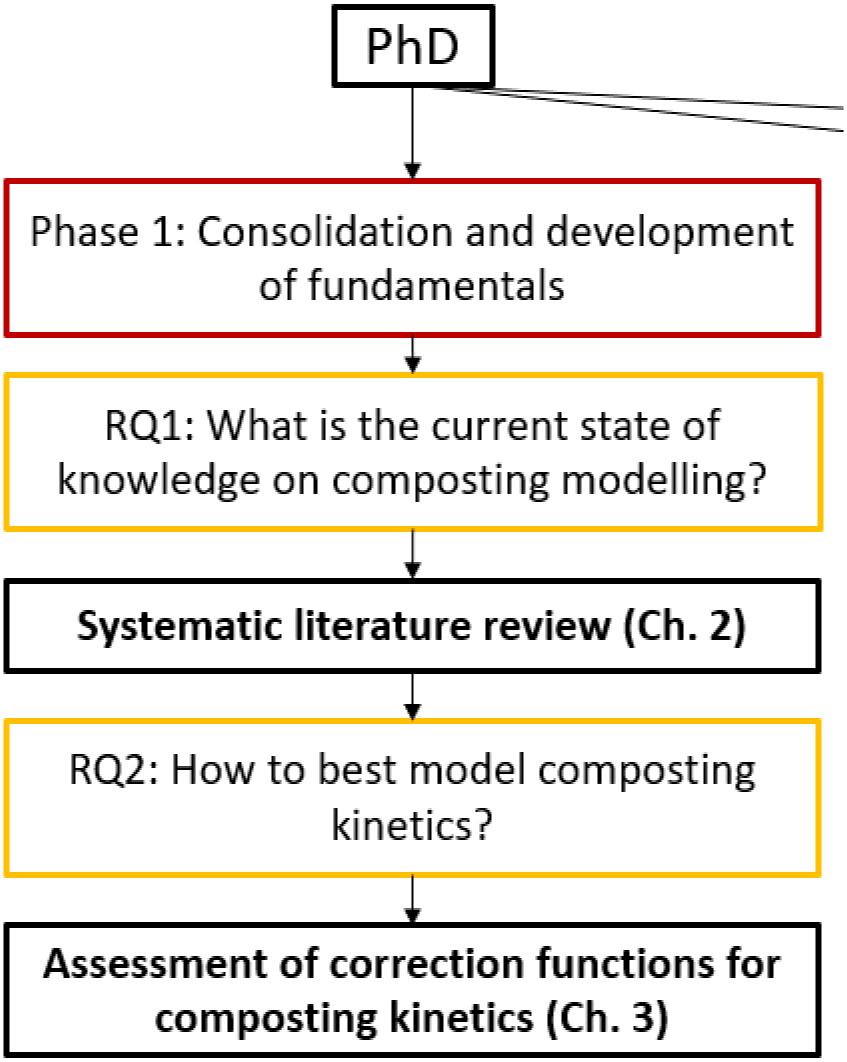


Figure 1. Dissertation layout.

Phase 1

Consolidation and development of the fundamentals of composting modelling



Chapter 1: General principles of composting, nutrient loss and transformation

The aim of this chapter is to provide general information on subjects at the core of this dissertation, particularly focusing on detailing what composting is, how the process operates on a fundamental level, and then exploring notions related to nutrient transformation and loss throughout the process, alongside gaseous emissions.

As detailed in the introduction, composting is an aerobic biodegradation process of organic matter, undertaken by a variety of microorganisms. Many composting systems exist, notably: windrow composting, static pile composting, in-vessel composting, tunnel composting, rotating drum composting, and vermicomposting (Gajalakshmi and Abbasi, 2008; Hay and Kuchenrither, 1990).

In general, the composting process can be divided into four stages: mesophilic, thermophilic, cooling, and curing (Abbasi et al., 2009; Chen et al., 2011; Tortarolo et al., 2008; Tortosa et al., 2017). The process is also often separated into two phases, an active and a passive one. The active phase, during which degradation occurs, encompasses the first two stages and part of the cooling stage, while the passive phase represents cooling and curing.

The process can be described as follows. During composting, mesophilic organisms, operating in the range of 25-45 °C, will start decomposing the substrate. This initial phase only lasts a few days during which short-chained organic compounds and easily biodegradable constituents are decomposed. As time progresses, the decomposition will lead the temperature to increase to around 50-60 °C, causing thermophilic organisms to take over the decomposition. During this phase, fungi, sporogenic bacteria, and actinomycetes decompose oils, proteins, and hemicellulose. The thermophilic phase is also responsible for the destruction of pathogens and seeds, which could hinder the on-field application of compost. Proper aeration is needed to maintain this phase of the process to ensure that the organisms receive enough oxygen to maintain an aerobic environment. Consequently, in systems with discontinuous aeration, such as windrows, temperature waves can be observed: the substrate is initially rich in oxygen, thus increasing in temperature, which subsequently declines as the oxygen is consumed for microbial activity, this pattern repeating at every mixing event (Abbasi et al., 2009).

Progressively, the temperature will decrease as less nutrients and energy are available for the organisms, leading into the cooling phase; mesophilic organisms taking up the reins once-again. The temperature will then stabilize, and the process enters the curing phase, which can last several weeks/months and increases the quality of the compost. During the curing phase, humic substances are formed by secondary reactions (condensation and polymerization of organic chains) (Gao et al., 2019; Wu et al., 2017; Xie et al., 2019) and the compost is made more suitable for agricultural application (improved pH, decreased C/N ratio) by decreasing the phytotoxicity. This is known as maturation of the compost. Figure 1.1 presents the general temperature profile during the composting process.

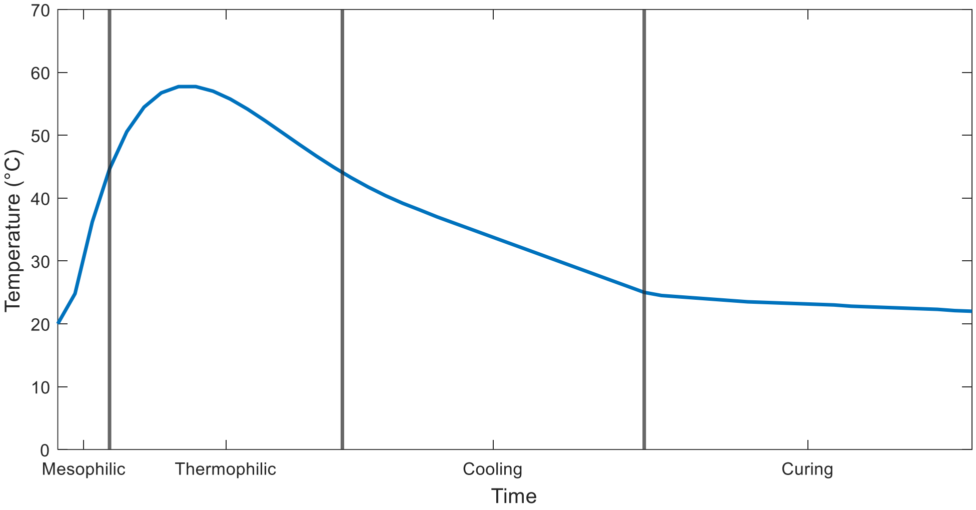


Figure 1.1 Temperature profile during the composting process.

Depending on the technology used, composting can either be a batch, semi-batch, or continuous process. Tunnel composters, in-vessel composters, and rotating drum composters can be operated continuously, reflecting the operation of a continuous stirred-tank reactor (CSTR) or a plug flow reactor (PFR) and allowing for continuous composting in the thermophilic phase (Gajalakshmi and Abbasi, 2008; Schulze, 1962; Xiao et al., 2009; Zarkadas et al., 2018). Windrow and static pile composting are more often operated in a batch setting. Indeed, the addition of fresh substrate can lead to negative consequences on the process due to modification in substrate composition and a decrease in temperature, reducing the efficiency of the microorganisms (Nakasaki et al., 1998; Sundberg and Jönsson, 2005; Wang et al., 2017). However, recent work has investigated using this decrease in temperature beneficially for low-temperature composting, to counteract the self-heating of the pile (Sun et al., 2019a).

Another important method of composting is vermicomposting, which operates in a very different manner; operating usually between 12 °C and 25 °C with the help of worms (Ndegwa and Thompson, 2001). The process and products are somewhat modified due to the needs and by-products of the worms, resulting in some benefits, such as reducing nitrogen loss and a higher accessible nutrient content, as well as drawbacks relating to a potentially reduced pathogen destruction, though more studies are needed in this area (Hénault-Ethier et al., 2016; Lazcano et al., 2009; Lim et al., 2016; Ndegwa and Thompson, 2001; Nigussie et al., 2016; Quaik and Ibrahim, 2013). One point of interest with vermicomposting is that it can be operated in batch, semi-batch or continuous modes (Abbasi et al., 2009). Though a very interesting and promising approach, vermicomposting and its modelling will not be explored in this dissertation due to its unique nature compared to the other modes of operation.

1.1 The biofilm: the seat of microbial activity and degradation and transformation during composting

Looking at the composting system more closely, it is possible to describe it as a three-phase system. There is a solid phase, made up of the organic matter, surrounded by an aqueous phase, in which the microorganisms are found, and a gaseous phase (air) passing throughout. The term biofilm is generally used to describe the layer of microorganisms that are in the aqueous phase and adsorbed onto the solid's surface. It is these microorganisms that are responsible for the degradation of the organic matter. Figure 1.2 presents a schematic overview of this.

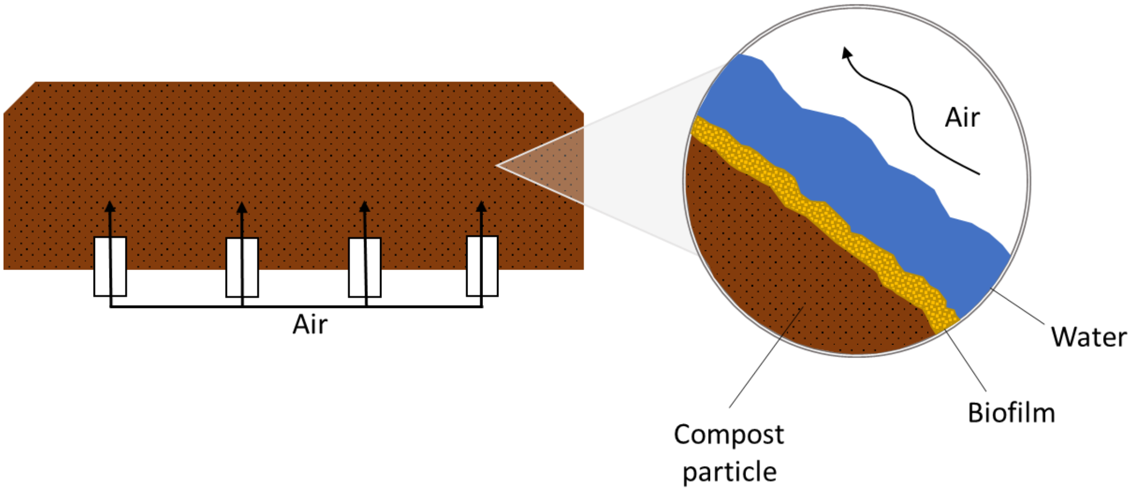


Figure 1.2 Conceptual model of organic matter in a composting heap and representation of the biofilm. On the left is a representation of the composting mound, while the right shows the interface between the gaseous, liquid, and solid phases (particle surface).

The microorganisms will initially colonize the solid substrate and proceed to multiply, forming the biofilm. This proliferation is due in part to the presence of carbon (C) and nitrogen (N) in the organic matter. The carbon serves as the primary energy source for the microorganisms, as well as a building block for their cells. In order for the substrate to be degraded, carbon must be taken up by the organisms in the biofilm. This process varies depending on the form of the carbon. Some carbon is considered to be easily and readily degradable, most-often being in soluble form, such as sugars and organic acids (Wang and Witarsa, 2016). This contrasts with the carbon found in more complex forms, such as hemicellulose, cellulose, and lignin. In these cases, the carbon can only be accessed by the microorganisms following disintegration and/or enzymatic hydrolysis, both of which happen extracellularly (Batstone et al., 2002).

Regardless of how it reaches the cells, the carbon uptake by the biofilm is then undertaken by aerobic organisms through microbial respiration. In this situation, oxygen (O_2) is consumed as an electron receiver and the carbon is mineralized into carbon dioxide (CO_2). The oxygen reaches the biofilm through dissolution in the aqueous phase. This highlights the necessity of proper moisture content and aeration. If one or both of these conditions fail, the aerobic microorganisms will be replaced by anaerobic ones, producing methane (CH_4) instead of CO_2. This is especially likely during the thermophilic phase of the process, given the proclivity of methanogens for higher temperatures (Megonigal et al., 2004), and greater oxygen consumption during this highly active period. However, if a process is well operated, it is generally expected that the large majority of carbon emissions will be as CO_2, with CH_4 emissions representing 0 to 10% of total C loss and production of volatile organics being below 5% of total C loss (ADEME, 2012; Walling and Vaneeckhaute, 2020b).

Nitrogen is also implicated in microbial activity, serving as an energy source for nitrifying organisms and as a metabolite for amino acid production. Nitrogen can be transformed or emitted through a variety of pathways in the composting process. These include ammonification/mineralization, immobilization, nitrification, denitrification, and volatilization. Figure 1.3 presents a conceptual overview of N transformation and loss during the composting process. During ammonification, also known as mineralization, organic nitrogen ($R\text{-}NH_2$) groups from the substrate are oxidized to ammonia (NH_3) or ammonium (NH_4^+), where ammonium can then be used for metabolic purposes, such as forming amino acids. When the microorganisms produce NH_3/NH_4^+ in higher quantities than needed, the surplus is excreted into the environment. The converse reaction is known as immobilization, where NH_4^+ is taken up by the microorganisms from their environment to produce organic N for their metabolism (amino acids). Ammonium can also be used through nitrification, where it is converted to nitrite (NO_2^-) and then nitrate (NO_3^-) in aerobic zones, to produce energy once again. This nitrate can then be converted through multiple steps into nitrous oxide (N_2O) followed by dinitrogen (N_2) through the denitrification process that occurs when the microorganisms use nitrate as a source of oxygen for their respiration in anoxic conditions.

The processes of mineralization and nitrification are important during composting, seeing how they produce NH_4^+ and NO_3^- that can easily be used by plants, whereas the other forms of nitrogen cannot be used directly. However, the main issue we encounter during composting is high volatilization of ammonia to the atmosphere. Indeed, as will be discussed in the following section, N-loss through volatilization can reach upwards of 90% in some cases (Eghball et al., 1997). Ammonia and especially nitrate can also be lost through leaching, when they are captured in water that flows through and leaves the composting pile. Though, generally speaking, N-loss through leaching for composting is very minor, accounting for about 0.5% of total nitrogen loss, with many studies even finding little to no production of leachate (Eghball et al., 1997; Trémier, 2004). Nitrogen loss as N_2O due to nitrification and denitrification generally tends to be low, usually below 15%, and happens mostly during the cooling phase. Nonetheless, it is possible to have very high N_2O emissions, even above 50% of initial nitrogen, depending on the substrate and operating conditions (ADEME, 2012).

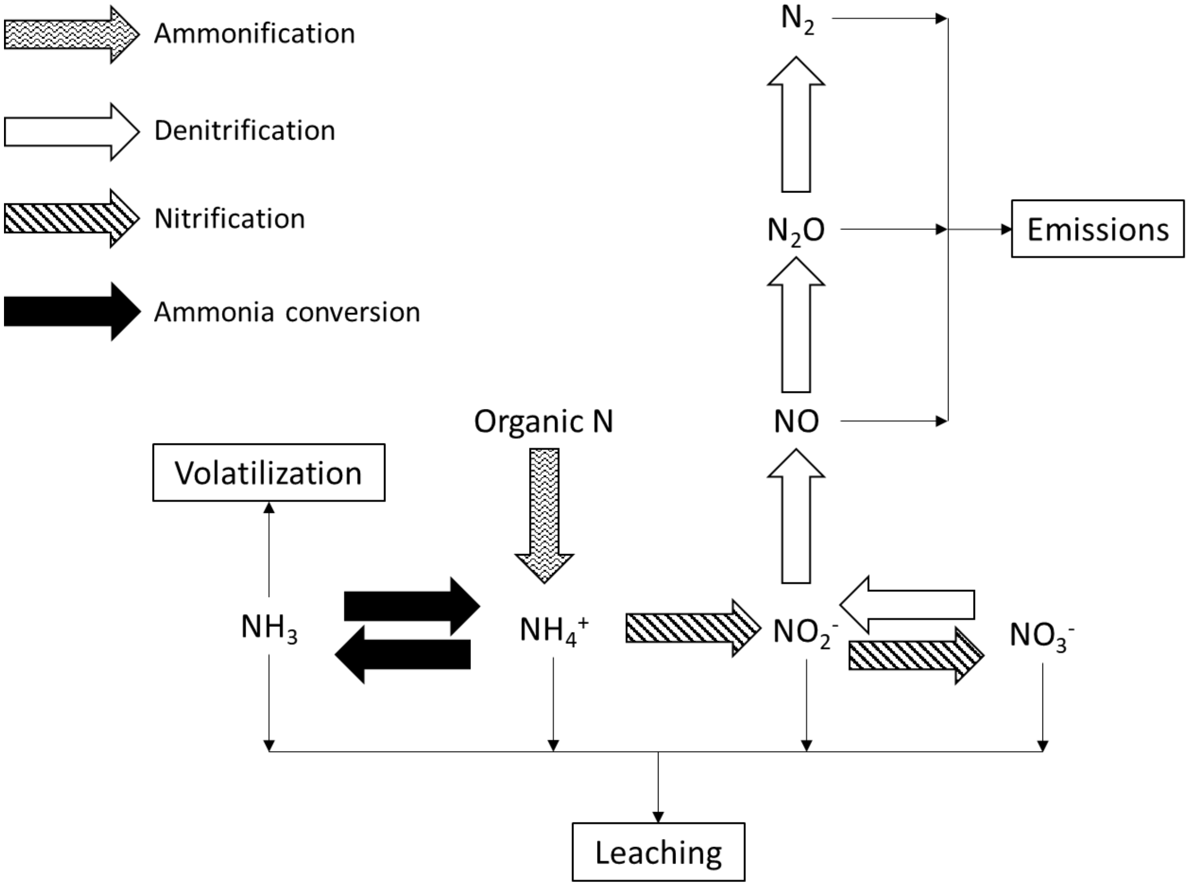


Figure 1.3 Nitrogen transformation and loss pathways, based on Walling and Vaneeckhaute (2021a).

The final nutrient that is of interest to us is phosphorus (P), given its importance as a macronutrient for plants and its role as one of the main limiting factors in fertilizer application legislation. Unlike carbon and nitrogen, phosphorus tends to be much more stable and is not subjected to volatilization or other complex transformations. The main pathway for P transformation and loss is through phosphate solubilizing microorganisms (Wei et al., 2018a). These organisms can transform nonbioavailable (insoluble) phosphorus into bioavailable (soluble) forms. It is this soluble form that is desirable from an agricultural perspective, given that nonbioavailable P cannot be used by plants. These microorganisms do not interact with the phosphorus directly, unlike what was described earlier for carbon and nitrogen. The main mechanism for P solubilization is through the release of compounds capable of chelating or reducing the pH of the environment to release the phosphorus from its mineral forms (Alori et al., 2017). This includes compounds such as organic and inorganic acids, siderophores, protons, hydroxyl ions, CO_2, and chelating substances. Though these bacteria are rarely reported on or investigated in the composting literature, there is an interesting and growing body of work looking into the inoculation of compost with phosphate solubilizing bacteria to increase the amount of plant-available phosphorus (Estrada-Bonilla et al., 2017; Kumar and Singh, 2001; Wei et al., 2018b).

Phosphorus loss during composting is also rarely reported, and its form is most often assumed to be stable throughout the process, with limited to no leaching. Some experiments have indeed reported light phosphorus loss, lower than 2% (Eghball et al., 1997), though others have found much more substantial loss through leaching, up to around 30% (Parkinson et al., 2004; Tiquia et al., 2002). Furthermore, despite the limited work on the speciation and characterization of phosphorus during composting, the assumption that it and its various fractions are stable appears questionable. For example, the research by Sharpley and Moyer (2000) and Lü et al. (2013) clearly highlight the mobility and the convertibility of P during composting. The prior examined the mobility of phosphorus in compost due to rainfall and found a removal of 59% to 95% of water extractable P, following five rainfall events. The fraction of water extractable P varied from 16% to 22% of total P, depending on the substrate (Sharpley and Moyer, 2000). Despite being very different from the dynamics of P leaching in a controlled process, the study highlights the potential for P mobility. Regarding P fractions, Lü et al. (2013) demonstrated the significant increase in phosphorus concentration during composting, given the relative decrease in organic matter. Among their findings was a large decrease in labile (both organic and inorganic) P as composting progressed, decreasing from around 56% to 29% of total P (48% (inorganic)/64% (organic) decrease over 49 days), with the traditional increase in pH observed during the process being attributed as one of the primary causes for this transformation. These labile forms were mainly transformed into recalcitrant fractions, either bound with calcium (Ca) and magnesium (Mg), or aluminium (Al) and iron (Fe). By the end of their 49-day composting trial, recalcitrant P had gone from 35% of total extracted P to 60%. This significant transformation from labile and easily extractable forms to recalcitrant forms can explain why P loss from composting is generally considered as being low, especially when compared to the significant organic matter loss during the process, but it remains of importance when considering the agronomic value of composts. Of note is that the substrate in Lü et al.'s (2013) study was pig manure, which is rich in Fe, Al, Ca, and Mg ions, and such a conversion might not be observed with other substrates. Indeed, the substrate and operating conditions have a significant impact on P fractions during composting, as underlined by the study of Gagnon et al. (2012). Table 1.1 presents the proportion of phosphorus fractions by extractability obtained in their study, following a modified Hedley sequential-phosphorus fractionation method (Hedley et al., 1982). From this table, we can see how easily extractable P (extractable by resin) made up between 22.5% and 74.2% of total P in final composts, depending on the substrate, while the most recalcitrant forms (extractable by HCl) also varied widely, from 5.5% to 46.3% (Gagnon et al., 2012). From all of the above, it is apparent that phosphorus is much more dynamic in composting, both in form and in mobility, than is widely assumed, and could therefore benefit from more research.

Table 1.1 Phosphorus fractionation (rounded) for various composts used in the study of Gagnon et al. (2012).

Extractable by	Potato process residues	Dairy manure	Beef manure	Swine manure	Lobster waste	Municipal biosolids	Poultry biosolids
Resin (%)	48.0	74.2	39.7	57.1	22.5	46.0	25.2
$NaHCO_3$ (%)	22.2	6.5	20.7	9.7	28.2	9.7	12.6
NaOH (%)	26.1	9.0	15.5	8.0	3.0	19.0	9.9
HCl (%)	5.5	10.3	29.0	27.7	46.3	25.4	52.3

1.2 Conclusion

This brief first chapter has painted a portrait of composting that should allow readers to better understand the dynamics and research areas that will be explored throughout the rest of this thesis. Key takeaways include that:

- Composting is a highly dynamic aerobic biodegradation process undertaken in a three-phase system (solid, liquid, air).
- Biodegradation is generally separated into four major phases (in order: mesophilic, thermophilic, cooling, curing), occurring through a variety of microorganisms found in the biofilm.
- Carbon and nitrogen are at the heart of this biodegradation, both being primordial for microorganism growth.
- Many operating parameters and variables influence composting, including temperature, aeration rate, moisture content, C/N ratio, pH, and bulk density.
- During optimal composting, the majority of mass loss should occur through the conversion of organic carbon to CO_2, though a conversion to CH_4 is possible in anaerobic pockets.
- Nitrogen transformation pathways found in composting are vast, including ammonification/mineralization, immobilization, nitrification, denitrification, and volatilization.
- Nitrogen loss during composting can vary significantly, generally being between 20% and 70%, going upwards of 90% in certain cases, mostly through volatilization.
- Phosphorus transformation and loss is an understudied area of the literature, though existing works point towards a progressive transition from labile to recalcitrant forms as the process progresses.
- Total phosphorus loss during composting has been reported as ranging from 2% to 30%, primarily through leaching.

The following chapter will build on this information, exploring how this complex process can be modelled mathematically, while highlighting areas that have seen less research, particularly regarding nutrients.

Chapter 2: A review of mathematical models for composting

2.1 Résumé

Le compostage est une méthode très utile pour traiter et valoriser les déchets organiques. Cependant, le procédé est défini par sa nature dynamique et régi par une multitude de paramètres de fonctionnement. Ainsi, la modélisation mathématique du procédé de compostage offre un outil puissant pour simuler et prédire les résultats variables du processus, permettant son optimisation. Cela peut inclure l'amélioration de l'efficacité, la réduction des coûts et la réduction de l'impact environnemental. Pour aider au développement de futurs modèles, nous fournissons ici une revue et une évaluation à jour de l'état de l'art de la modélisation du compostage. En révisant 40 ans de littérature, cette revue dresse le portrait le plus complet du domaine à ce jour. Cela comprend une analyse des tendances de la modélisation du compostage: examinant le type de systèmes ciblés, l'objectif des modèles et les approches de la cinétique et du transfert de masse et de chaleur. Concernant les approches de modélisation, nous explorons le fractionnement à la fois des substrats et des micro-organismes, les processus de dégradation biologiques qui peuvent être inclus (désintégration, hydrolyse, absorption et mort) et leur cinétique (de premier ordre, de type Monod), les bilans énergétiques (génération biologique, convection, conduction) et les bilans de masse. Nous fournissons également une évaluation des résultats des analyses de sensibilité effectuées sur les modèles de compostage, constatant que les modèles sont les plus sensibles à la croissance microbienne et aux taux de mortalité, ainsi qu'aux taux de consommation et aux rendements des produits. Dans la dernière partie de la revue, nous identifions, explorons et fournissons des recommandations directrices pour les travaux sur les domaines émergents et les domaines à développer dans la modélisation du compostage (changement de volume, pH, maturation, intelligence artificielle, etc.).

Mots-clés : biodégradation aérobique; modélisation; simulation; prédiction; intelligence artificielle; stochastique

2.2 Abstract

Composting is a valuable method to treat and valorize organic waste. However, the process is defined by its dynamic nature and governed by a multitude of operating parameters. As such, mathematical modelling of the process offers a powerful tool to simulate and predict the variable outcomes of the process, allowing for its optimization. This can include improving efficiency, lowering costs and reducing environmental impact. To aid with the development of future models, we provide an up-to-date review and assessment on the state of the art of composting modelling. By reviewing 40 years of literature, this review paints the most complete picture of the field to date. This includes an analysis of trends in composting modelling: looking at the type of systems that are targeted, the aim of the models and the approaches to kinetics and mass and heat transfer. Regarding modelling approaches, we explore the fractionation of both substrates and microorganisms, the biological processes that can be included (disintegration, hydrolysis, uptake, and death) and their kinetics (first-order, Monod-type), energy balances (biological generation, convection, conduction) and mass balances. We also provide a review of the results of sensitivity analyses performed on composting models, finding that models are most sensitive to microbial growth and death rates, as well as consumption rates and product yields. In the final portion of the review, we identify, explore, and provide guiding recommendations for work on emerging areas and areas requiring development in composting modelling (volume change, pH, maturation, artificial intelligence, etc.).

Keywords: aerobic biodegradation; modelling; simulation; prediction; artificial intelligence; stochastic

2.3 Introduction

To favor the development and implementation of composting processes, mathematical models have been developed over the past few decades. These models aim at furthering our understanding of the processes, consequently reducing the time and energy spent on their optimization and allowing for simulation and assessment of process modifications. To date, only three reviews have explored the modelling of composting: Hamelers (2004) reviewed the approaches for modelling composting kinetics, notably focusing on the differences between inductive and deductive models. This was followed by Mason (2006) who looked at the structure and kinetic foundations of composting models, paying attention to their simulation capabilities and performance. The more recent review by Li et al. (2013) examined the importance of certain factors and their impact on the composting of food waste, as well as looking at modelling approaches and how models deal with uncertainty. However, since these reviews, there has been significant work in the field of composting modelling, with over 1600 papers having been published on the subject since 2013, more than the amount (1450) published between 1990 and 2010 (based on the Web of Science database).

Given these recent developments and the increasing growth in the field, a new review on the current state of composting modelling would be very beneficial. Therefore, the aim of this chapter is to review and examine the state of the art while highlighting areas requiring further development. Section 2.4 presents the methodology used during the review process, as well as general trends identified from the composting literature. Section 2.5 investigates in detail the mathematical modelling of the composting process, providing a comprehensive overview of the work that has been done in this field by focusing on kinetics, heat and mass balances, and the significance of model parameters, gleaned from an assessment of sensitivity analyses. Section 2.6 identifies and discusses emerging areas and areas requiring development in the field of composting modelling, while section 2.7 provides some concluding remarks.

2.4 Material and methods

This review focuses on literature from the emergence of composting modelling to the present day. The choice to consider such a large span of literature instead of basing this work on the previous reviews and completing with more recent information was to provide a truly comprehensive interpretation of the state of composting literature. This is most notably portrayed in section 2.5.1 that presents the trends in composting literature and throughout section 2.6 on emerging areas and areas requiring development, something that the prior reviews lack. Furthermore, this has allowed the work to provide a much stronger quantitative support for its claims and comments on all aspects of composting modelling.

To undertake the review, the Web of Science database was queried using the "advanced search" function. The search term was as follows: TS=(compost* AND (model* OR simulat*)), yielding 3217 results at the time of writing this. The addition of search terms and Boolean operators was found to be counterproductive and so the author decided to use the original search and do a manual selection of the works that appeared to be of interest for our review. Of the 3217 papers resulting from the query, 209 were identified as being potentially pertinent for this work, based on their titles, abstracts, and keywords. These works, ranging from 1980 up to June 2019, were all published white literature and written in English. Figure 2.1 presents the distribution of these publications over time.

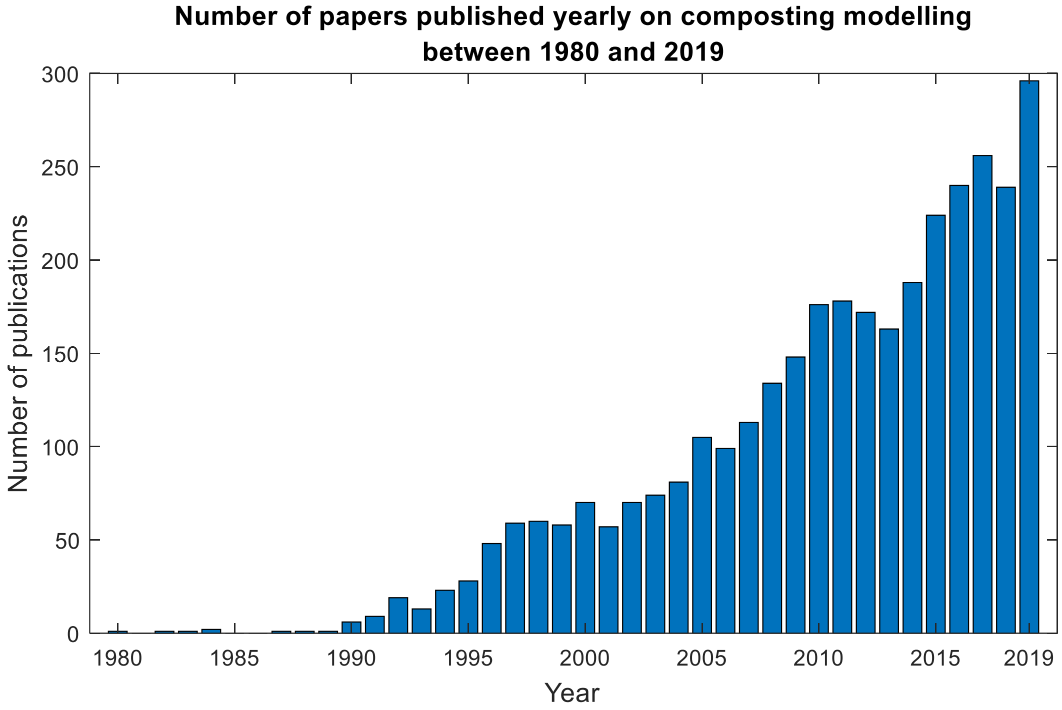


Figure 2.1 Temporal distribution of papers on composting modelling between 1980 and 2019 identified using the Web of Science database using the advanced search query: TS=(compost* AND (model* OR simulat*)). Of the papers published in 2019, 34% were assessed during the review process (published by June of 2019).

These papers then underwent a preliminary analysis to determine whether they were "pertinent", "somewhat pertinent", or "non pertinent" for this work. An article was considered pertinent if it presented a mechanistic, i.e., based on theory and a mathematical description of the process, or mixed mechanistic-empirical model on the composting process. These articles would then be fully investigated by the authors. Somewhat pertinent papers were those that provided either empirical or structural equation models and were considered when looking at general trends in the modelling literature, while non pertinent works were those that had little to no relation to mathematical modelling and were discarded. In all, 123 articles were found to be pertinent to this work, 54 were considered to be somewhat-pertinent, and 27 were deemed non-pertinent. Furthermore, 5 papers were inaccessible. The temporal distribution of these reviewed papers can be found in figure 2.2.

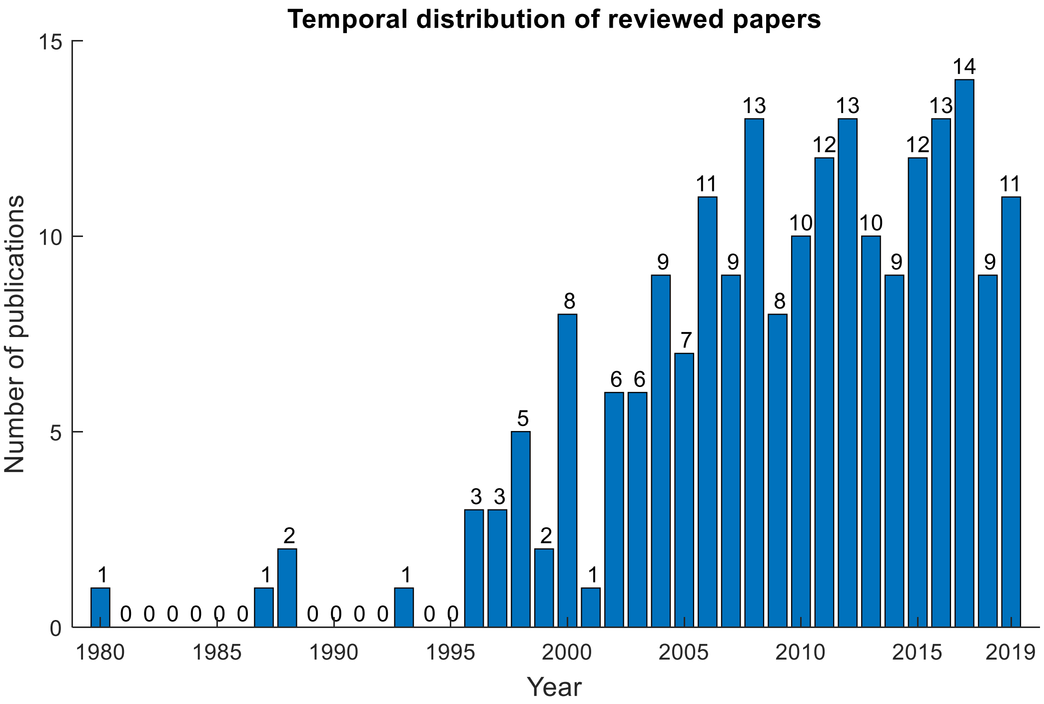


Figure 2.2 Temporal distribution of reviewed composting papers, ranging up until June of 2019.

2.5 Modelling the composting process

Composting is a process marked by multiple dynamic changes due to diverse and deeply interrelated phenomena. These changes include a characteristic temperature profile, transitioning between mesophilic and thermophilic temperature ranges (also reflected in the change in microbial community), an initial decrease in pH followed by a slow increase due to a release and then consumption of short-chained organic acids, a decrease in mass, free air space (space between particles) and generally moisture content, a constant change in composition, the emissions of various gases, and the production of leachate. These changes are due to three main phenomena: microbial biodegradation, heat transfer, and mass transfer. Microorganisms, including bacteria, fungi, and actinomycetes, degrade the organic matter, leading to the change in composition and a release of energy and water. This energy, combined with heat transfer through pathways such as convection, conduction, and evaporation, contributes to a net temperature change in the process. Furthermore, compounds such as volatile solids and soluble compounds can be lost during the process through volatilisation or by leaching. Therefore, when developing mathematical composting models, the aim is to capture this complex reality through kinetic modelling combined with mass and heat balances.

A very general and conceptual way of representing the numerical pathway taken to model the composting process is presented in Figure 3. This iterative process can be described as follows: based on the substrate composition and temperature (and potentially moisture content and oxygen concentration), the mass of substrate degraded within a time interval dt can be calculated using degradation kinetics. This substrate consumption can then be linked (either empirically or theoretically using stoichiometry) to the consumption of oxygen, the metabolic production of water, and the amount of heat generated by the microorganisms during this time interval. Mass and energy balances can then be applied to determine the net change in these variables within the timeframe, providing a new set of values that can then pass through the same process for a subsequent time interval. All of these processes will be described throughout section 2.5.

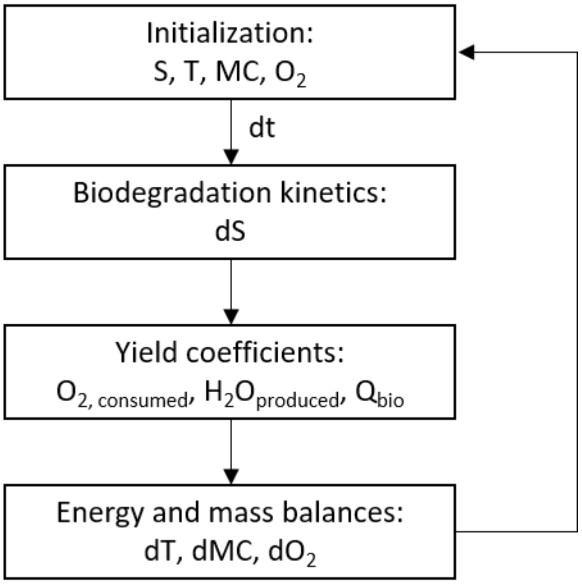


Figure 2.3 A general pathway to the numerical solution of mechanistic composting models. The terms are defined as follows: S (substrate), T (temperature), MC (moisture content).

The following section starts with a description of trends in composting modelling (section 2.5.1), followed by a detailed overview of the three main pillars of composting, i.e. substrate degradation (section 2.5.2), heat and energy balances (section 2.5.3), and mass balances (section 2.5.4). We also review sensitivity analyses in section 2.5.5 to highlight some of the most important parameters and general considerations when developing composting models.

2.5.1 Trends in composting modelling

During the preliminary analysis, in the aim of getting a clearer grasp on the state of composting modelling, the way each paper approached the modelling situation was identified. This included categorizing them based on their purpose (control, impact evaluation, predictive), their structure (deterministic vs stochastic, mechanistic vs empirical, structural equations), the type of system they were based on (reactor/in-vessel, pile, landfill, unspecified), the dimensions that were considered (heat and mass transfer and biological activity/degradation), and their “focus” (temperature, oxygen/aeration, kinetics, pathogen inactivation, odours, emissions, runoff/leaching, etc.).

From the overview of the literature, a few interesting trends have become apparent. Firstly, an overwhelming majority of papers (95%) focused on predictive modelling, while 3% were specifically aimed at process control and 2% at impact evaluation. The most common model types were deterministic and mechanistic in nature (70%), followed by empirical (regression-based) models (30%), though some studies combined both approaches (7%). Structural equation models were used in 3% of cases and models implementing fuzzy or stochastic methods were only used 10% of the time.

In terms of the type of system that was studied or that the models were based on, reactors or in-vessel systems were by far the most popular, representing 63% of cases, followed by piles (windrows or static) at 28% and landfills at 2% (7% were unspecified). For mechanistic models, heat and/or mass transfer were considered, to varying degrees, in approximately 62% of cases, while growth and/or degradation kinetics were considered 89% of the time. Mass and energy balances were combined with kinetics in 60% of cases, kinetics oftentimes being studied independently (28%), or balances being used without explicit kinetic modelling to consider temperature or aeration (12%). Regarding the modelling of microbial growth and substrate degradation, first-order kinetic equations were the most prominent, finding use in 52% of cases. This was followed by Monod/Michaelis-Menten kinetics in 30% of cases, with a variety of other models (Contois, Tessier, non-first-order, empirically derived) making up the remainder. First-order and Monod kinetics were combined in 15% of cases.

Finally, with respect to model focus, degradation kinetics and compost "quality" were the most studied subjects, being considered in 75% of papers. This was followed by temperature (64%) and oxygen concentration (55%). These three main focuses make up the bulk of the reviewed literature on composting modelling and can be considered as the pillars of a general predictive model. Other areas of interest included emissions from composting (13%), notably as either NH_3 or CO_2, runoff water and leaching (7%), pathogen elimination (5%) and odour emissions (3%).

2.5.2 Substrate degradation

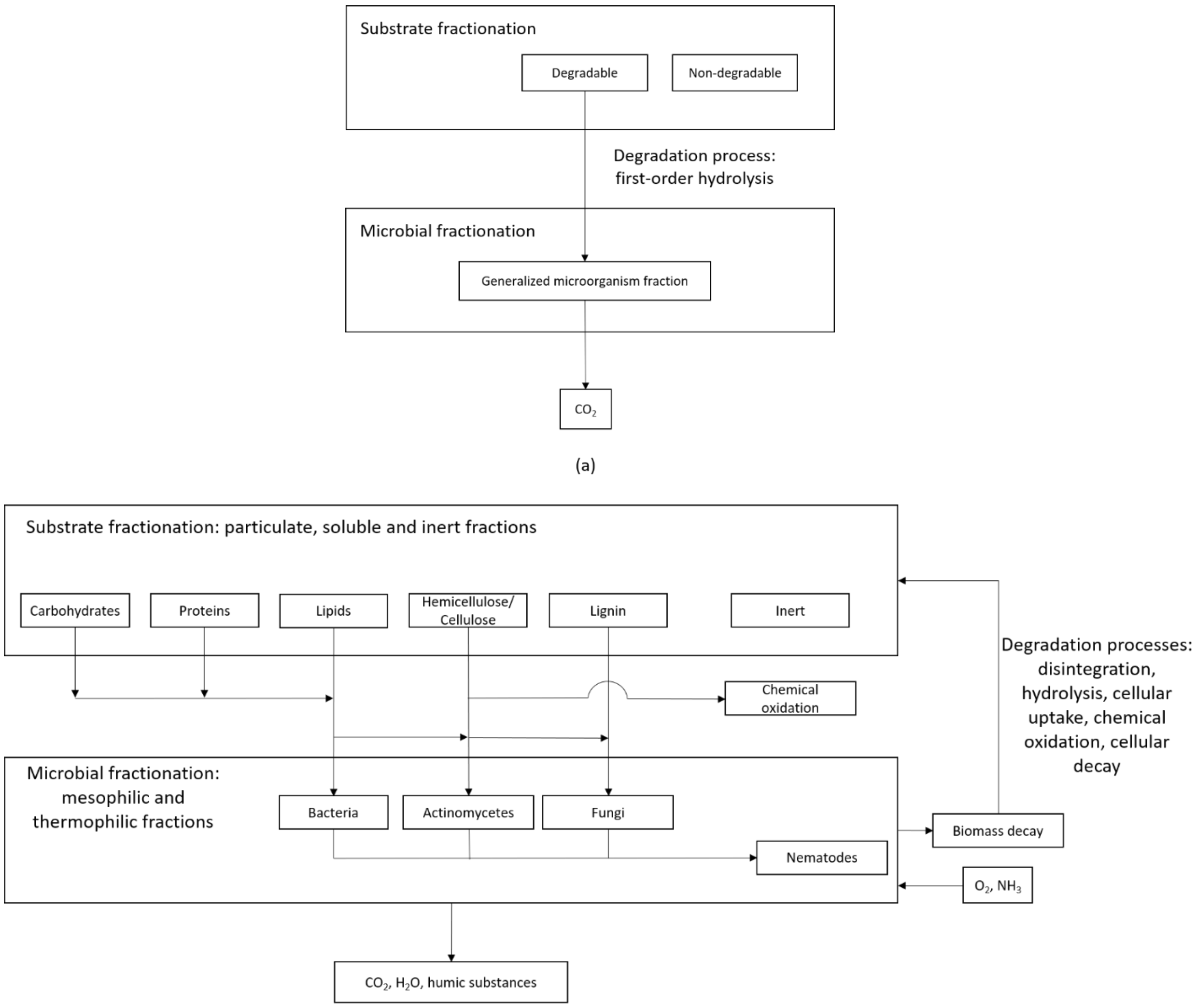
To model substrate degradation, three important considerations must be addressed by modellers. The first is determining how the substrate will be fractionated, i.e. how will the substrate be represented and what will be input into the degradation model. The second is to determine the microbial fractionation, i.e., what will be degrading the substrate. The third is to determine what degradation processes will be considered in the model, i.e., how the substrate will be transformed. These can then be used to model the degradation through kinetics, as presented in section 2.5.2.1. Figure 2.4 presents a conceptual overview of how the biological components of composting models can greatly vary in scope and complexity, highlighting the wide range of choices we discuss in this sub-section.

For substrate fractionation, the organic matter can be divided into multiple fractions, ranging in complexity. Basic fractionations can simply consider a degradable and a non-degradable fraction. For example, Tremier et al. (2005b) used the same fractionation as the Activated Sludge Models (ASM) (Henze et al., 2000) for their composting model, dividing the substrate into a directly biodegradable, a hydrolysable, and an inert fraction. Significantly more complex fractionations have also been proposed, such as separating the substrate into carbohydrates, lipids, proteins, hemi-/cellulose, lignin, and sometimes going into specific chemical species, as well as using biochemical or chemical oxygen demands (BOD/COD) (Francou et al., 2008; Kaiser, 1996; Orrico Junior et al., 2018; Sole-Mauri et al., 2007; Woodford, 2009).

The case is similar for microbial fractionation. Microbial diversity and succession are responsible for dynamic changes in the rate of substrate degradation. In reality, the microbial community is diverse and dependent on various process parameters (Chen et al., 2019; Ince et al., 2018; Ki et al., 2017; Ryckeboer et al., 2003; Steel et al., 2013; Vieira and Pecchia, 2018; Zhao et al., 2019), though this complexity often far outweighs the capabilities of composting models. Many composting models have generalized this microbial diversity through general reaction coefficients, representing the entire microbial community as one entity. Though mechanistically flawed, these models have proven to be accurate if sufficient data exists to properly fit the reaction rates. More mechanistically inclined models have, however, provided more detailed fractionations of the microbial community (Fontenelle et al., 2011; Kaiser, 1996; Sole-Mauri et al., 2007;

Wang and Witarsa, 2016). An early example of this comes from Kaiser (1996) who considered four types of microorganisms that were responsible for substrate degradation: bacteria, actinomycetes, brown-rot fungi and white-rot fungi. In this case, each organism had their own kinetics and was associated with different substrate fractions, as well as having an order of precedence between microorganisms acting on the same substrate fraction. Building off of this notion of microbial fractionation, Sole-Mauri et al. (2007) also included a mesophilic and thermophilic fraction for actinomycetes, fungi, and bacteria (a total of six fractions), aiming to better represent the process.

Finally, regarding degradation processes, multiple pathways exist for substrate degradation. These processes are mainly biological, though chemical pathways have also been used in the literature. Biological processes include disintegration, hydrolysis, both of which occur extracellularly (Batstone et al., 2002), cellular uptake (microbial growth), and cellular decay (endogenous respiration or lysis), as well as considerations for inhibition by overcrowding in the biofilm and energy requirements for cell maintenance. There has also been some efforts to model anaerobic degradation in aerated environments, though this has seen limited interest in composting literature (Rafiee et al., 2018), finding more prominence in a landfilling context (Obersky et al., 2018; Rafiee et al., 2017). Chemical pathways have also rarely been considered, though chemical oxidation (of cellulosic material) has seen particular interest in a small subset of the field, particularly for prediction of self-ignition of composting heaps (Aganetti et al., 2016; Luangwilai et al., 2018; Moraga et al., 2009; Nelson et al., 2003; Sidhu et al., 2006; Zambra et al., 2011; Zambra et al., 2012).



(a)

(b)

Figure 2.4 Schematic representation of the variability in biological modules of composting models: (a) demonstrates the conceptual pathway of a very simple model that divides the substrate into a degradable and non-degradable fraction, the degradable fraction being hydrolyzed by a general microbial mass to degrade the substrate and produce CO_2. (b) shows a much more complex modelling pathway with multiple substrate fractionations, each associated to various microbial fractions and with various degradation processes. These biological modules can then be integrated with heat and mass balances as detailed in the following sections.

2.5.2.1 Kinetics

Multiple kinetic models have been used to describe the composting process. The most basic composting models will often consider hydrolysis as the sole degradation process, seeing how it is generally the rate-limiting step (Batstone et al., 2002; Wang and Witarsa, 2016). Though it has rarely been expressed as hydrolysis, the rate-limiting step has most often been represented by a first-order kinetic expression (eq. 2.1). The second most common expression are the Monod-type equations (eq. 2.2). Beyond this, there are also a few works that have used the Contois expression to take into account overcrowding by microorganisms at the surface of the substrate (Bialobrzewski et al., 2015; He et al., 2018; Qin et al., 2007; Seng et al., 2016; Sole-Mauri et al., 2007; Vidriales-Escobar et al., 2017; Wang and Witarsa, 2016).

$$R_{\mathrm{degradation,\ first-order}} = -\frac{d[S_i]}{dt} = k_i \cdot [S_i] \tag{2.1}$$

$$R_{\mathrm{degradation,\ Monod}} = -\frac{d[S_i]}{dt} = \mu_i \frac{X_i}{Y_{S_i}} = \frac{\mu_{\max,i}[S_i]}{K_{s,i} + [S_i]} \frac{X_i}{Y_{S_i}} \tag{2.2}$$

The variables and parameters of equations 2.1 and 2.2 are as follows (the index i is used here to represent a specific microorganism growing on a specific substrate): In equation 2.1, k_i is the (hydrolysis) rate constant (s^{-1}). In both equations, $[S_i]$ is the concentration of the substrate (kg m^{-3}) and t is the time (s). In equation 2.2, X_i is the biomass concentration (kg m^{-3}); μ_i and $\mu_{\max,i}$ are the specific and maximum growth rate of the microorganisms (s^{-1}), respectively; $K_{s,i}$ is the half-velocity constant (kg m^{-3}) (or $K_{M,i}$ in the Michaelis-Menten equation, representing the Michaelis constant) and Y_{S_i} is the yield coefficient (kg kg^{-1}), representing the mass of biomass produced over the mass of substrate consumed. Such yield factors are highly used throughout the field to link the consumption or production of various compounds to the reaction rates. The most commonly used ones are for oxygen consumption and water production, but they can be used for any reaction and are especially present in more complex models implementing successive reactions. For example, rates of biological oxygen consumption (equation 2.3) and water production (equation 2.4) can be simply linked to degradation rates as follows, using an oxygen consumption/water generation coefficient (Y_{O_2}/Y_{H_2O}):

$$R_{O_2\ \mathrm{consumption}} = Y_{O_2} R_{\mathrm{degradation}} \tag{2.3}$$

$$R_{H_2O\ production} = Y_{H_2O} R_{degradation} \tag{2.4}$$

Such coefficients have also been used to estimate a variety of other metabolic products, such as the emission of carbon dioxide (CO_2) in a multitude of models, and methane (CH_4) in Ge et al.'s (2016) model, the latter being directly related to the rate of hydrolysis.

Furthermore, as highlighted by Wang and Witarsa (2016), disintegration and uptake are also involved in the degradation process and these researchers found disintegration to be rate-limiting for soluble substrate uptake. Disintegration has almost never been explicitly included in the reviewed composting models, with the exception of the model developed by Denes et al. (2015) (expressed as two subsequent hydrolysis steps) and Wang and Witarsa (2016). In the latter case, the authors expressed disintegration as a function of (hemi)cellulose and lignin hydrolysis instead of the commonly used (in other fields) first-order equation (Batstone et al., 2002). Cellular uptake of soluble compounds (microbial growth) has been considered in addition to hydrolysis in a few more cases (Denes et al., 2015; Lashermes et al., 2013; Lin et al., 2008; Sole-Mauri et al., 2007; Vasiliadou et al., 2015; Zhang et al., 2012) and is generally represented by a Monod kinetic. A Tessier expression to take into account the energy needed to maintain cell activity, thus lowering the maximum growth rate if the substrate is lacking or if there is competition between organisms, has also been considered by Wang and Witarsa (2016).

Decay and release of cellular compounds has also been considered in many models. In this case, the cellular compounds are returned as substrate for other microorganisms. This has generally been represented using a negative growth rate (Herbert or Pirt model), though endogenous respiration (where cells oxidize their own cellular material instead of new organic matter from the environment) has also been used (Gujer et al., 1999; Wang and Post, 2012). Decay is often simply represented in the following form (eq. 2.5) by a first-order equation, where b_i is the microbial death rate (s^{-1}):

$$R_{decay} = b_i X_i \tag{2.5}$$

2.5.2.2 Correction functions

Given the important variation in operating parameters during the composting process, it is essential to capture this change on the reaction rate. Therefore, modellers implementing simple first-order or Monod-type models can use correction functions (also referred to as adjustment factors or growth-limiting functions) to consider the change in degradation rate as a function of various operating conditions. Corrections can be applied based on temperature, moisture content, free air space (porosity), pH, specific substrate, and oxygen limitation. The rate of degradation can thus be rewritten as:

$$\mathrm{R}'_{\mathrm{degradation}} = \mathrm{R}_{\mathrm{degradation}} \mathrm{f}_{\mathrm{T}} \mathrm{f}_{\mathrm{MC}} \mathrm{f}_{\mathrm{O_2}} \mathrm{f}_{\mathrm{FAS}} \mathrm{f}_{\mathrm{pH}} \tag{2.6}$$

Despite the seemingly widespread use of correction functions noted by Mason (2006), only 46% of the reviewed models (n = 56) used one or more correction functions. The rate of implementation has been relatively consistent over time, with no significant increase or decrease in use over the past decade compared to the 1990's and 2000's. There were two main reasons for the omission of correction factors that were explicitly addressed in the literature. First is the case where a thorough mechanistic model was developed, making the correction unnecessary. This was the case, for example, for Fytanidis and Voudrias (2014) who incorporated a complex flow module into their model, therefore removing the need for a free air space correction. The second case is a more novel approach to kinetic model design highlighted by Ebrahimzadeh et al. (2017). In their work, Ebrahimzadeh et al. (2017) circumvented the use of correction functions by using elementary chemical equations (zero, first, second and n-th order equations) with experimental data on volatile solids change over time to produce an accurate kinetic model.

Regarding the application of correction functions, there does not appear to be any significant difference between the use of correction functions alongside first-order vs Monod-type kinetics. Nevertheless, the number of models that did not implement any type of correction was high. There can be valid reasons to not implement correction functions, notably when aiming for a model with a minimal number of parameters and when operating at relatively optimal conditions; the benefit of many of these correction functions often being most impactful at the extremes in operating parameters (such as a cut-off at high and low temperatures and moisture content). However, correction functions can be a powerful tool to solidify the model's accuracy, especially to increase its range of applicability.

The most common type of corrections are temperature corrections (n=54) (e.g. Baptista et al., 2010; Keener et al., 2005; Petric and Selimbašić, 2008; Sánchez Arias et al., 2012; Seng et al., 2016; Vasiliadou et al., 2015; Vlyssides et al., 2009; Wang and Witarsa, 2016). Three main methods are predominant: cardinal temperature corrections (the Rosso model) are the most common, followed by corrections using the Arrhenius equation, and a variety of empirical corrections. Equations considering cardinal temperatures (Rosso et al., 1995; Rosso et al., 1993) tend to offer the best representation of the composting process seeing how they can better represent the behaviour of the composting pile at extreme temperatures (Mason, 2008; Richard and Walker, 2006). Newer temperature corrections have also been proposed (Bialobrzewski et al., 2015; Bonifacio et al., 2017a; Lin et al., 2008; Petric et al., 2015; Petric and Selimbašić, 2008; Zhou et al., 2014a), though it would be beneficial to have a comparative study of their performances, especially compared to the cardinal temperature method. Some models have also implemented different corrections for different processes (Fytanidis and Voudrias, 2014; He et al., 2018; Lin et al., 2008; Seng et al., 2016; Wang and Witarsa, 2016; Yu et al., 2009). As an example, Seng et al. (2016) corrected their growth expression with the Arrhenius equation, their decay rate with Ekinci's (2003) correction, and their rate of hydrolysis with Haug's (1996) correction. A full list of correction functions used throughout the reviewed literature is presented in the appendix of this paper.

The second most common corrections are moisture content corrections (n=28) (e.g. Bonifacio et al., 2017a; Keener et al., 2005; Malamis et al., 2016; Mohee et al., 1998; Richard et al., 2002; Seng et al., 2016; Sole-Mauri et al., 2007; Vasiliadou et al., 2015), followed by oxygen limitations (n=24) (e.g. Ekinci et al., 2004b; Keener et al., 2005; Seng et al., 2016; Talib et al., 2014; Zhang et al., 2016). Moisture corrections have all been empirical in nature, with the most common being the logistic curve proposed by Haug (1993), with a variety of other empirical models being used, but none finding any significant traction (n>2). On the other hand, oxygen corrections have mainly been mechanistic, most-often through a Monod expression, with Baptista et al.'s (2010) modified Monod expression having found strong use during the past decade. These expressions have been found to provide the best results, despite the existence of empirical corrections (Baptista et al., 2010; Richard et al., 1999).

The last of the “major” corrections to find somewhat frequent use (n=14) is for free air space (e.g. Ekinci et al., 2006; Liang et al., 2004; Malamis et al., 2016; Ndegwa et al., 2000). Haug’s (1993) model has been used in every case, except for one who used Ekinci’s (2001) function. A more recent empirical model has been developed by Yu et al. (2009) for passively aerated systems.

Only two of the reviewed models implemented a pH correction (Liang et al., 2004; Petric et al., 2015). There has also been cases of corrections for consideration of inhibition by specific (phenolic) compounds (Vlyssides et al., 2009) and consideration of other substrates (such as ammonia nitrogen) limitation (Sole-Mauri et al., 2007) through Monod expressions.

2.5.3 Heat balance

Heat balances have also come in a variety of forms. A traditional and generalized heat balance that has been used often throughout the literature is presented in equation 2.7.

$$\frac{\mathrm{d(mcT)}}{\mathrm{dt}} = \mathrm{G(H_i - H_0) - UA(T - T_a) + Q_{bio}} \tag{2.7}$$

In this balance, m is the mass of the substrate (kg), c is the heat capacity of the substrate (kJ kg^{-1} °C^{-1}), T is the temperature (°C), G is the airflow through the system (kg s^{-1}), $\mathrm{H_i}$ and $\mathrm{H_0}$ are the enthalpies of the gas at the inlet and outlet of the system (kJ/kg), U is a global heat transfer coefficient (kW m^{-2} °C^{-1}), A is the area of the system (m^2) and $\mathrm{T_a}$ is the ambient temperature (°C).

This form has remained relatively unchanged for many of the mechanistic composting models, with just over 50% of the evaluated models implementing a similar heat balance. In this expression, the term on the left represents accumulation, while the first term on the right is for convection, the second term is conduction, and the last term is biological heat production. Most often, equation 2.7 is further simplified by assuming that the mass (m) and the heat capacity (c) are constant through time, allowing them to be sent to the right side of the equation and leaving a simple differential equation that can be solved through traditional numerical approaches, e.g., through finite differences.

There are, however, some novel areas that have seen more development recently. This notably includes the modelling of chemical oxidation (Aganetti et al., 2016; Luangwilai et al., 2018; Zambra et al., 2012) and multi-dimensional models, with various works looking at 1D systems (Bari and Koenig, 2012; Fytanidis and Voudrias, 2014; Henon et al., 2009; Luangwilai et al., 2010; Sidhu et al., 2006; Stombaugh and Nokes, 1996; Tremier et al., 2005a; Van Lier et al., 1994; VanderGheynst et al., 1997b), and very limited work on 2D (Das and Keener, 1997a; Kuwahara et al., 2009; Moraga et al., 2009; Putranto and Chen, 2017; Sidhu et al., 2006; Sidhu et al., 2007; Zambra et al., 2011) and 3D modelling (Zambra et al., 2012; Zambra et al., 2015). The multi-dimensional (1 to 3D) balances tend to be significantly more complex than the more common 0D models in terms of numerical solution given that they are usually composed of systems of partial differential equations. The most common approaches used in the reviewed literature are the finite volume (e.g. Zambra et al., 2015) and the finite element (e.g. Putranto and Chen, 2017) methods. An example of a multi-dimensional energy balance whose form has been the most prevalent through the literature is presented in equation 2.8. This specific form is from Luangwilai et al.'s (2018) work on self-heating in the composting pile, integrating cellulosic oxidation:

$$\begin{aligned}(\rho \mathrm{C})_{\mathrm{eff}}\frac{\partial T}{\partial t} = k_{\mathrm{eff}}\nabla^2 T - \varepsilon\rho_{\mathrm{air}}\mathrm{C}_{\mathrm{air}}U\frac{\partial T}{\partial x} + Q_C(1-\varepsilon)\rho_{\mathrm{C}}A_{\mathrm{C}}\mathrm{O}_2\exp\left(-\frac{E_C}{RT}\right)\\ +Q_b(1-\varepsilon)\rho_b\left[\frac{A_1\exp\left(-\frac{E_1}{RT}\right)}{1+A_2\exp\left(-\frac{E_2}{RT}\right)}\right]\\ +L_V\left(\varepsilon Z_c V-(1-\varepsilon)Z_e W exp\left(-\frac{L_v}{RT}\right)\right) \qquad (2.8)\end{aligned}$$

Without going into much detail (interested readers are highly recommended to consult the works of Luangwilai (2010, 2013, 2018), Zambra (2011, 2012, 2015), Nelson (2007, 2008), and Sidhu (2006, 2007), which have all implemented similar balances), the first term on the right represents conductivity, the second term depicts airflow through the system (convection), the third term portrays oxidation of cellulosic materials, the fourth term characterizes biological heat generation and the fifth term is associated with energy change from evaporation and condensation.

Heating and heat transfer, generally for temperature estimation, have also been the main focus for a variety of works. This includes general works such as those of VanderGheynst et al. (1997b), De Guardia et al. (2012), Luangwilai et al. (2013) and Wang et al. (2016), while certain modellers have expanded in more specific areas, such as considering or deepening notions related to radiation (Ahn et al., 2007), convection (Ge et al., 2016b), condensation (Luangwilai et al., 2018) and biological heat generation (self-heating) (Bialobrzewski et al., 2015; Fontenelle et al., 2011; Luangwilai et al., 2013; Luangwilai et al., 2010; Luangwilai et al., 2018; Nelson et al., 2007; Nelson et al., 2003; Sidhu et al., 2006; Sidhu et al., 2007). There has also been a recent "simple" model devised by Ro et al. (2018) that aimed at estimating ammonia emissions. This model simply considered heat loss by implementing a ratio between ammonia concentration and Henry's law constant at different temperatures.

Generally, heat generation ($\mathrm{Q_{bio}}$) is calculated from respiration kinetics, either from O_2 consumption or CO_2 production rates (Kaiser, 1996; Nakasaki et al., 1987) or directly from substrate degradation rates (Haug, 2018; Higgins and Walker, 2001; Mason, 2006; Mason and Milke, 2005). Equation 2.9 can be used to represent this biological heat generation:

$$\mathrm{Q_{bio}} = -\Delta \mathrm{H_S} \frac{\mathrm{dS}}{\mathrm{dt}} \tag{2.9}$$

Where $\Delta \mathrm{H_S}$ is the biological heat generation coefficient (kJ/kg substrate), representing the amount of energy generated by mass of substrate consumed. As mentioned, this equation can be rewritten with O_2 consumption or CO_2 production by using appropriate heat generation coefficients.

Indeed, given equation 2.9, the value of the biological heat generation coefficient can be a very important part of estimating the temperature in the composting pile (De Guardia et al., 2012; Wang et al., 2014). Table 2.1 presents some of the estimates identified in the literature, while the values that have been most frequently used in the reviewed literature are 16 000 kJ/kg of substrate (Haug, 1993), 18 090 kJ/kg of substrate (Ekinci, 2001) and 22 097 kJ/kg of substrate (Zhang et al., 2010). However, these values are unlikely to be constant. Indeed, Wang et al. (2014) obtained coefficients of 18 000 kJ/kg of degraded biodegradable volatile solids at the beginning of their experiments, dropping to 16 000 kJ/kg by the end, similarly to Ahn et al. (2007) who found a range of 16 830 – 19 700 kJ/kg for poultry manure with wood shavings. To deal with this variability, Wang et al. (2014) have proposed an empirical equation to measure the biological heat generation coefficient through time. However, the alternative of using values based on oxygen consumption could present some advantages. Verification in the composting context is necessary, but based on general work in biochemistry, it would seem that these respiration rates should be relatively constant (Gnaiger, 1983). These values have ranged from 9 760 to 14 000 kJ/kg O_2 (Mason, 2006), though the latter (from Finstein (1986)) seems to have been used more frequently in the reviewed literature and is in line with substrate specific coefficients reported in Gnaiger (1983). Therefore, when feasible, we recommend that modellers use a biological heat generation coefficient based on oxygen consumption data instead of substrate consumption.

Table 2.1 Values of the biological heat generation coefficient ($\mathbf{\Delta H_S}$) used in the reviewed literature.

References	**Biological heat generation coefficient ($\mathbf{\Delta H_S}$)**	**Units**
Rongfei et al. (2017)	302 to 19 700	kJ/kg of substrate
Wang et al. (2014)	16 000 to 18 000	kJ/kg of substrate
Ahn et al. (2007)	16 830 to 19 700	kJ/kg of substrate
Haug (1993)	16 000	kJ/kg of substrate
Ekinci (2001)	18 090	kJ/kg of substrate
Zhang et al. (2010)	22 097	kJ/kg of substrate
Mason (2006)	9 760 to 14 000	kJ/kg O_2

2.5.4 Mass balance

Mass transfer is one of the most variable areas in the literature, being dependent on the scope of the model. The most common mass balances are global balances (assuming the pile to be homogenous) applied for water and oxygen transfer. A general form of these equations (Higgins and Walker, 2001) is presented below.

$$\frac{dH_2O_s}{dt} = \frac{G\big(H_s(T_a) - H_s(T)\big) - Y_{H_2O} \cdot {dS}/{dt}}{\rho_{DM} V} \tag{2.10}$$

$$\frac{dO_2}{dt} = \frac{G\big(X_{O_2,in} - X_{O_2,out}\big) - Y_{O_2} \cdot {dS}/{dt}}{V \varepsilon \rho_a(T)} \tag{2.11}$$

Where $\mathrm{H_2O_s}$ represents the amount of water in the substrate (kg H_2O/kg dry matter), $\mathrm{O_2}$ is the oxygen content of the dry air (kg O_2/kg dry air), G is the mass airflow (kg dry air/s), $\mathrm{H_s}$ is the saturated humidity of the air (kg H_2O/kg dry air), T and $\mathrm{T_a}$ are the temperature of the system and the ambient temperature (°C), respectively, $\mathrm{Y_{H_2O}}$ is the metabolic production of water (kg H_2O/kg S) and $\mathrm{Y_{O_2}}$ the consumption of oxygen (kg O_2/kg S), V is the volume of the system (m^3), ρ_{DM} is the density of the dry matter (kg m^{-3}), ρ_{a} is the density of the air (kg m^{-3}) and ε is the porosity of the bed (-).

Equations 2.10 and 2.11 offer a basic and simplified representation of the mass transfer, the first terms on the right of the equation being the mass that gets transferred in and out of the system through the airflow, with the second term being the amount produced/consumed by the system. However, they fail to take into account the heterogeneous nature of the composting pile. Despite this, other than for a few specific purposes such as pathogen elimination, mixing, or very accurate temperature profiles, homogenous (0D) models have generally offered satisfactory results for global temperature and moisture mass balances, as well as predictions for a variety of other variables. As is the case with the energy balance, these equations can generally be easily solved through a finite difference approach or a differential equation solver.

Some studies have used more detailed and diverse transport models, including a variety of other compounds such as emissions (CO_2, CH_4, NH_3, N_2O) and nutrients (phosphorus and nitrogen) (see section 4 for more details), considerations of heterogeneity through a spatial description of the system, and other transfer processes such as diffusion and multiphase (between water and air) transport. These include some detailed one-dimensional airflow and transportation models (Bongochgetsakul and Ishida, 2008; Fytanidis and Voudrias, 2014; He et al., 2018; Luangwilai et al., 2018; Tremier et al., 2005a), as well as some of the 2 and 3D models mentioned previously (Kuwahara et al., 2009; Moraga et al., 2009; Zambra et al., 2011; Zambra et al., 2012; Zambra et al., 2015).

There are also rare efforts that have focused on liquid transfer through the composting pile, something that is nearly never considered. These works include Seng et al. (2012) who developed a water flow model to predict moisture content (including diffusion and percolation of liquid) and Zambra et al.’s (2015) bioleaching model.

2.5.5 Parametrization and sensitivity of composting models

Composting models vary widely in complexity. With the development of mechanistic models, the size of these models has tended to grow significantly, requiring more and more state variables and parameters. Indeed, it is common to see models with over 40 parameters and state variables. Despite the presence of parameter-heavy models, model identifiability has seen very limited interest in the reviewed papers, while Hamelers (2004) has already provided a fantastic overview of this subject for composting kinetic modelling.

Therefore, instead of focusing on identifiability, it can be beneficial to explore the parameters that have the most significant impact on a model's output. This has been explored multiple times through sensitivity analyses, though they have been presented in only a surprisingly small portion of the reviewed literature (26%, n = 32). One major challenge with applying sensitivity analysis to composting is that, given the multiple interactions that exist within a composting model, it can often be difficult to gain meaningful understanding from the analysis (Kaiser, 1996; Petric and Mustafić, 2015; Sole-Mauri et al., 2007).

Nevertheless, some relatively consistent results have been found. The most consistent finding is that the maximal growth rate and/or hydrolysis rate constant are amongst the most important parameters affecting the process (temperature variation, emissions, moisture variation) (Denes et al., 2015; Ge et al., 2015; Liang et al., 2004; Lin et al., 2008; Ma et al., 2018; Petric and Mustafić, 2015; Sole-Mauri et al., 2007; Stombaugh and Nokes, 1996; Vasiliadou et al., 2015; Vidriales-Escobar et al., 2017; Zavala et al., 2004; Zhang et al., 2012), as well as death rate constants (Denes et al., 2015; Lashermes et al., 2013; Liang et al., 2004; Lin et al., 2008; Vidriales-Escobar et al., 2017; Zhang et al., 2012), while initial biomass concentration has a very limited effect (Bialobrzewski et al., 2015; Denes et al., 2015; Ge et al., 2015; Kaiser, 1996; Lashermes et al., 2013; Petric and Mustafić, 2015; Xi et al., 2005). Yields and consumption rates have also been noted multiple times as having a high impact, such as the O_2 uptake rate (Higgins and Walker, 2001), activation energy of the biomass (Luangwilai et al., 2010), assimilation rate of substrate/product yield (He et al., 2018; Lashermes et al., 2013; Vasiliadou et al., 2015; Zhang et al., 2012), and biological heat generation coefficient (De Guardia et al., 2012; Wang et al., 2014).

Further studies have also focused their analyses on the impact of certain modifications that they brought to traditional composting models, highlighting the impact of design decisions. For example, Ge et al. (2016b) noted the high sensitivity of convection to the heat transfer coefficient and how this could seriously impact the heat balance. Further examples in this vein include those of Seng et al. (2012) and Bonifacio et al. (2017b) who found ambient weather (temperature, rain) to be amongst the main sources of variability within their models. There is also the works of Zavala et al. (2004) and Fontenelle et al. (2011) that provide some interesting results regarding the biological side of the process. Zavala et al. (2004) developed a model that used three processes (hydrolysis followed by uptake (growth) followed by endogenous respiration) and noticed that the parameters associated to hydrolysis were significant, while those associated to growth were not. This was due to hydrolysis being the rate limiting step. Fontenelle et al. (2011) instead implemented three different microbial populations (yeast, bacterial and fungal) and determined that bacterial population had the most sizable impact on the outputs, while the model was less sensitive to changes in fungal population. These results were expected given that the bacterial community had the most dominant role during their experimental study.

2.6 Emerging areas and areas requiring development

Beyond the traditional composting models presented throughout the paper, often seeking to predict degradation, temperature and moisture content, other models have been designed for or have included more niche considerations. This includes prediction of self-ignition of composting piles (Aganetti et al., 2016; Luangwilai et al., 2018; Moraga et al., 2009; Nelson et al., 2003; Sidhu et al., 2006; Zambra et al., 2011; Zambra et al., 2012), pathogen or pollutant destruction/evolution (Gea et al., 2007; Lashermes et al., 2013; Pandey et al., 2016a; Pandey et al., 2016b; Sadef et al., 2014; Zhang et al., 2014), odour emissions (Gutiérrez et al., 2014; Gutiérrez et al., 2017; Heinemann and Wahanik, 1998; Rincón et al., 2019), gaseous emissions (Asadi et al., 2017; Asadollahfardi et al., 2015; Ge et al., 2016a; Liang et al., 2004; Oudart et al., 2015; Rafiee et al., 2017; Ro et al., 2018; Wilshusen et al., 2004), leachate/runoff water modelling (Duncan et al., 2013; Seng et al., 2012; Tollner and Das, 2004; Zambra et al., 2015), and nutrient transformation and loss (Bonifacio et al., 2017a; Bonifacio et al., 2017b; Oudart et al., 2015; Vasiliadou et al., 2015; Vlyssides et al., 2009).

Furthermore, many areas still require significant development. These areas include modelling for different composting systems (windrows, piles, rotating drums), predicting variations in free air space and volume, end quality and maturity, physicochemistry and pH, and biodegradability. There are also different modelling approaches, notably using stochastic or artificial intelligence, that have seen some interest over the years. This section will provide a detailed overview of these areas of research.

2.6.1 Consideration of the different composting processes

In-vessel (reactor) composting is disproportionately studied in the literature (63% of reviewed papers) compared to practical implementation of the process which also involves an important amount of windrow and static pile systems (28% of reviewed papers). A reason for this is the obvious ease and control of studying the process in a closed system, but this has left certain systems woefully understudied. This is notably the case for rotating drum (Oliveira et al., 2018; Varma et al., 2017; Villaseñor et al., 2012) and naturally aerated composting (Oudart et al., 2015). This is important seeing how composting models will generally only be applicable to the system they were designed around. This has to do with how aeration is undertaken in each system and with the important differences in the system boundaries, requiring significant redefinition of mass balances and potentially heat balances as well.

2.6.2 Consideration of physical parameters impact and variation

Another area that could see significant development is the modelling of free air space and volume change during the process. During composting, the mass of the pile will be reduced by about 10 to 50% (Breitenbeck and Schellinger, 2004; Tiquia et al., 2002; Van Lier et al., 1994), with a reduction in pile height of between 15 and 60% (Breitenbeck and Schellinger, 2004; Van Lier et al., 1994; Yue et al., 2008). This compacting will reduce the free air space and will lead to significant changes in many parameters, such as reducing effective airflow (oxygen diffusion and heat convection), increasing the heat conductivity of the pile and modifying mass transfer (notably gaseous exchange and water loss) (Das and Keener, 1996; El Kader et al., 2007). Beyond the work on compacting's influence on aeration by Das and Keener (1997b) and Yu et al. (2008), the development of a correction factor for degradation by Yu et al. (2009) and the response regression model for initial free air space by Soares et al. (2013), of the reviewed literature, only the work of Illa et al. (2012) sought to model the change in dimensions as a function of time and to link it to biological activity. Vasiliadou et al. (2015) also included a general volume change within their models based on the destruction of insoluble particulate matter, without looking at it from a dimensional perspective or the change in free air space. The capacity to predict and integrate free air space changes could be beneficial for process control and optimization, notably regarding mixing and moisture control (Das and Keener, 1996; El Kader et al., 2007). Further work in this area could be guided by the plethora of efforts to model compacting in soil sciences (e.g. Nawaz et al., 2013; Vereecken et al., 2016).

2.6.3 Prediction of quality and nutrient composition of composts

Prediction of the specific end quality of compost has also seen barely any work, despite the focus on modelling degradation. Modelling of the maturation (humification and biosynthesis) process is basically non-existent. Only one identified model sought to predict humic matter development, which was undertaken through structural equation modelling (Xie et al., 2019). The model of Kujawa et al. (2014) also managed to analyse compost maturity through neural analysis, though this does not provide much information on the actual quality of the final compost. Similarly, even though compost is used as a soil conditioner, modelling interest on the fate of nutrients during the process has been minimal. The two most advanced models with respect to nitrogen transformation and loss are currently those of Oudart et al. (2015) and Bonifacio et al. (2017a,b), considering ammonification, volatilization, nitrification, and denitrification to some degree, though with some significant and limiting assumptions. Phosphorus has seen even less interest, being considered only superficially through basic mass balances in two models (Vasiliadou et al., 2015; Vlyssides et al., 2009), whereas we have seen no mention of potassium or any of the micronutrients in the literature.

This can also be generalized to a lack of physicochemical considerations, notably through the omission of pH. pH impacts many important processes by affecting the activity of microorganisms (Smårs et al., 2002; Sundberg et al., 2004; Sundberg et al., 2013), as well as playing a key role in certain transformation processes, such as volatilization and solubilization of various compounds. Therefore, pH exercises a strong influence on the rate of decay, odour emissions, and nutrient transformation and loss during the process, as well as being an important marker for agronomic quality. Only one model has included pH other than through correction factors (Liang et al., 2004). Further work in this vein could also take inspiration from efforts in wastewater treatment and anaerobic digestion modelling that have already implemented pH (Batstone, 2009; Batstone et al., 2002; Rosen et al., 2006; Serralta et al., 2004; Yu et al., 2010), with notable work by Flores-Alsina et al. (2015), Huber et al. (2017) and Vaneeckhaute et al. (2018a) to include chemical speciation, activity corrections and ion-pairing for robust speciation and pH prediction. Chemical speciation during the composting process could be especially beneficial for models seeking to describe the transformation, loss and availability of certain compounds, such as heavy metals and nutrients, as various experiments have demonstrated (Eghball et al., 1997; Fang et al., 1999; Sharpley and Moyer, 2000; Wu et al., 2017; Xuejiang et al., 2008). Furthermore, the ability to model the influence of pH on composting could lead to the development and implementation of novel process control and optimization methods by pH control. These methods could be addressed at decreasing odours, reducing emissions, and increasing process efficiency and product quality. Indeed, methods such as addition of alkaline (Fang et al., 1999; Lei and VanderGheynst, 2000; Nakasaki et al., 1993; Yu and Huang, 2009) or acidic (Chen et al., 2010; Fangueiro et al., 2015; Kithome et al., 1999) amendments have been studied, as well as the use of magnesium (struvite formation) and zeolites as control strategies (Chan et al., 2016; Jeong and Kim, 2001; Lim et al., 2017; Wang et al., 2013b; Witter and Lopez-Real, 1988), and inoculation of the system with acid-tolerant bacteria (Kuroda et al., 2015; Nakasaki et al., 2013; Nakasaki et al., 1996).

2.6.4 Further needs of research in terms of modelling the substrates biodegradability

The final knowledge gap to be highlighted is the prediction of biodegradability of substrates. As discussed in section 2.5, various fractionations have been used to represent composting substrates. The aim of these fractionations, whether simple or detailed, are often to produce the most generalizable representation of the substrate given the wide variability in composition of organic wastes and bulking agents. Without being able to generalize the process kinetics, many composting models are only applicable to the waste sources they were developed and calibrated for. This is a significant limitation that currently plagues the field. This limitation is due to the biodegradability of organic matter (i.e., only a certain portion will be degraded, regardless of how long the process lasts) that can hinder the biodegradation of the substrate. A variety of methods can be used to determine biodegradability, such as BOD, COD, and respirometric methods (Tremier et al., 2005b), but they can be resource intensive and need to be repeated for different substrates. The ability to model biodegradability would be of considerable benefit to the field and could allow for models to be more generalizable to various waste sources. However, modelling efforts in the composting field have been non-existent. There have nonetheless been some efforts in the field of anaerobic digestion that could potentially serve as inspiration. For example, various studies have linked biochemical characterisation to biodegradability (Chandler et al., 1980; Denes et al., 2015; Liu et al., 2015; Mottet et al., 2010), while recent work by Bareha et al. (2019) also evaluated the prediction of organic nitrogen biodegradability. Bioaccessibility can also present another issue for composting, though this has generally been addressed through the use of Contois kinetics in a few composting models, with the model of Wang and Witarsa (2016) likely offering the best mechanistic framework due to the consideration of disintegration before hydrolysis as well.

2.6.5 Choice of the modelling approach

Regarding modelling approaches, despite the variability present throughout the composting process, stochastic approaches have been rare (Asadi et al., 2017; Fernández et al., 2016; Giusti and Marsili-Libelli, 2010; Neugebauer et al., 2018; Qin et al., 2007; Seki, 2000; Sun et al., 2011; Xi et al., 2008). These models have mostly been designed as a response to the inherent randomness of state variables in composting systems. Seki (2000) provided an early foray into this area of modelling. Seki’s model was based on a traditional deterministic and mechanistic model, following the fundamentals described earlier in the paper (Monod growth kinetic, first-order death, general heat balance). This model was then extended to a stochastic model by following a Marcovian process where the variable concentration terms used in the model were replaced to become probabilistic. The newly obtained balance equation of the probability distribution was then converted into the Fokker-Planck equation to facilitate their numerical solution. These added steps to render the deterministic model stochastic thus allowed the model to predict both the expected values and standard deviations of the state variables.

Since Seki’s (2000) work, research into stochastic modelling of composting has been split in approach. Some modellers have followed with the approach of converting deterministic and mechanistic models into stochastic ones, such as Qin et al.'s (2007) and Xi et al.'s (2008) integration of a fractional fuzzy vertex method to their models to characterize the effects of uncertainty. However, a variety of other approaches have appeared over time, especially in more recent work (after 2010). For example, Giusti and Marsili-Libelli (2010) used a Gustafson-Kessel clustering algorithm combined with linear autoregressive consequents to develop a dynamic model composed of three fuzzy rules that are associated to a linear autoregressive model based on temperature and pressure input data, following a more empirical than mechanistic approach. Sun et al. (2011) also implemented a cluster analysis, in this case applying a genetic algorithm to search for the optimal sets of state variables and parameters from the stepwise cluster analysis. Another stochastic modelling approach was undertaken by Fernández et al. (2016), seeking to expand on the ability of stochastic models to predict long-term behaviour during composting, something that prior models failed at achieving. This model combines Markov processes and Monte-Carlo simulations to deal with incomplete data based on previous observations for long term (> 200 days) composting, providing predictions for physical and biochemical characteristics (pH, electrical conductivity, total organic matter, carbon and nitrogen concentrations, and temperature). However, the two most recent works have gone back to focusing on more short-term predictions, with Asadi et al. (2016) comparing Lagrangian and Gaussian stochastic models to predict short range ammonia emissions from composting, and Neugebauer et al. (2018) exploring fuzzy modelling for heat recovery and aeration control during the process. The case of Neugebauer et al. (2018) also presents an interesting application of linguistic variables to the composting scenario in a novel way.

When compared to deterministic models, stochastic models offer the benefit of producing a much greater depth of secondary knowledge about the process, such as the variance of the state variables. This, however, generally comes at the cost of a more complex model, which may be undesirable given complexity of existing composting models. Nevertheless, stochastic models can be beneficial in certain situations. One of the main draws of modelling with uncertainty is that these models can address systems with incomplete data and, when combined with inductive approaches, can be alluring for practical application. They can also provide valuable operating insight for composting by identifying whether observed performances fall within the system's range of uncertainty, or whether there may be another (optimizable) factor at play (Qin et al., 2007). Though the ability to produce accurate long-term predictions has been lacking (Giusti and Marsili-

Libelli, 2010), recent efforts seem to be making good progress in this area as well (Fernández et al., 2016). Despite these properties, the use of stochastic methods in many composting applications can be challenging. The variability of an input or an operating condition could be considered by the model, but this variability is often associated with many important changes that the model may not be able to deal with, notably relating to kinetics. For example, a variable substrate composition, such as a change in the C/N ratio, moisture level, or mixing, can lead to significant kinetic changes that may not be captured through a stochastic approach. However, artificial intelligence, an extension of stochastic processes, can offer many of the same advantages, while circumventing some of the drawbacks.

Artificial intelligence as a modelling approach has also seen relatively limited development, though interest has been growing over the past decade (Alavi et al., 2019; Boniecki et al., 2013; Boniecki et al., 2012; Díaz et al., 2012; Faverial et al., 2016; Kujawa et al., 2014; Liang et al., 2003b; Tang et al., 2006; Varma et al., 2017; Yildiz and Degirmenci, 2015). These models have been aimed at a variety of aspects of composting modelling and have provided some innovative ways to follow the process. For example, the early models of Liang et al. (2003b) investigated various backpropagation networks (a form of artificial neural network) that could estimate the O_2 uptake rate, and thus microbial activity, during biosolids composting, using only temperature, moisture content, and process duration as inputs. Díaz et al. (2012) used an adaptive neural fuzzy inference system to optimize pH, temperature, and CO_2 evolution based on aeration, moisture content, particle size and composting time as inputs, similarly to Varma et al. (2017) who used a radial basis functional neural network to optimize volatile solids, soluble biochemical oxygen demand and CO_2 evolution during the process. Some studies have focused on more specific parameters, such as Boniecki et al.'s neural networks to predict ammonia emissions (Boniecki et al., 2012) and heat loss (Boniecki et al., 2013), and Yildiz and Degirmenci's (2015) work on predicting oxygen exchange through regression analysis and artificial neural network modelling, the latter noting the benefits of the neural approach over the regression analysis. Other neural models have also aimed at predicting the end-quality of the compost. These include the models of Kujawa et al. (2014), Faverial et al. (2016), and Alavi et al. (2019). Of these works, Kujawa et al.'s (2014) model based on neural image analysis provides a great example of the benefits of these artificial intelligence methods and how they differentiate themselves from traditional mechanistic modelling.

In their work, Kujawa et al. (2014) combined computer image analysis with neural modelling to classify the stage of maturation of compost, an area that was identified as lacking in research in section 2.6.3. The models were developed by analysing the colour and texture of images of compost (sewage sludge and maize straw) at various stages of maturation. These analyses included greyscale, RGB (red-green-blue), contrast, and other visual variables that were found to be relatable to the stage of maturation. This information was then fed into a neural model (based on the multilayer perceptron typology) that was trained to identify which data sets reach the desired maturation stage. Of the 21 models generated by the researchers, the best model has a reported classification error rate of 1.56%, demonstrating the potential accuracy of these neural approaches.

As highlighted by the above-mentioned papers, intelligence algorithms can present a very alluring approach to model many of the complex processes taking place during composting. Their ability to rely on measurable variables (such as temperature, pH, microbial population, carbon, nitrogen, or even images) without requiring the knowledge of parameters or even mechanisms is of clear practical advantage. Such systems that develop through inductive learning (training) could also be beneficial for the development of knowledge for later use in deductive models through the patterns that they identify. However, the development and application of an intelligence algorithm is not without issues, as will be discussed in chapter 6 (Walling and Vaneeckhaute, 2020a). These systems require a substantial amount of calibrated data to properly train them and to ensure their accuracy, significantly more than would be used to design a mechanistic model (for example, Alavi et al. (2019) used 567 experimental sets to train their artificial neural network, while Liang et al. (2003b) used 8760 data patterns for their network). This issue is compounded by the relative rigidity of intelligence systems, these systems potentially not being transferable to other (similar) cases due to data variations because of limitations to their training. This could be problematic given the huge variability at many steps of the composting operation (substrates, bulking agents, moisture content, temperature, pH, etc.). Furthermore, even when these systems are accurate, they can run the risk of being labeled as black boxes, possibly limiting their implementation. Nevertheless, artificial intelligence provides a very interesting (and different) path forward for composting modelling. Developers should not favor developing either mechanistic or artificial intelligence models, but instead use both in tandem to support development in the composting field. Intelligence systems can be used to produce easy to use models and to identify patterns, while mechanistic models can be used to learn (validate and test theory) and to allow for robust control and optimization.

Concerning empirical vs mechanistic modelling, Mason (2006) had noted that the most successful models at the time implemented either empirical kinetic expressions or first-order models with empirical corrections, despite the limited evidence “for the applicability of a first-order model to substrate degradation”. This trend was not observed in a major portion of our reviewed literature, with a significant increase in accuracy of mechanistic models, especially those implementing Monod-type kinetics, as of the mid 2000’s. This is also supported by the work of Fytanidis and Voudrias (2014) who compared both first order and Monod kinetics and found Monod kinetics to be slightly more accurate. The author hypothesizes that the initial shortcomings of mechanistic models were due to a lack of proper understanding of how degradation in these systems occurred, alongside numerous (questionable or wrong) assumptions. As mechanistic models started to implement more representative microbial fractionations and faulty assumptions were reduced, their predictive capabilities significantly increased.

2.7 Conclusions

This review aimed at providing a comprehensive and consolidated view of the state of composting modelling, a field that has seen consistent development over the past 40 years. Multiple aspects of composting modelling have been highlighted throughout this review:

1. A majority of composting models have sought to combine degradation kinetics with dynamic heat and mass balances in a deterministic fashion to predict temperature, moisture and substrate degradation through time. There has also been a growing body of work on multidimensional (1, 2 and 3D) systems in more recent years.
2. Degradation kinetics have been represented through either first-order or Monod-type kinetics and have been a more contentious area than the well agreed upon heat and mass balances. Despite stronger theoretical support and some evidence that Monod-type kinetics should offer the most realistic results, both approaches have shown good success. Multiple degradation processes have been considered, including disintegration and hydrolysis of particulate substrate, cellular uptake of soluble compounds, cellular death, and chemical oxidation, in both aerobic and anaerobic conditions.

3. The use of correction functions to adjust microbial kinetics is divided. Nearly half of the reviewed literature implemented some form of correction functions, while the other half completely neglected their use. A multitude of correction functions are available to take into account the impact of temperature, oxygen content, moisture content, free air space and pH, a list of which is presented in the appendix of this work. Further research should investigate and compare the use of these various correction functions to provide modellers with better guidance as to which functions to select.
4. Sensitivity analyses have been undertaken in only a small portion of the reviewed papers, despite the value of these assessments in providing an understanding of the impact of certain parameters and of design choices.
5. Areas of research that could benefit from more development include: modelling for different composting systems (windrows, piles, rotating drums), predicting variations in free air space and volume, end quality and maturity, physicochemistry and pH, and biodegradability.
6. The growing interest in stochastic and artificial intelligence modelling approaches can provide powerful new tools to develop knowledge in the field. These approaches should be used in tandem with mechanistic modelling to provide the greatest level of learning and adaptability by using the advantages of each approach to counteract the drawbacks of the other.

Chapter 3: Modelling composting kinetics: An evaluation of temperature, moisture, and oxygen corrections

3.1 Résumé

Ce chapitre présente une évaluation des fonctions de correction utilisées dans la modélisation mathématique du compostage. Sur la base des données expérimentales de diverses expériences à l'échelle pilote, des modèles de dégradation de premier ordre corrigés ont été développés et évalués pour chaque combinaison de fonction de correction (96 par essai) et pour deux approches de modélisation distinctes (k_{max} fixe vs optimisé). Les résultats de ces modèles ont ensuite été évalués par une approche de l'erreur quadratique moyenne normalisée (Normalized Root Mean Squared Error) et une enquête plus approfondie sur l'ensemble optimal (10 premiers) pour chaque essai. Il a été constaté que le modèle de Haug (1993) et la correction de température cardinale (modèle de Rosso) pour la température ont de bonnes performances dans les deux cas, tandis que l'équation d'Arrhenius est parmi les plus performantes lorsque k_{max} est fixé. L'équation de Monod était la meilleure fonction de correction pour la limitation de l'oxygène dans tous les cas, tandis que les résultats pour les corrections d'humidité étaient plus variables. Des appariements préférentiels de corrections de température, d'humidité et d'oxygène sont fournis.

Mots clés: biodégradation aérobique, état solide, modèle, facteur d’ajustement, simulation, limitation de croissance

3.2 Abstract

This chapter presents an assessment of the correction functions used in mathematical composting modelling. Based on experimental data from various pilot scale experiments, corrected first-order degradation models were developed and evaluated for every combination of correction function (96 per trial) and for two separate modelling approaches (fixed vs optimized $\mathrm{k}_{\mathrm{max}}$). The results of these models were then assessed through a Normalized Root Mean Squared Error (NRMSE) approach and further investigation of the optimal set (top 10) for each trial. It was found that the Haug (1993) and the cardinal temperature correction (Rosso model) for temperature have strong performances in both cases, while the Arrhenius equation is amongst the most successful when $\mathrm{k}_{\mathrm{max}}$ is fixed. The Monod equation was consistently the best correction function for oxygen limitation across all cases, while results for moisture corrections were more variable. Preferential pairings of temperature, moisture and oxygen corrections are provided.

Keywords: aerobic biodegradation, solid state, model, adjustment factor, simulation, growth limiting

3.3 Introduction

Chapter 2 has provided us with an extensive overview of composting modelling, yet many important questions were also highlighted. Beyond the interest in developing a generalizable composting model to predict GHG emissions and nutrient loss/transformation, an important amount of doubt seems to surround the validity of certain modelling approaches, notably related to the use of correction functions for factors such as temperature, moisture, and oxygen content.

As detailed in chapter 2, the most commonly used model for degradation kinetics throughout the composting literature is a first order expression. Therefore, the prediction of substrate degradation over time can be expressed as detailed in Eq. 3.1:

$$\mathrm{R_{degradation}} = -\frac{\mathrm{d[S_i]}}{\mathrm{dt}} = \mathrm{k_i} \cdot [\mathrm{S_i}] \tag{3.1}$$

where $[\mathrm{S_i}]$ is the concentration of biodegradable substrate, t is time and $\mathrm{k_i}$ is the (degradation/hydrolysis) rate constant.

However, the above expression represents an "ideal" degradation, unaffected by the many dynamic process variables that influence biodegradation, such as temperature, moisture, and oxygen content. Modellers have therefore taken to implementing correction functions to consider the influence of a variety of factors and to better represent reality, as was touched on in chapter 2. These correction functions are either mechanistic or empirical factors that vary between 0 and 1 and are used to constrain the degradation. Therefore, when implementing correction factors, the degradation rate can be rewritten as follows, with $\mathrm{f_i}$ referring to correction functions for temperature, moisture content (MC), oxygen content, free air space (FAS) and pH:

$$\mathrm{R'_{degradation}} = \mathrm{R_{degradation} f_T f_{MC} f_{O_2} f_{FAS} f_{pH}} \tag{3.2}$$

These correction functions ensure that the composting model does not assume that degradation always happens at a maximal rate, thus limiting degradation outside of optimal ranges. For example, composting is known to operate optimally at temperatures between 50 and 60 °C (Eklind et al., 2007; Miyatake and Iwabuchi, 2006; Nakasaki et al., 1985), moisture contents of 40 and 70% (Haug, 2018; Richard et al., 2002; Tiquia et al., 1998) and oxygen contents above 5-10% (Bertran et al., 2004; Haug, 2018), with growth being significantly limited above and below these conditions. These functions propose to offer some method of representing these constraints. Despite the benefits of correction functions and their widespread implementation that had been previously noted by Mason (2006), the review of chapter 2 makes it clear that this area requires further research. Indeed, only 46% of the reviewed models implemented correction functions, while a plethora of functions were utilized (15 different functions for temperature, 10 for moisture content and 5 for oxygen content). Despite prior work by Richard et al. (1999; 2006) and Mason (2008) that sought to investigate the impact of temperature and oxygen on composting kinetics, there has not been any work seeking to assess the various correction functions used throughout the field in a concerted manner. These earlier works have led to increased support for the cardinal temperature correction (the Rosso model) (Rosso et al., 1995; Rosso et al., 1993) for temperature correction (Mason, 2008; Richard et al., 2006), while the Monod expression was determined by Richard et al. (1999) to be the most accurate for oxygen, with Baptista et al.'s (2010) modified Monod expression gaining prominence in recent years. Regarding moisture corrections, to the best of our knowledge, there has not been any work on assessing their use. However, given recent developments in composting modelling and the limited number of correction functions evaluated in these studies, an up to date and consolidated evaluation would be of great benefit to the field.

This chapter therefore seeks to provide guidance on the use of correction functions in composting modelling, notably by assessing the use of 21 correction functions (11 for temperature, 7 for moisture and 3 for oxygen content) used in composting literature (some had to be omitted given a lack of information, detailed in section 2.2). We aim to provide insight as to the benefits and drawbacks of these functions, how they interact with one-another, and hope to provide guidance for future modellers in selecting the correction functions that can provide the most accurate results. The work undertaken in this chapter is based on the quantitative and qualitative assessment of the ability of a first-order kinetic model to accurately predict experimental results. Every combination of correction functions has been tested on data from the literature based on four experimental trials, the resulting models were then analyzed numerically using the normalized root mean square error (NRSME). Optimal solution sets (top 10 for each trial) were then identified to further validate the results of the NRSME assessment. As such, this chapter identifies the most accurate correction functions, both individually and jointly, as well as providing guidance for model developers in selecting these functions for their models.

This chapter is divided as follows: section 3.4 presents the materials and methods used to undertake this assessment, followed by a detailed presentation of our results and discussions around them in section 3.5, with concluding remarks being presented in section 3.6.

3.4 Materials and methods

The experimental data used for this study comes from the work of Malamis et al. (2016). This article was chosen following the review process of chapter 2 (Walling et al. (2020)) where it was identified as presenting the best data for this type of analysis, given Malamis et al.'s (2016) thorough follow through and clear presentation of temperature, moisture content, oxygen content, degradation rate and organic matter loss, all of which was replicated over four trials. Detailed information on their experimental work can be found in their paper, but it consisted in four 20 to 25-day trials of sewage sludge and agricultural waste composting in an in-vessel (reactor) system with a working volume of 2.4 m^3. Based on these experimental results, the following work was undertaken.

3.4.1 Kinetic modelling

A first-order equation was applied to model the process. First-order equations have been by far the most prominent in the field, likely due to hydrolysis being the rate-limiting step of the process (Walling et al., 2020). The first-order model presented in Eq. 3.1 was therefore applied, using the form employed by Malamis et al. (2016):

$$\frac{\mathrm{d}[\mathrm{BOM}]}{\mathrm{dt}} = -\mathrm{k_d} \cdot [\mathrm{BOM}] \tag{3.3}$$

where BOM is the biodegradable organic matter (kg), $\mathrm{k_d}$ is the first-order biodegradation rate (day^{-1}), and t is time (day).

$\mathrm{k_d}$ is then adjusted with correction functions for temperature, moisture content and oxygen content, more details of which can be found in section 3.4. $\mathrm{k_d}$ can therefore be expressed as follows, where $\mathrm{k_{max}}$ is the maximal biodegradation rate (day^{-1}):

$$\mathrm{k_d} = \mathrm{k_{max}}\, \mathrm{f_T f_{MC} f_{O_2}} \tag{3.4}$$

Though implemented in a very limited amount of literature, free air space (FAS) and pH corrections can be applied. However, the only FAS correction function to find any traction is that of Haug (1993), while pH has only been corrected for twice (in Liang et al. (2004)

and Petric et al. (2015)). Due to their limited application and the lack of necessary data, these functions were omitted from this study. However, even if the necessary data was available to implement a FAS correction, prior studies have indicated that it may not be a significantly limiting factor (Baptista et al., 2010; Zhang et al., 2010).

Though Malamis et al. (2016) state that they integrated Eq. 3 to obtain a traditional rate law, we doubt the validity of such an approach given the time dependency of $\mathrm{k_d}$, seeing how temperature, moisture and oxygen content all vary in time. We therefore proceeded to solve Eq. 3.3 by using the finites differences method by calculating d(BOM)/dt, $\mathrm{f_T}$, $\mathrm{f_{MC}}$ and $\mathrm{f_{O_2}}$ for every time step of 1 day.

Two separate modelling approaches were used regarding $\mathrm{k_{max}}$: (1) in the first approach, $\mathrm{k_{max}}$ was given a fixed value across all model combinations within a same trial based on the experimentally observed degradation rate. In this case, $\mathrm{k_{max}}$ was set at 15% higher than the highest observed degradation rate, observed around 60 °C in every case, which coincides with the optimal temperature range for composting (Eklind et al., 2007; Miyatake and Iwabuchi, 2006; Nakasaki et al., 1985). The advantage of this approach is that it is easily generalizable if values of $\mathrm{k_d}$ or $\mathrm{k_{max}}$ are known, allowing for application in a variety of contexts (different wastes or system configurations). (2) In the second approach, values of $\mathrm{k_{max}}$ were optimized for each combination using the Excel Solver add-in by minimizing the Normalized Root Mean Squared Error (NRMSE) (discussed in section 2.3) by varying $\mathrm{k_{max}}$. The benefit of the second approach is that it produces more accurate predictions and, for our assessment, allows us to identify which model combinations provide the optimal shape relationship. However, the values of $\mathrm{k_{max}}$ can vary widely, which can limit the generalizability of such models given that these values might have little bearing on the actual maximum degradation rate (the model is based around a very specific case).

3.4.2 Correction functions

The correction functions used in Eq. 3.4 were selected based on the list of correction functions applied in composting literature identified in chapter 2. Of these identified functions, a few were not included in this study given the lack of information necessary to use them. These include the temperature corrections by Petric et al. (2015) due to unclear values for the coefficients used in the equation and Yu et al. (2009) due to a microbial fractionation that we could not simulate with this data; and moisture corrections by Shishido (1999) and Kaneko and Fujita (1986) due to a lack of information on the ranges of applicability of these functions. The list of functions tested for temperature, moisture and oxygen content can be found in tables 3.1 through 3.3. In total, 21 correction functions were assessed.

In the equations presented in table 3.1, T is the temperature in °C. For the cardinal temperature correction (Rosso model), T_{max} is set to 71.6 °C, T_{min} is 5 °C and T_{opt} is 58.6 °C, as these are the most commonly used values in the literature following the work of Richard and Walker (2006). The reference temperatures (T_{R1} and T_{R2}) in the Haug (1993) model are given values of 50 and 60 °C, respectively. Though T_{R1} is usually given a value of 20 °C (e.g. Petric and Selimbašić, 2008; Wang et al., 2016; Zhou et al., 2014a), given that we used $\mathrm{k_{max}}$ instead of the traditional degradation rate at 20 °C ($\mathrm{k_{20}}$), the value of 50 °C was found to be more appropriate. In the Stombaugh and Nokes (1996) correction, the proposed values of T_1 = 0 °C, T_2 = 30 °C and T_3 = 55 °C were used (Stombaugh and Nokes, 1996). An important note regarding the application of the Arrhenius equation: whereas all of the correction functions in table 3.1 can simply be applied using the temperature at a specific time, the Arrhenius equation requires the knowledge of A (pre-exponential factor) and $-E_a/R$ (activation energy). These values can be simply determined with experimental data if the rate of degradation is measured, where the equation can be rewritten as follows:

$$\mathrm{ln(k_d) = ln(A) - \frac{E_a}{R}\left(\frac{1}{T + 273}\right)} \tag{3.5}$$

Given the form of Eq. 3.5, by plotting $\mathrm{ln(k_d)}$ as a function of $\mathrm{1/(T + 273)}$, we can obtain a relatively linear plot whose y-intercept is equal to $\mathrm{ln(A)}$ and slope is $\mathrm{-E_a/R}$. The Arrhenius equation can then be applied using these values, with the important note that, in this case, the Arrhenius equation replaces $\mathrm{k_{max}\, f_T}$ in Eq. 3.4, seeing how it offers an estimate of $\mathrm{k_d}$, though it is uncorrected for moisture or oxygen content.

Table 3.1 Temperature correction functions used in this study from most to least used. T is expressed in degrees Celsius.

Temperature correction function	**References**
$f_T = \frac{(T - T_{max})(T - T_{min})^2}{(T_{opt} - T_{min})[(T_{opt} - T_{min})(T - T_{opt}) - (T_{opt} - T_{max})(T_{opt} + T_{min} - 2T)]}$	(Rosso et al., 1995; Rosso et al., 1993)
$k_d = Ae^{\frac{-E_a}{R(T+273)}}$	Arrhenius equation
$f_T = C_1^{T-T_{R1}} - C_2^{T-T_{R2}}$; often, $C_1 = 1.066$ and $C_2 = 1.21$.	(Haug, 1993)
$f_T = 0.0182T$	(Haug, 1996)
$f_T = -3.11 \times 10^{-4}T^2 + 3.48 \times 10^{-2}T + 0.0265$	(Lin et al., 2008)
$f_T = 2.142 \times 10^{-4}T^2 - 2.356 \times 10^{-2}T + 1.348$	(Ekinci, 2001)
$f_T f_{MC} = 0.089 \exp\left(-0.5\left[\left(\frac{MC - 44.22}{19.87}\right)^2 + \left(\frac{T - 58.31}{16.72}\right)^2\right]\right)$	(Ekinci et al., 2004b)
$f_T = -8 \times 10^{-6}T^3 + 0.008T^2 - 0.0238T - 0.2643$	(Mohee et al., 1998)
$f_{T,bacteria} = T(80 - T)/1600 \;\; T < 80$ $f_{T,actinomycetes\ and\ fungi} = T(60 - T)/20(80 - T) \;\; T < 80$	(Kaiser, 1996)
$f_T = \begin{cases} T/(T_2 - T_1) & T_1 < T \leq T_2 \\ 1.0 & T_2 < T \leq T_3 \\ 3.75 - T/(T_2 - 10) & T_3 < T \end{cases}$	(Stombaugh and Nokes, 1996)
$f_T = \exp(-(T - 57)^2/254))$	(Smith and Eilers, 1980)

In the correction functions of table 3.2, MC refers to the moisture content of the composting system. It is either expressed as a value between 0 and 1, or a percentage between 0 and 100%. All functions except those of Haug (1980), Ekinci et al. (2004b) and Mora-Naranjo et al. (2004) use an MC ranging between 0 and 1. For the Stombaugh and Nokes (1996) correction, the proposed values of $m_1 = 0$, $m_2 = 0.2$ and $T_3 = 0.4$ were used (Stombaugh and Nokes, 1996).

Table 3.2 Moisture correction functions used in the reviewed literature from most to least used.

Moisture content correction function	**References**
$f_{MC} = \dfrac{1}{\exp(-17.684MC + 7.0622) + 1}$	(Haug, 1993)
$f_{MC} = \begin{cases} 0 & m_1 < m \leq m_2 \\ m/m_2 - 1.0 & m_2 < m \leq m_3 \\ 1.0 & m_3 < m \end{cases}$	(Stombaugh and Nokes, 1996)
$f_{MC} = \begin{cases} 1 - 17.3(1 - m/100)^{6.94} & m \geq 40 \\ 20.6614(m/100)^{4.06} & m < 40 \end{cases}$	(Haug, 1980)
$f_T f_{MC} = 0.089 \exp\left(-0.5\left[\left(\dfrac{MC - 44.22}{19.87}\right)^2 + \left(\dfrac{T - 58.31}{16.72}\right)^2\right]\right)$	(Ekinci et al., 2004b)
$f_{MC} = 0.012m - 0.18$	(Mora-Naranjo et al., 2004)
$f_{MC} = -56.97 + 57.98 \exp[(-0.5(m - 0.56)/1.52)^2]$	(Mohee et al., 1998)
$f_{MC} = \exp(-10.973(FS - 0.3)^2)$	(Smith and Eilers, 1980)

Finally, in table 3.3, three oxygen corrections are presented. In these equations, O_2 represents the oxygen content of the environment, expressed as a % v/v. Two of these expressions are mechanistically derived: the traditional Monod expression had found the most use in the literature until the advent of Baptista et al.'s (2010) modified Monod, which has seen strong use over the past decade (Walling et al., 2020). In the Monod expression, the most common value for k_{O_2}, the oxygen half-saturation coefficient, is 2% v/v, following the works of Haug (1993) and Richard et al. (2006). In the Higgins and Walker (2001) correction, temperature and moisture also intervene, though this function is not a temperature correction (Higgins and Walker used the cardinal temperature function to correct for temperature). In this case, moisture content is represented as a percentage.

Table 3.3 Oxygen content correction functions used in the reviewed literature in order of use.

Oxygen content correction function	**References**
$f_{O_2} = \dfrac{O_2}{O_2 + k_{O_2}}$	Monod expressions
$f_{O_2} = \dfrac{O_2}{\left(\dfrac{20.95}{0.83 + 20.95}\right)(0.83 + O_2)}$	(Baptista et al., 2010)
$f_{O_2} = \dfrac{O_2}{0.79 - 0.041T + 0.040MC + O_2}$	(Higgins and Walker, 2001)

3.4.3 Modelling assessment

Using the experimental data provided in Malamis et al. (2016), reaction kinetics for each of the four trials were modelled using the numerical process detailed in section 3.4.1 and implementing every combination of the correction functions presented in section 3.4.2. However, an early assessment of the correction functions was undertaken to validate their individual use. This assessment consisted in implementing the correction functions individually with the experimental data. In the case of temperature corrections, it was found that the models of Ekinci (2001), Mohee et al. (1998) and Smith and Eilers (1980) provided non-sensical corrections, Ekinci's (2001) function constantly tending towards 0 and Mohee et al.'s (1998) and Smith and Eilers' (1980) functions always providing results above (and significantly greater than) 1. In the case of Kaiser (1996), which provides two functions based on microbial fractionation, we took the average of the bacterial and fungal corrections. For moisture corrections, the functions by Smith and Eilers (1980) and Mohee et al. (1998) once again had to be dismissed given that the prior stayed constant at 0 and the latter was constantly above 1. No issues were found with the oxygen corrections.

Following this initial assessment, simulations were ran for every kinetic model based on the daily temperature, moisture, and oxygen content data provided in Malamis et al. (2016). In total, 768 simulations were undertaken (96 per trial (8 temperature x 4 moisture x 3 oxygen) x 4 trials x 2 $\mathrm{k_{max}}$). The results of these simulations predicting biodegradation over time were then compared to the experimental results. Quality of fit was determined quantitatively using the normalized root mean square error (NRMSE), using equations 3.6 and 3.7:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(\mathrm{BOM_{loss,model,i}} - \mathrm{BOM_{loss,exp,i}}\right)^2}{n}} \tag{3.6}$$

$$\mathrm{NRMSE} = \frac{\mathrm{RMSE}}{\mathrm{BOM_0}} \times 100 \tag{3.7}$$

Where $\mathrm{BOM_{loss}}$ refers to the cumulative amount of biodegradable organic matter loss at a time i (%), $\mathrm{BOM_0}$ represents the initial biodegradable organic matter content (%), and n is the amount of data points.

Using the NRMSEs obtained for every simulation, average NRSMEs were determined for each correction function, both by trial and averaged over the four trials. Furthermore, in the aim of shedding some light on what combinations of correction functions provided the most accurate results, the top ten models (based on NRMSE) were identified for each trial, forming what will be referred to as "optimal sets".

3.5 Results and discussion

3.5.1 Correction function profiles

Figure 3.1 through 3.3 present the profiles of each correction function with respect to their correction variable (in plots (a)), and the result of the correction functions, as expressed through a correction factor, for trial 1. Trial 1 was selected simply for visualization purposes.

Starting with temperature corrections, presented in Figure 3.1, both plots highlight the impact that the functions have on the degradation rate. From the top plot, (a), we can observe three general behaviours, i.e., functions that are: (1) slightly restrictive, such as those of Stombaugh and Nokes (1996) and Kaiser (1996), which are barely inhibitor in normal operating ranges (> 25 °C), though the latter becomes inhibitory at a much lower "high" temperatures than the other functions; (2) moderately restrictive, such as those of Haug (1996) and Lin et al. (2008); and (3) highly restrictive, such as those of Haug (1993) and the cardinal temperature correction, with the prior being the most restrictive of the functions assessed. Based on Figure 3.1 (b), we can see that the Arrhenius equation also fits into the category of "highly restrictive".

When looking at how this impacts the estimated degradation, Figure 3.1 (b) shows how the outputs of these functions translate to a real case, during a full composting trial. At day 0, given the low temperature, the highly restrictive functions limit the reaction rate down to about 20% of k_{max}, (cardinal temperature, Haug (1993), Arrhenius), while the moderately restrictive ones limit it to 50% to 70% (Haug (1996) and Lin et al. (2008)), and the slightly restrictive functions reduce it to 80% to 90% (Stombaugh and Nokes (1996) and Kaiser (1996)). During the thermophilic phase, the main impacting factor is what the functions consider to be the "maximum" temperature of composting, which appears as a sharp drop-off in most of the curves of plot (a). The most high-temperature restrictive function is that of Kaiser (1996), which starts to decrease degradation at 40 °C, with the Haug (1996) model being at the opposite end of the spectrum, never decreasing. Though, for the Haug (1996) equation, given that it does predict a rate above k_{max}, it would be pertinent to limit the correction factor to 1 above a certain temperature. When looking at Figure 3.1 (b), the curve of Kaiser's (1996) function clearly highlights the impact that a "maximum" temperature can have, significantly inhibiting the rate of degradation, while most other models considered a near maximal degradation rate. Finally, for the passive phase of the composting process (when the temperature starts to decrease back down), we can see that the functions mirror the earlier stage, though at a more subdued rate, given the much slower decrease in temperature than increase. This allows us to see the different behaviour of the correction functions very clearly in plot (b), especially the three that were highly limiting early on (Arrhenius, Rosso, Haug (1993)). Indeed, though more limiting, the correction function produced by the Arrhenius equation decreases more slowly than that of the Haug (1993) model, while the cardinal temperature correction remains the least limiting of these three.

For moisture corrections, these functions tend to be less variable and more restrained than those for temperature, emphasising the much greater impact of temperature correction functions (and thus the importance of selecting an accurate model). Figure 3.2 (a) shows the profiles obtained by the four assessed moisture corrections over the entire possible range of moisture. We once again note the same three behaviours: (1) slightly restrictive functions, such as the Stombaugh and Nokes (1996) equation; (2) moderately restrictive functions, such as those of Haug (1980 and 1993), both giving nearly the same results; and (3) highly restrictive functions, such as that of Mora-Naranjo et al. (2004), which sets the optimal moisture content at 100%. Note that, in a composting setting, this makes no sense, as will be treated later in this chapter. However, given that this function has been used in the literature, it was assessed alongside the others. Regarding the results of these corrections as applied on a real case, shown in Figure 3.2 (b), moisture content in the experiments never decreased below 50%, so growth was not significantly limited in most cases. The Stombaugh and Nokes (1996) model maintains the correction factor at 1 throughout the experiments, given that its cut-off for low moisture is at 40%, while the Mora-Naranjo et al. (2004) correction was drastically more restrictive throughout the entirety of the experimental run than the other three functions.

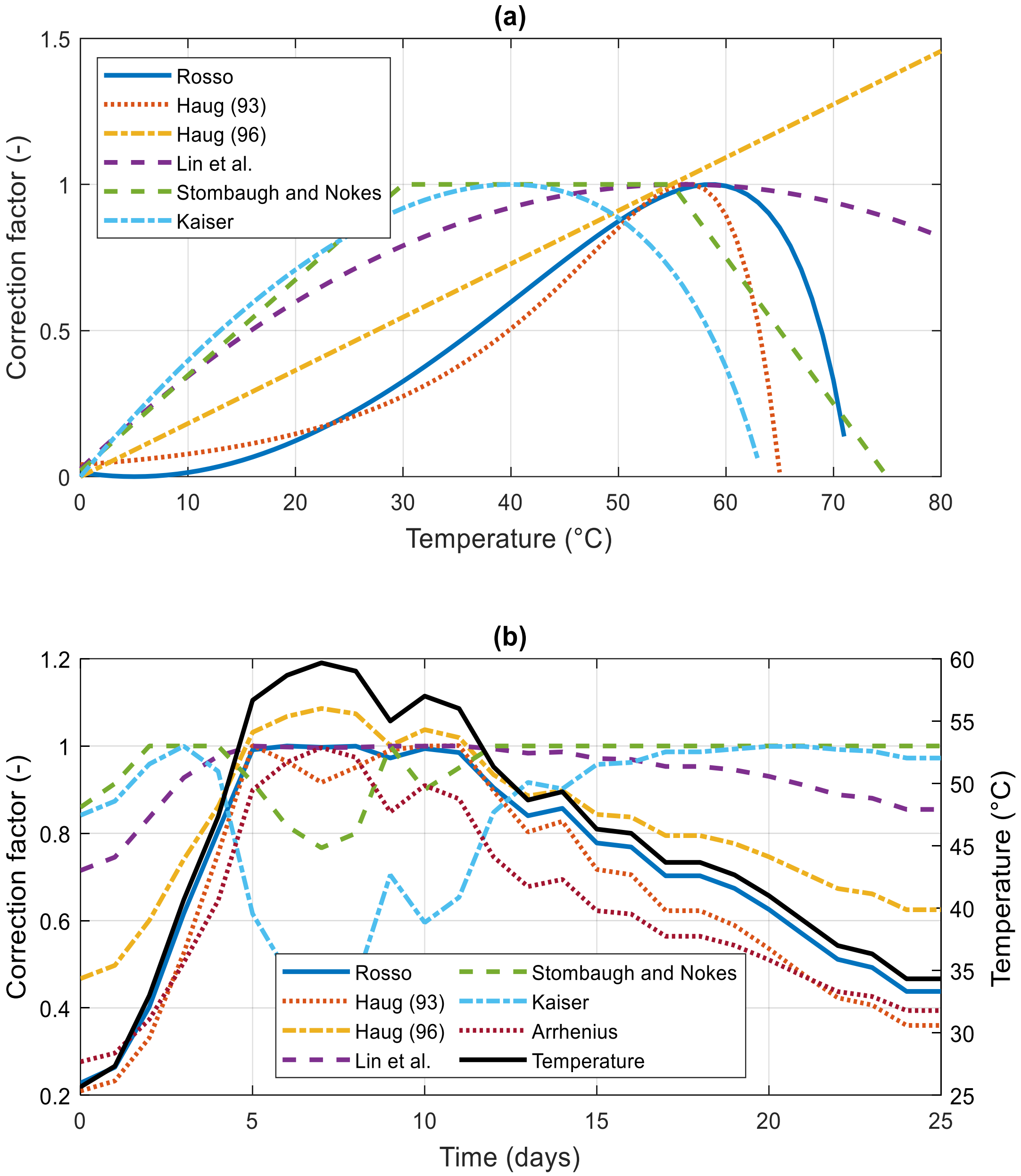


Figure 3.1 (a) Profiles of the assessed temperature correction functions. (b) Results when applied to trial 1, alongside experimental tempertaure. To plot the values for the Arrhenius equation, the values of k_d have been divided by k_{max}.

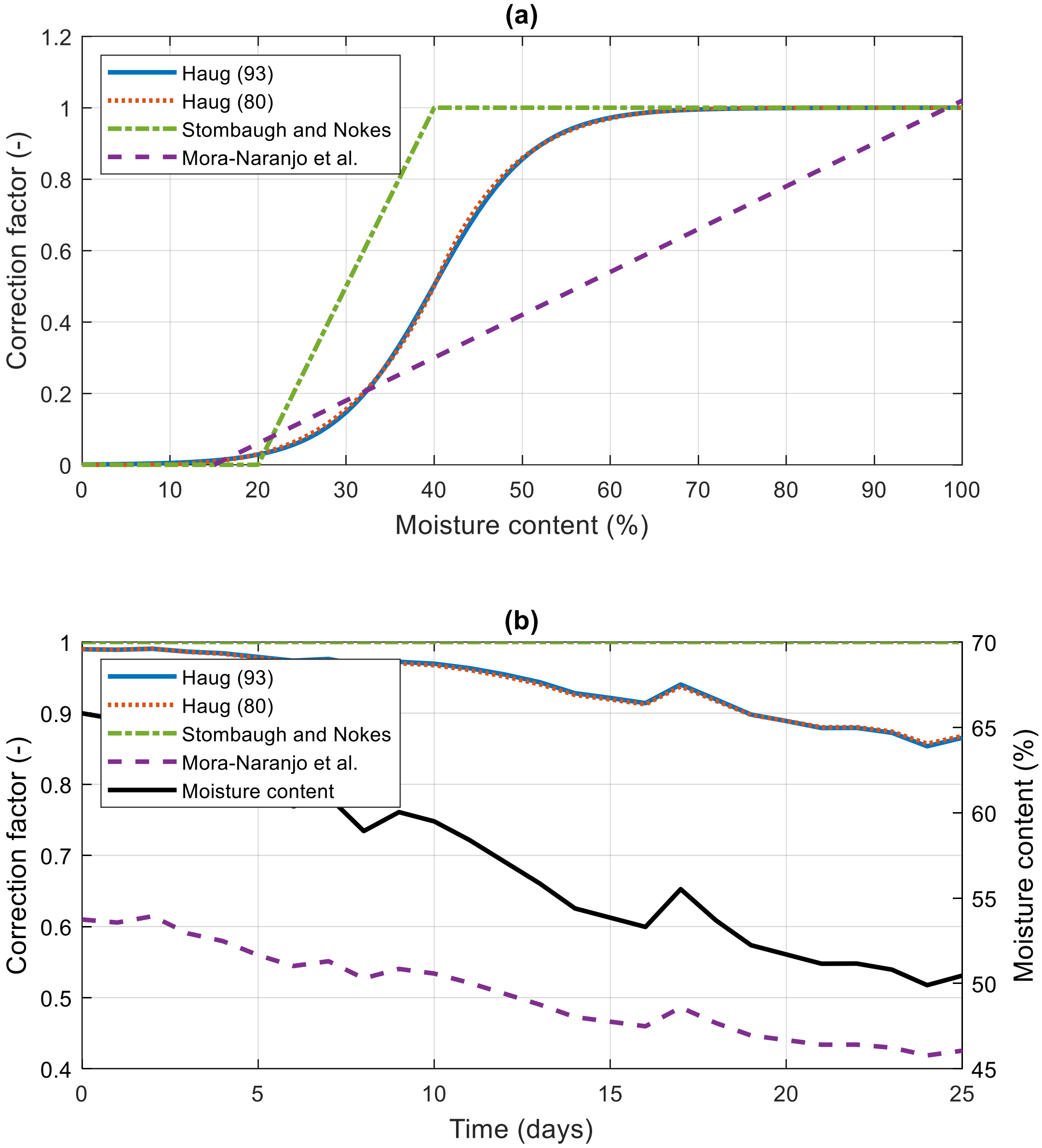


Figure 3.2 (a) Profiles of the assessed moisture correction functions. (b) Results when applied to trial 1, alongside experimental moisture content.

Finally, regarding oxygen corrections, Figure 3.3 (a) highlights how similar the three equations behave, with the Monod equation being more restrictive than the model of Baptista et al. (2010). However, plot (a) does not account for the impact of temperature and moisture on the Higgins and Walker (2001) correction, having been plotted for a constant T = 55 °C and MC = 60% (noninhibitive for both). Indeed, Figure 3.3 (b) shows how this inclusion of temperature and moisture modifies the model, giving it a unique profile compared to the other two, which share a shape (Monod being more pronounced), and making it more inhibitive than the Baptista et al. (2010) equation. It could loosely be considered as a middle ground between the Monod equation and Baptista et al.'s (2010), as will be further discussed in section 3.5.

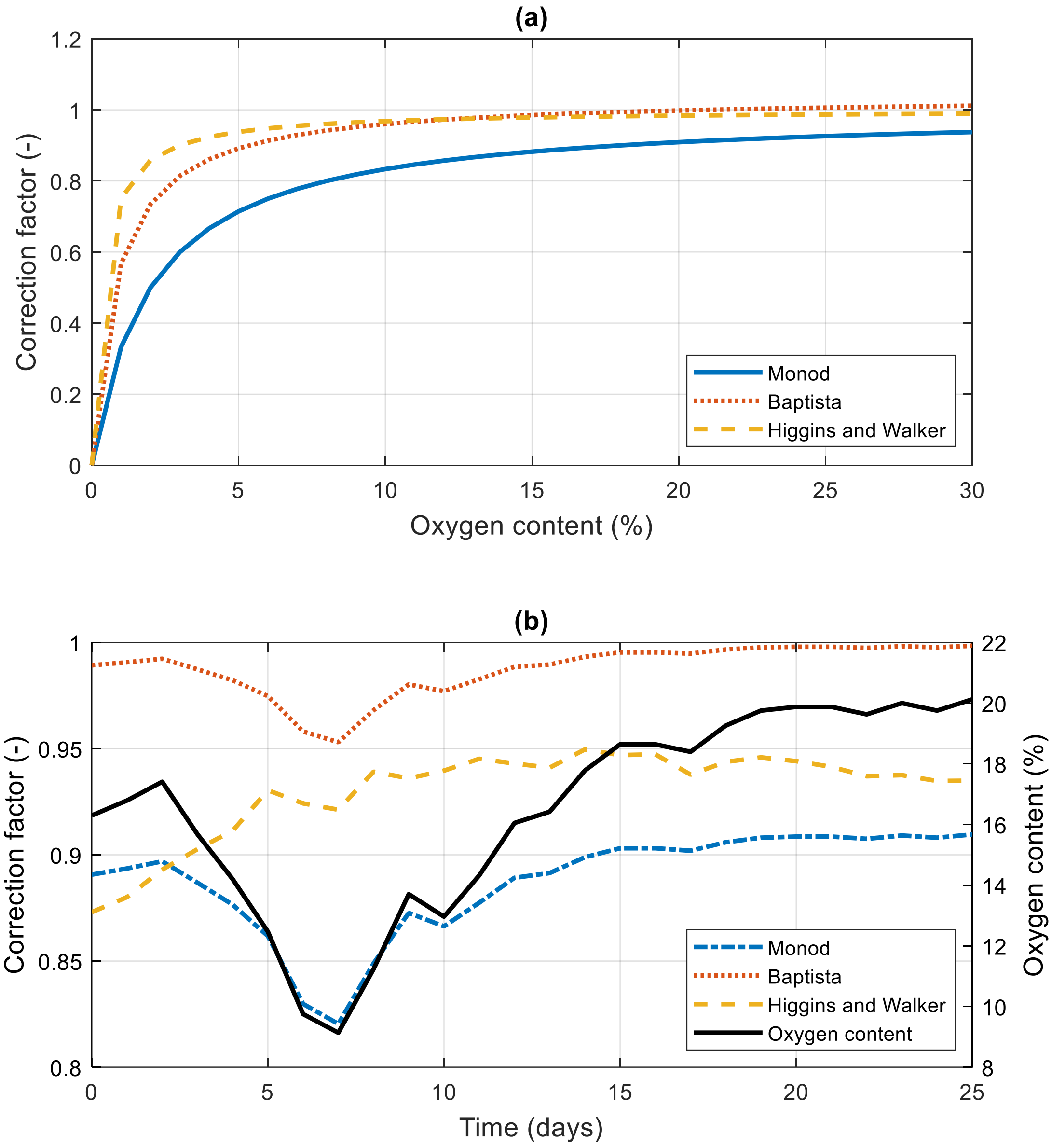


Figure 3.3 (a) Profiles of the assessed oxygen correction functions. (b) Results when applied to trial 1, alongside experimental oxygen content.

3.5.2 NRMSE assessment

Moving on to the quantitative analysis of the correction functions, Table 3.4 presents the averaged NRMSEs for a correction factor applied in combination with two other correction factors (one for temperature, moisture, and oxygen) across all trials. Firstly, it is important to note that the averaged % error presented in these tables is not representative of the actual error to be expected from these functions, given the interaction between so many "suboptimal" correction functions. Indeed, the optimal solutions produced significantly lower NRMSEs in every case, with full details on these combinations and their errors being provided in Appendix B.

Table 3.4 highlights the important difference in the general accuracy of the two modelling approaches taken (fixed vs optimized k_{max}), though this is expected. In both cases however, similar results are obtained regarding the relative performance of the correction functions. Most moisture corrections seem to provide similar results, with the exception of Mora-Naranjo et al.'s (2004) correction. As highlighted in Figure 3.2, this function is much too aggressive, likely due to the expression apparently not originally being intended for composting, though it has been applied in the composting context before (Ma et al., 2018). Oxygen corrections all offer very similar errors as well. Regarding temperature corrections, it would appear that the cardinal temperature correction, the Haug (1993 and 1996) models, and, in the case of a fixed k_{max}, the Arrhenius equation, all provide more accurate results than the other three corrections (Lin et al. (2008), Stombaugh and Nokes (1996) and Kaiser (1996)).

Table 3.4 Average NRMSE for each correction function across all the trials.

		Average NRMSE (% error)	
	Correction function	**Fixed k_{max}**	**Optimized k_{max}**
Temperature functions	Cardinal temperature correction	18.11	4.86
	Haug (1993)	18.12	4.80
	Haug (1996)	19.79	5.72
	Arrhenius equation	19.91	19.91
	Lin et al. (2008)	22.17	8.15
	Stombaugh and Nokes (1996)	23.68	10.80
	Kaiser (1996)	24.32	14.75
Moisture functions	Haug (1980)	16.43	7.91
	Haug (1993)	16.45	7.83
	Stombaugh and Nokes (1996)	16.89	7.74
	Mora-Naranjo et al. (2004)	36.85	13.66
Oxygen functions	Monod	18.27	9.21
	Higgins and Walker (2001)	19.00	8.89
	Baptista et al. (2010)	20.66	9.03

Given the close range of many of the NRMSEs and the potential for experimental and data processing error, a deeper assessment is called for. Therefore, in order to provide a clearer analysis and get a better picture of the most accurate models, as well as combinations, the 10 model combinations providing the best results based on NRMSE for each trial were identified, forming what we will call the "optimal set". These models were, in general, much more accurate than the averages reported in Table 3.4 and presented some very interesting findings. Indeed, despite the relatively high NRMSEs shown in Table 3.4, the range for the top 10 models was generally much lower, a list of these combinations and their NRSMEs being presented in the Appendix B. The list of the frequency of each correction function in the optimal set can be found in Table 3.5.

Table 3.5 Frequency of individual correction functions in the optimal set (top 10 of each trial).

		Fixed k_{max}		**Optimized k_{max}**	
	Correction function	**Total**	**% of total**	**Total**	**% of total**
Temperature functions	Arrhenius equation	14	35	1	2.5
	Haug (1993)	14	35	14	35
	Cardinal temperature correction	12	30	16	40
	Kaiser (1996)	0	0	0	0
	Lin et al. (2008)	0	0	0	0
	Stombaugh and Nokes (1996)	0	0	0	0
	Haug (1996)	0	0	9	22.5
Moisture functions	Haug (1980, 1993)	22	55	14	35
	Stombaugh and Nokes (1996)	18	45	18	45
	Mora-Naranjo et al. (2004)	0	0	8	20
Oxygen functions	Monod	19	47.5	14	35
	Higgins and Walker (2001)	11	27.5	12	30
	Baptista et al. (2010)	10	25	14	35

From Table 3.5, we can note that, for a fixed k_{max}, the Arrhenuis equation, the Haug (1993) and the cardinal temperature correction were all present at approximately the same rate in the optimal set. Oxygen and moisture corrections remain relatively divided, though Haug's (1980, 1993) corrections and the Monod equation were the most prevalent.

In the cases with optimized values of $\mathrm{k_{max}}$, the Haug (1993) and cardinal temperature corrections provided the most accurate models, demonstrating their ability to more accurately predict the degradation profile and supporting the findings of Richard and Walker (2006) and Mason (2008). Indeed, we can note a significant decrease in the presence of the Arrhenius equation, given that it does not rely on $\mathrm{k_{max}}$ and therefore cannot be optimized in the same manner.

In both cases, oxygen and moisture corrections were present at similar rates, mirroring the results of Table 3.4. One interesting finding here, which simultaneously highlights the strength and issue with the approach of optimizing $\mathrm{k_{max}}$, is how the Mora-Naranjo et al. (2004) moisture correction managed to make up nearly 20% of the optimal sets. In these cases, the optimized $\mathrm{k_{max}}$ was often double that of the ones determined using the other equations. Though this may seem like a one-off, it might underline one of the reasons why laboratory-scale composting experiments throughout the literature have provided an incredibly large range of $\mathrm{k_{max}}$'s, varying upwards of 3900% for similar substrates and conditions in certain situations, as determined by the review of Baptista et al. (2012). Indeed, given a lack of standardization in modelling and reporting of composting kinetics, we recommend against trying to obtain usable or transferable degradation rates from these works.

Returning to the optimal sets, though Haug's 1980 and 1993 corrections often provided near identical results, the 1980 function generally outperformed the 1993 correction in the case of a fixed $\mathrm{k_{max}}$, while the 1993 function provided more optimal results for an optimized $\mathrm{k_{max}}$, as highlighted in table 3.4, though the difference in performance was mostly negligible.

3.5.3 Determining which correction functions to use together

From the results provided above, some general recommendations can be formulated as to the selection of correction functions to model composting using first-order kinetics. It is important to note, however, that the results were still very variable and that these recommendations are general guidelines aimed at consistently ensuring accurate results, though more optimal combinations may exist. Table 3.6 provides the combinations most likely to provide consistently accurate and higher ranked results, based on our assessment. The table can be used in tandem with Figures 3.1-3.3 to aid in selecting correction functions. If ever a model is overly aggressive or lenient, then a simple fix could be to switch out the moisture or oxygen corrections. For example, a Monod equation could be replaced with the equation of Higgins and Walker (2001) if the model is too restrictive (underpredicting degradation), or the Haug (1980, 1993) moisture corrections can be used if a model implementing the Stombaugh and Nokes (1996) correction overpredicts the biodegradation rate.

In the case where a modeller seeks to follow the first approach of using a fixed $\mathrm{k_{max}}$, then the recommendations are rather clear. For temperature corrections, the Arrhenius equation should be prioritized, though Haug's (1993) correction or the cardinal temperature correction can also be used with success. For moisture corrections, all the assessed models except for the Mora-Naranjo et al. (2004) correction provided similar results. Based on the optimal sets, the Arrhenius equation should be used in tandem with Stombaugh and Nokes' (1996) moisture correction and the Monod equation. For the Haug (1993) and cardinal temperature corrections, the Haug (1980, 1993) models should be favored alongside a Monod oxygen correction, though the Stombaugh and Nokes (1996) correction managed to perform decently as well in the case of the Haug (1993) temperature correction. The clearest takeaway in the case of a fixed $\mathrm{k_{max}}$ approach is the dominance of the Monod equation as an oxygen limitation. It managed to provide the best two solutions in every trial, while also making up more than 50% of the optimal sets and generally outperforming the other similar combinations (temperature + moisture) with different oxygen corrections.

In the case where $\mathrm{k_{max}}$ is optimized, the recommendations are a bit less strict. The cardinal temperature and Haug (1993) models both performed very well, though, based on our results, the Haug (1993) model led to more optimal solutions, higher ranked solutions, and a lower average NRMSE. The Haug (1996) correction also provided 8 of the 10 optimal solutions for trial 2, though it never made it into the optimal sets for any of the other trials. Despite this result and given its higher average NRSME, its lack of representation in the other trials, and the close performance of the cardinal temperature model in trial 2, we would not recommend favoring the Haug (1996) over the other two. Therefore, when $\mathrm{k_{max}}$ is optimized, we recommend the use of the Haug (1993) or cardinal temperature (Rosso) models. Regarding moisture and oxygen corrections, the Haug (1993) model worked best alongside the Stombaugh and Nokes (1996) moisture correction, while the cardinal temperature function performed better with the Haug (1993) moisture correction. Indeed, in every trial, the combinations of the Haug (1993) temperature correction and the Stombaugh and Nokes (1996) moisture correction, regardless of oxygen correction, outperformed every other moisture correction function.

The cardinal temperature correction did not behave in such a clear fashion. It performed well in some trials alongside the Mora-Naranjo et al. (2004) moisture correction but, as mentioned earlier, this correction likely leads to a significant overestimation of $\mathrm{k_{max}}$ (which may or may not be an issue for certain modellers). None of the moisture corrections consistently outperformed all the others. Once again, the Monod equation for oxygen limitation was found to nearly always outperform the Baptista et al. (2010) and the Higgins and Walker (2001) corrections.

Table 3.6 Recommended combinations of correction functions.

Modelling Approach	**Temperature**	**Moisture**	**Oxygen**
Fixed $\mathrm{k_{max}}$	Arrhenius	Stombaugh and Nokes (1996)	Monod
	Haug (1993)	Haug (1993)/ Stombaugh and Nokes (1996)	Monod
	Cardinal temperature	Haug (1980)	Monod
Optimized $\mathrm{k_{max}}$	Haug (1993)	Stombaugh and Nokes (1996)	Monod
	Cardinal temperature	Haug (1993)/ Stombaugh and Nokes (1996)	Monod

We also assessed the individual use of the most accurate temperature corrections, to see whether they benefited from the addition of the other (moisture and oxygen) corrections. In the cases of both fixed and optimized $\mathrm{k_{max}}$, none of the individual models managed to outperform combinations with moisture and oxygen corrections. The one exception to this that was consistently observed, based on the optimal sets, was that the individual application of the Haug (1993) temperature correction outperformed its application alongside the Haug (1993) moisture correction and Baptista et al.'s (2010) oxygen correction.

Finally, the aspect of practicality is also worth mentioning. Though the Arrhenius equation might offer better results for modelling with a fixed $\mathrm{k_{max}}$, it is also the only one of these functions that requires empirical data to use. Though not necessarily difficult to obtain, this can pose an unwanted challenge for modellers and might reduce the generalizability of the model compared to the Haug (1993) and cardinal temperature correction models, who only require the value of the temperature. It is important to note however that the coefficients (C_1 and C_2) of the Haug (1993) model can also be determined empirically through a regression analysis (Wang et al., 2014; Wang and

Witarsa, 2016), though the values used in this study have been the most prevalent in the literature. Furthermore, all of the models assessed in this paper, with the possible exception of the Arrhenius equation, are extremely easy to apply and implement into composting models, if temperature, moisture, and oxygen data are present (either predicted or determined in-field). Given that these equations simply multiply the degradation rate, modellers could evaluate their implementation for a given case, without having to go through the same process undertaken in this study, as highlighted in Table 3.6 and by switching some of the correction functions if necessary.

3.5.4 Limitations and further research

Further research would be needed to expand this work and investigate into the kinetic foundations of composting as well. A variety of kinetic expressions can be used to represent the composting environment (first-order, Monod, Contois, Tessier, etc.), as detailed in chapter 2, and it is unlikely that these models will respond to correction functions in the same way as the first-order model assessed here. We also highlight that, despite having a variable and representative range of temperatures in our trials, these models were not evaluated for extreme conditions during the process (other than initial and final low temperature). It is possible that some of the functions might not provide responses that are as accurate for processes that can see sharp changes in some of these operating variables, presenting a potential limitation of our work. Examples could include semi-batch composting that can lead to sharp temperature decreases, naturally aerated systems or windrows that can see more significant oxygen and moisture depletion, as well as more novel approaches to composting such as hyperthermophilic composting.

3.6 Conclusion

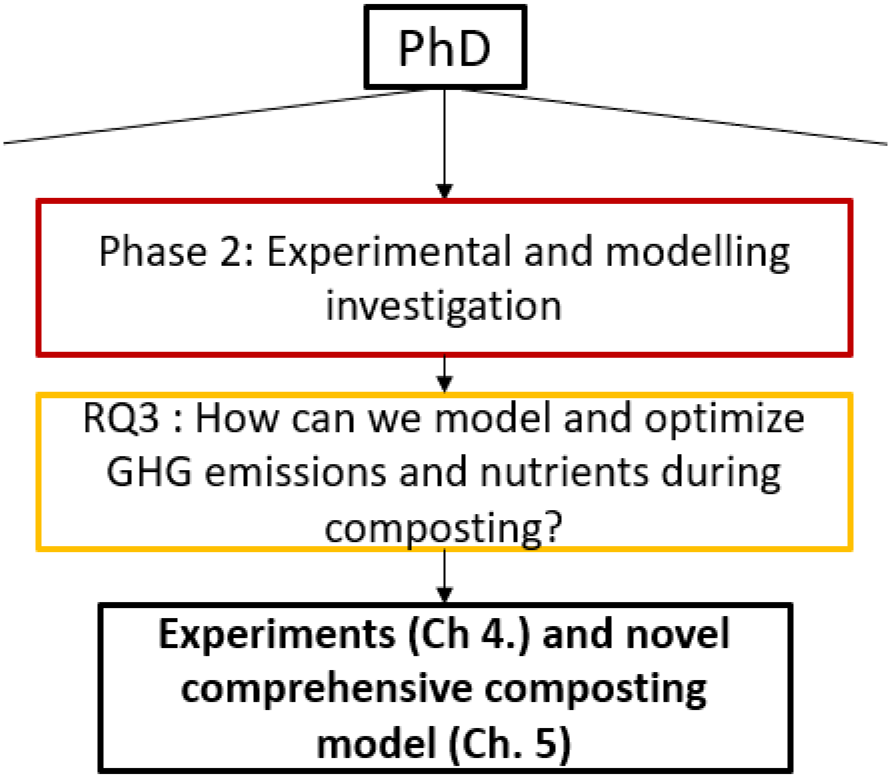
Despite significant growth and development in the field of composting modelling, the use of correction functions to modulate degradation rate based on certain operating variables such as temperature, moisture content and oxygen content has been a woefully understudied area of the literature. This chapter aimed at providing guidance on the use of these correction functions by assessing the application of different correction functions (12 for temperature, 8 for moisture, and 3 for oxygen) applied together with a first-order kinetic expression to predict degradation based on experimental composting results.

As highlighted in our results and discussion, throughout the four trials, there was some variability in results. Therefore, general recommendations for selecting correction functions were proposed, instead of being able to pinpoint a unique and optimal combination of correction functions. These recommendations include favoring the Arrhenius equation, the Haug (1993), or the cardinal temperature corrections for temperature, when modelling with a fixed $\mathrm{k}_{\mathrm{max}}$. In the case of numerically optimized $\mathrm{k}_{\mathrm{max}}$'s, the Haug (1993) model provided the best performance, followed by the cardinal temperature correction. In all cases, the Monod equation was found to be the best oxygen limitation function, nearly always outperforming the other oxygen corrections. Regarding moisture corrections, some preferential pairings were proposed with the above-mentioned temperature corrections, though emphasis was placed on the potential benefit of testing multiple moisture corrections.

In spite of the variability in results, we believe that the results highlighted in this chapter are likely to hold true for many composting models implementing first-order degradation kinetics (the majority of models). This is since, other than maximal reaction rates ($\mathrm{k}_{\mathrm{max}}$), the evaluated models had no input that was substrate specific or particular considerations for mechanisms that would or would not be involved in certain scenarios.

Phase 2

Experimental and modelling investigation of nutrient loss and GHG emissions during composting



Chapter 4: Proposition for experimental work to investigate nutrient loss, transformation and GHG emissions from composting aiming at model calibration and validation

4.1 Introduction

Following the work undertaken in the previous chapters, we can move into the second phase of this PhD, which aims at applying the knowledge gained in phase 1 to develop the composting models which are at the heart of this thesis. The first step of this second phase was set to be an experimental investigation of nutrients and emissions throughout composting, which would then be used to calibrate and/or validate the composting models. However, as mentioned in the statement on the impacts of the COVID-19 pandemic, the planned experiments were delayed by over a year, meaning that they would not be completable within the timeframe of this PhD. Despite this, significant work had gone into planning the experiments, designing the reactors, and putting everything in place. Therefore, the author believes that presenting this information can be of benefit, if only to further consolidate knowledge on composting research. More specifically, the hope is that this chapter can be of particular interest and benefit to people still developing their knowledge in the field (such as graduate students), given that the only reviews on the design of composting experiments are those of Petiot and De Guardia (2004), Mason and Milke (2005) and Li et al. (2013). The prior references focus only on reactor operation, while the latter mainly focuses on composting recipes, without discussing methodology. This chapter seeks to bridge the gap, serving as a "mini-review" of sorts and an experimental methodology, and is the distillation of months worth of research and planning on an optimal approach to designing composting experiments. Furthermore, for those unfamiliar with composting research, it can provide additional context to understand how the data used throughout the following chapters, especially chapters 5, 7, and 8, are generated.

This chapter will go over the primary design, planning, operating choices, and recommendations for laboratory and pilot-scale composting systems aimed at following nutrients and greenhouse gas emissions during the composting process, seeking to provide guidance for future composting modellers and researchers. We will start by exploring the necessary considerations for composting experiments design in section

4.2, followed by the designed and implemented experimental setup and plan in section 4.3.

4.2 Considerations for designing composting experiments

4.2.1 The type of composting system

The first question to be asked when designing composting experiments is: what type of system are we seeking to simulate? As mentioned in chapter 1, this can range from in-vessel composting, static pile and windrow composting, rotating drums, vermicomposting, aerated sacs, etc.

In chapter 2, we highlighted that the most studied composting environment is the reactor/in-vessel system, given the ease of implementing it at laboratory scale. A schematic representation of the general layout of laboratory and pilot-scale composting reactors is presented in Figure 4.1 (a), most often used to study in-vessel and static pile composting. However, even at smaller scales, alternate systems have been envisioned. Of the various types of composting systems, the ones that have received the least attention at bench scale are systems based on piles, such as windrows and naturally or passively aerated piles, given that they have key geometric features and boundary conditions not seen in most of the other, more controlled, environments. For example, unlike in-vessel systems or aerated sacs, which tend to be packed with organic matter and held within the confines of their systems, piles must be able to stand on their own, imposing some geometric restrictions, as well as influencing boundary conditions (heat and mass transfer with ambient and uncontrolled conditions, unlike reactors). This has, however, not stopped researchers from designing systems capable of representing windrows and piles at small scales. Indeed, Figure 4.1 (b) presents the setup that has most often been applied to study windrows in laboratory or small-pilot scale processes, as applied by Hogan et al. (1989) and Magalhaes et al. (1993). This second orientation provides the advantage of allowing for symmetry to be assumed, especially if placed in a rectangular reactor, and, if sufficient similitude is achieved (section 4.2.3), it can be used to assess profiles (temperature, degradation, etc.) and process operation at a small scale. However, the first orientation presented in Figure 4.1 (a) is by far the most used, with the assumption that mixing will homogenize the environment enough as to minimize large gradients in the environment.

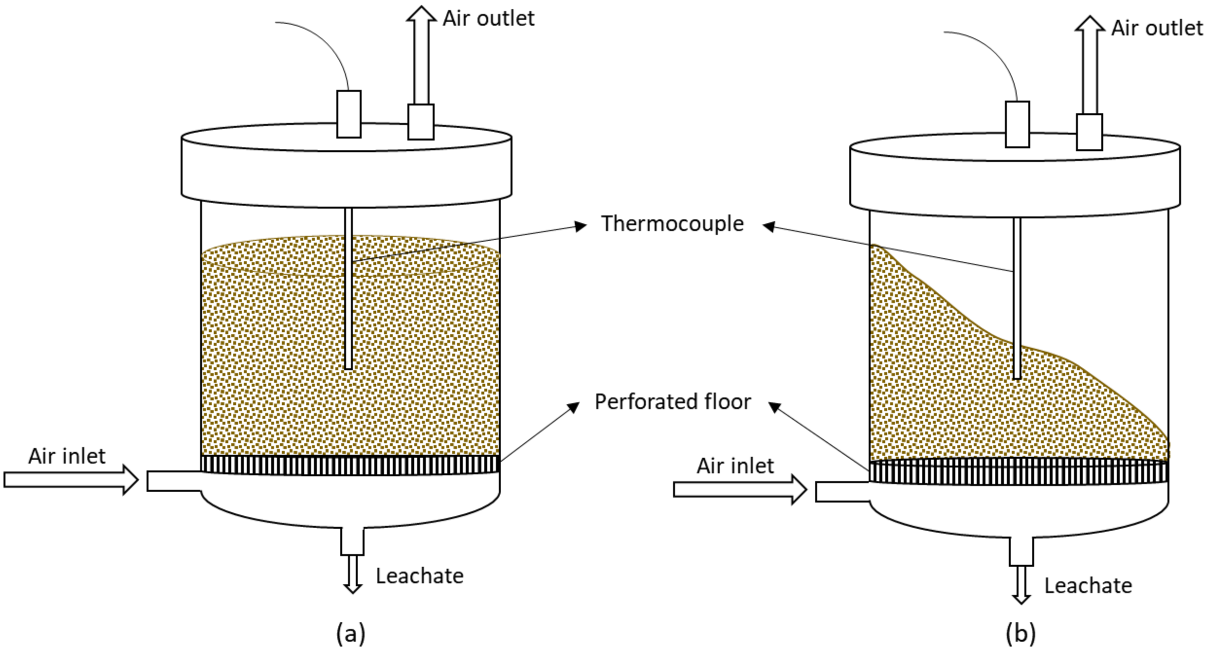


Figure 4.1 Schematic of laboratory composting reactor configurations. (a) is the most common setup and is mainly used to evaluate in-vessel composting and static pile composting; while (b) has seen some implementation to model piles, such as windrows.

4.2.2 Process size

Following determination of the type of system, process sizing is the next major step. Sizing of composting systems for research can be extremely variable, and each offer unique advantages and disadvantages. A very loose categorization of composting system sizes, as defined by the author and based on the ranges used throughout literature and the results they allow to obtain, is presented in Table 4.1, alongside an overview of the advantages, disadvantages, and recommended uses of these sizes:

Table 4.1 Loose categorization of composting system sizes and their respective advantages, disadvantages, and recommended use-cases.

Scale	Size (m^3)	Advantages	Disadvantages	Recommended use
Laboratory	0 – 0.2	Easy and thorough control and monitoring	Significant differences from full-scale processes, which lead to important variability across different experimental	Development of fundamental knowledge: e.g., evaluation of how factors influence process variables, such as temperature, moisture, and

			setups and when compared to real-world applications. Limited to no information on techno-economic considerations.	oxygen content on degradation rates, GHG emissions, nutrient transformation, etc. **Not to be extrapolated to full-scale systems.**
Pilot	0.2 – 5.0	Good physical representation of the composting environment (adequate heterogeneity, insulation). Can provide valuable information for techno-economic assessments (energy use, mixing, aeration strategies). Retains a good level of control and ease of sampling.	Significantly increased costs and logistics (particularly regarding substrate management) when compared to laboratory-scale.	A great middle ground between the laboratory- and full-scale systems. Can provide information on the physical, chemical, and biological behaviour of the composting environment, though differences will remain compared to full-scale. Can be extrapolated to full-scale systems, though differences must be accounted for (e.g., dead zones which might be more likely at full-scale).
Full	> 5.0	Truest representation of real composting processes	Challenging to determine specific information, complex sampling, elevated costs.	Best method to follow large-scale phenomena, such as heat and mass transfer, real degradation rates and profiles, final compost quality, pathogen elimination, etc. Can be difficult when seeking to develop fundamental theory given that balances (mass and energy) are likely to be difficult to close.

Beginning with the **laboratory-scale**, these systems are perfectly suited to study and monitor the composting process in great detail and with great precision in measurements and control. However, their small size and this ease in control also make these systems very different from full-scale applications, leading to deviations from the latter. These differences can happen in a few key areas, and it is important to be aware of them and to work to counteract them. These areas mostly pertain to the physical restrictions of the setup and how this can affect the process. This can notably be felt in the heat exchange of these systems. Indeed, at small scale, such as 0.05 m^3, a reactor would only have about 25 kg of substrate, making it very unlikely for the system to generate and retain enough heat to ensure a normal composting temperature profile. Indeed, at smaller scales, the surface area to volume (SA:V) ratio will most likely be significantly larger than those of full-scale processes (Mason and Milke, 2005), while self-insulation is nearly non-existent (Petiot and De Guardia, 2004). Other issues with the laboratory scale are that it is very difficult to replicate the heterogeneity of a real composting system in this restricted environment. This, in turn, can impact mass and heat transfer, making these systems less suited to assess temperature or local degradation profiles. Furthermore, the responsive control applied at this scale is often much more effective than what could be achieved at larger scales, resulting in much more reactive systems.

Indeed, laboratory composting setups should be prioritized to study aspects of composting that are not hindered by assuming a homogeneous and tightly controlled environment. However, this scale should be avoided for any variable that is affected by the heterogeneity of the environment, notably air/heat flow and temperature characterizations. Care should also be taken when assessing factors that are linked to such aspects, such as drawing conclusions on pathogen elimination for a whole system when temperature profiles play an intrinsic role in this (Hénon, 2008). Laboratory-scale systems are perfect to understand how operating conditions or changes to the environment or substrates can impact other factors in the process, such as determining how temperature impacts moisture or kinetics or how moisture content can promote or inhibit certain transformation pathways, such as the production and release of methane or (de)nitrification, for example. However, this represents a development of fundamental knowledge. Hence, great care should be taken when seeking to extrapolate results of laboratory systems to larger scales. Indeed, in their analysis of laboratory and full-scale composting kinetics, Baptista et al. (2012) found that variations in degradation rates reported at laboratory-scale were extremely large, at a factor of 39, while the rates reported at full-scale processes only varied 3-fold. Furthermore, they also noted that degradation rates obtained at laboratory-scales were, on average, significantly faster than those reported for full-scale systems, being 5.7 times faster for similar substrates (or 1.9 times faster for municipal solid wastes). This was noted as being due to the better management of the composting conditions through strict control, being about 50% more efficient at laboratory than at full-scale.

At the other end of the scale, **full-scale** experiments are obviously the best representation of real composting processes. However, the size of these processes can make it difficult to ascertain specifics, especially given the generally "open'" nature of composting operations, leading to many potential sources of interference on measurements. Furthermore, their size can lead to significant costs, even if only for sampling. Indeed, sampling can be one of the most challenging aspects of full-scale systems, given their significant size and heterogeneity. Full-scale processes are best suited to follow general characteristics of composting, or large-scale phenomena, such as heat and mass transfer, degradation rates and profiles, and general characterizations, such as C/N ratio, organic matter (OM) content, and such. Where full-scale experiments are less useful is in working out specific mechanisms and exploring theory in depth, though they can be a great source of validation for laboratory and pilot-scale work in this area. For example, and pertinent to this dissertation, exploring pathways for nutrient transformation during composting is much easier and more precisely measured at laboratory and pilot scales than it would be at full-scale. However, studies on pathogen elimination, "real" degradation, and temperature distributions will benefit from being undertaken at full-scale.

Finally, the middle ground between laboratory and full-scale experiments, the **pilot-scale** manages to compromise between the advantages and disadvantages of both laboratory and full-scale systems. Being larger in size than laboratory-scale setups, in the case of composting, pilots tend to offer a much better physical representation of the composting environment. Indeed, with the increased mass of substrate used in these systems, they are generally capable of self-heating to the same extent as a full-size process, without requiring additional temperature control, as well as having surface area to volume ratios more similar to those of full-scale applications (Mason and Milke, 2005). From pilot scale systems, it is also possible to ascertain information related to energy use, mixing, aeration strategies, etc., that can be used in technical and economic evaluations; information that would not be available from the laboratory scale and that are important before transitioning to full-scale implementation. The main disadvantage of pilot-scale composting systems, when compared to laboratory-scale, is the generally significant increase in costs and experiment duration, as well as the added logistics associated with getting and storing enough waste to operate the system, though these are necessary to gather the full-breath of information allowed through these systems.

4.2.3 Ensuring similarity

Regardless of the scale chosen, ensuring similarity between the experimental setup and the evaluated environment is necessary. For composting, this is most often ensured through insulation, in cases where the system is not capable of maintaining its heat, and grinding and sieving of substrates and bulking agents to meet a specific size distribution. Indeed, throwing fully intact banana peels into a 10 L reactor alongside wood chips would not allow for a representative assessment of the composting of this mixture, given that conduction, convection and diffusion of heat, moisture, and oxygen would all be grossly misrepresented compared to a full-scale process.

The first aspect to consider is the **geometry** of the designed systems. The most common reactor shape is cylindrical (vertical for reactors, horizontal for rotating drums), given that they minimize surface area to volume (SA:V) ratio, decreasing heat loss. However, apart from heat loss, this design consideration is rather unimportant at laboratory scales, other than if aiming to study key geometric features that require a rectangular/trapezoidal pile, as shown in Figure 4.1 (b). Nevertheless, for larger systems, the added heat loss can be important, making the difference between a system that can operate solely on self-heating and -insulation or one requiring added temperature control. Indeed, in a comparison of cylindrical and rectangular composting vessels (60 L), Qasim et al. (2019) obtained a heat loss of about 17% higher in the rectangular reactor than the cylindrical reactor, at optimal aeration. In this case, the SA:V was about 10% higher for the rectangular system than the cylindrical one, leading to quicker temperature decreases and less time spent in the thermophilic phase.

For **insulation and temperature control**, a variety of alternatives are possible, especially for reactor/in-vessel systems. The aim of these is to maintain desired boundary conditions regarding temperature. For pilot systems, the vessels can often be insulated with traditional insulants and left to self heating. However, insulation on its own is unlikely to be enough for smaller, laboratory-scale, systems. Indeed, at this size, biological heat generation is rarely enough to overcome the heat-loss of the system. For this reason, three reactor formats, in addition to self heating systems, have become widely used throughout the field (Mason and Milke, 2005): (1) fixed temperature reactors, (2) controlled temperature difference (CTD) reactors, and (3) controlled heat flux reactors. These designs are a way of controlling and ensuring desired boundary conditions, and will be explored more in detail in section 4.2.5.

Regarding **particle size**, full-scale composting operations generally operate with particles ranging from 3 or 4 mm up to 75 mm (Alberta Environment and Parks, 2018). For smaller scale systems, experiments can generally be designed following one of two approaches: (1) maintaining a similar particle distribution as a full-scale process and assuming that the experiment represents a certain cross-section of a larger process; or (2) maintaining an equivalently scaled-down particle distribution, as well as aeration rate, in the aim of emulating the full process at a smaller scale. In the first case, experiments can still seek to determine optimal process conditions for a variety of scenarios or evaluate specific behaviour, such as heat transfer. However, it is important to be aware of the boundary conditions of these systems and how they differ from the case of full-scale processes, given that profiles (degradation, temperature, moisture, oxygen) will be greatly impacted by these conditions. In the second case, boundary conditions and process geometry seek to emulate that of a full-scale system, allowing for more realistic profiles throughout the system, though this approach has been very rare in the literature. Indeed, oftentimes, many researchers use the first approach of maintaining a similar particle size distribution while attempting to emulate a full-scale process at significantly reduced size. This was exemplified by Lashermes et al. (2012) who sought to assess the reproducibility and compare the results of six small-scale (4 L) composting reactors with full-scale systems. The experimental reactors demonstrated strong reproducibility, but the system limitations did cause them to differ from full-scale processes. Indeed, such limitations included a shorter thermophilic phase and a decrease in the degradation of lignin, with the authors also pointing to the lack of colonization by macrofauna as being another potential source of deviation (Lashermes et al., 2012). As highlighted by both Lashermes et al. (2012) and Baptista et al. (2012), laboratory-scale results simply cannot be generalized to full-scale systems, especially when process similarity is not ensured.

4.2.4 Operating conditions

Operating conditions are the most studied aspect of composting, given that they regulate how the process unfolds. The main operating conditions and control variables include temperature, moisture content, aeration rate, bulk density, C/N ratio, and pH. Generally, optimal ranges for these conditions have been reported as being: between 50 and 60°C for temperature (Eklind et al., 2007; MacGregor et al., 1981; Miyatake and Iwabuchi, 2006; Nakasaki et al., 1985; Strom, 1985), between 40 and 70% for moisture (Guo et al., 2012; Jiang et al., 2011; Kim et al., 2016; Kumar et al., 2010; Liang et al., 2003a; Tiquia et al., 1998), oxygen contents above 12% (Alberta Environment and Parks, 2018; Haug, 2018), which generally seem to be achieved by aeration rates around 0.2 and 1 L_{air} min^{-1} kg organic $matter^{-1}$ (Chen et al., 2015; De Guardia et al., 2008; Gao et al., 2010; Guo et al., 2012; Petric and Mustafić, 2015; Rasapoor et al., 2009; Yamada and Kawase, 2006), bulk density between 300 and 700 kg m^{-3} (Alberta Environment and Parks, 2018), initial C/N ratio of 20 to 35 (Guo et al., 2012; Huang et al., 2004; Kumar et al., 2010; Onursal and Ekinci, 2017; Yan et al., 2015; Zhu, 2007), and pH around basic or mildly acidic environments. For pH, the optimal range is based on the preference of the microorganisms in the environment, with bacteria tending to prefer neutral pH, while fungi have a better activity in mildly acidic environments (de Bertoldi et al., 1983). Some work has also gone into modifying the microbial ecology to operate optimal in specific conditions, such as through inoculation with acid-tolerant bacteria (Kuroda et al., 2015; Nakasaki et al., 2013; Nakasaki et al., 1996).

4.2.5 Process control

Of the operating conditions highlighted in the previous section, temperature, moisture content, and aeration tend to be actively controlled throughout the process, while bulk density, C/N ratio, and pH tend to be modified prior to the process. Regarding the latter, **initial property modification** is mostly undertaken through the addition of bulking agents, to modify both bulk density and C/N ratio, while pH is sometimes modified by addition of alkaline substances, such as fly ash, NaOH and lime (Fang et al., 1999; Lei and VanderGheynst, 2000; Nakasaki et al., 1993; Yu and Huang, 2009), or acidic amendments (Chen et al., 2010; Fangueiro et al., 2015; Kithome et al., 1999). Table 4.2 provides an example of substrate and bulking agents N contents, C/N ratios, moisture contents, and bulk densities, provided by the Northeast Regional Agricultural Engineering Service (NRAES) (Rynk et al., 1992). Regardless of real-world or laboratory evaluation and application, this modification remains the same.

Table 4.2 Common substrate and bulking agent properties, adapted from Rynk et al. (1992).

Substrate/Bulking agent	%N dry weight	C/N ratio[a]	Moisture content (%)	Bulk density (kg/m^3)
Mixed slaughterhouse waste	7-10	2-4	-	-
Fish wastes	6.5-14.2	2.6-5	50-81	-
Poultry carcasses	2.4	5	65	-
Activated sludge	5.6	6	-	-
Sewage sludge	2-6.9	5-16	72-84	638-1040
Digested sewage sludge	1.9	16	-	-
Food waste	1.9-2.9	14-16	69	-
Tree trimmings	3.1	16	70	769
Swine manure	1.9-4.3	9-19	65-91	-
Grass clippings	2.0-6.0	9-25	-	178-297
Cattle manure	1.5-4.2	11-30	67-87	785-993
Paunch manure	1.8	20-30	80-85	866
Fruit waste	0.9-2.6	20-49	62-88	-
Horse manure	1.4-2.3	22-50	59-79	721-961
Shrub trimmings	1.0	53	15	254
Paper mill sludge	0.56	54	81	-
Leaves	0.5-1.3	40-80 (54)	-	59-178
Corn stalks	0.6-0.8	60-73	12	32
Corn cobs	0.4-0.8	56-123 (98)	9-18	330
Straw	0.3-1.1	48-150 (80)	4-27	34.5-224
Sawdust	0.06-0.8	200-750 (442)	19-65	207-267
Corrugated cardboard – uncompacted	0.1	563	8	30-90
Corrugated cardboard – compacted	0.1	563	8	180-300
Rice hulls	0-0.4	113-1120 (121)	7-12	185-219
Bark – hardwoods	0.1-0.4	116-436 (223)	-	-
Bark – softwoods	0.04-0.39	131-1285 (496)	-	-
wood chips/shavings - hardwoods	0.06-0.11	451-819 (560)	-	-
wood chips/shavings - softwoods	0.04-0.23	212-1313 (641)	-	-

[a] Values in parentheses are average values.

For **active control**, however, there are many options that lend themselves to researchers, all of which can have an important impact on the outcome of the composting process. Regarding **temperature control**, the two main pathways for process operation are either (1) self-heating or (2) controlled temperature. In the case of self-heating systems, the systems are left to generate their own heat through biodegradation, while insulation may be added to mitigate heat loss. This insulation is especially pertinent at smaller scales, where the surface area to volume ratio may be higher than that of a full-scale system. The second alternative, that of controlling the systems temperature directly, is especially common at laboratory and small pilot-scales. This is not to say that full-scale composting processes do not implement temperature control, most often achieved through a regulation of aeration and moisture, but the control applied at laboratory and pilot scales can be, and is often, far more rigorous than that of full-scale processes (reminder of the 50% higher control efficiency at laboratory-scale noted by Baptista et al. (2012)). Of the temperature control schemes applied for composting reactors, three major alternatives have been most prevalent throughout the literature, as detailed by Mason and Milke (2005): (1) fixed temperature systems, (2) controlled temperature difference (CTD) systems, and (3) controlled heat flux systems. Fixed temperature systems, as the name implies, operate at an imposed temperature, maintained by heating or cooling of the system. Though uncommon in practice, some composting processes can operate at a fixed temperature, something that is seeing particular interest in the field of high-temperature (hyperthermophilic) composting (Cui et al., 2019; Liao et al., 2018; Yu et al., 2018). Controlled temperature difference reactors are designed to limit heat loss and achieve and maintain self heating at smaller scales, acting as a form of controlled insulation. In these systems, a temperature difference between or throughout the system is set and maintained by providing heat to compensate for heat losses. As such, even with small amounts of substrates, the heat generated by biodegradation is mostly kept in the system, allowing for it to heat up and to replicate self-heating and self-insulation that would only be achievable and maintainable at much larger process sizes. Finally, the controlled heat flux approach is a deviation on the controlled temperature difference, with a constant and pre-determined heat-flux being maintained through the reactor’s walls instead. As noted, temperature can also be controlled through aeration and inlet air temperature, influencing both convection through the environment and evaporation, though this control may not limit heat losses enough to allow for self heating, and is therefore mostly implemented at larger scales.

For laboratory and pilot-scale work, controlled temperature difference (CTD) reactors are recommended to best emulate large-scale composting processes (Mason and Milke, 2005), while fixed temperature systems are very useful to determine parameters, such as degradation rates at fixed temperatures, microbial diversity, the impact of process additives, etc.

For **moisture control** during the process (it is often modified before the process as well), water is generally added to the environment in one of two ways: (1) spraying of water onto the composting matrix, or (2) humidification (saturation) of inlet air. The first method is more reactionary than the second, but in any case, automated moisture control of composting is a rarity, given that moisture measurements are most often done by periodically extracting and drying a compost sample for 24 hours.

Finally, for **oxygen control**, this is mainly achieved through aeration strategies. Once again, smaller systems and research-oriented applications tend to have a much greater ability and access to oxygen measurement methods. Many laboratory and pilot-scale processes use oxygen sensors to measure oxygen levels of the exhaust gas, but such measurements are very rarely done in the field. Therefore, oxygen control is dependent on good aeration strategies. Multiple strategies exist, being generally classed as active/forced, passive or natural methods (Alberta Environment and Parks, 2018; Fernandes and Sartaj, 1997). Active aeration strategies are the most common for large scale operations and can take various forms. The most common of these strategies are either through frequent mixing and turning, as used during windrow composting, where the oxygen is replenished in the environment through this action, or through blowing or drawing air through the system, most often applied with static pile or in-vessel systems. In these systems, air is blown (positive aeration) or drawn (negative aeration) through pipes placed throughout the system. Though both positive and negative forced aeration are often used, positive aeration offers the benefit of being able to preheat and humidify the air entering the system, allowing for better control of the system, though additional heating may be necessary near the pipes to ensure pathogen destruction (Hénon, 2008). Note that there is no consensus on whether turning/mixing a pile, such as windrows, is an active or passive strategy and can often be found classified in both categories. Given the "active" nature of the management of the composting involved in these strategies, the author prefers to classify it alongside the active approaches, similarly to Larney et al. (2000), Amlinger et al. (2008), and Varma et al. (2018). Indeed, passive aeration approaches tend to use a temperature gradient between the composting environment and perforated pipes placed throughout the system, drawing air through the environment by convection. Finally, naturally aerated systems have no means to facilitate aeration and are totally dependent on diffusion within the system, operating in a similar manner to passively aerated systems, but without means to facilitate heat and mass transfer through the piles.

For systems using forced aeration, a few important design questions must be considered (Ekinci et al., 2004a): (1) is airflow provided continuously or discontinuously (intermittent)? (2) is the air recirculated? (3) is the direction of the airflow ever reversed? Each of these choices can lead to significant changes in process operation, as studied by Ekinci et al. (2004a). From the literature reviewed throughout the course of this dissertation, laboratory-scale experiments seemed to implement continuous and discontinuous aeration at similar rates, as well as recirculation, though a more systematic review of literature on composting experiments would be warranted at this point. Regarding the first of these choices, intermittent aeration can be useful to achieve a more uniform temperature profile throughout the environment, notably near air inlets that remain at lower temperature, which can decrease pathogen elimination. Further benefits include less convection through the system, decreasing overall moisture loss and ammonia loss (Ekinci et al., 2004a), which are both direct functions of airflow rate. For recirculation, this strategy aims at decreasing temperature and moisture gradients throughout the system, the pile heating the air as it passes through it, which would then heat the new incoming air. The most important aspect when using recirculation is to make sure that adequate oxygen is provided to the system, given that it is possible to accumulate heat and moisture in the system, while depleting oxygen. Finally, regarding reversed-direction airflow, this is the least common of the above considerations, and with good reason. Indeed, this operating strategy, which periodically reverses the direction of airflow, is intended to achieve a more uniform moisture distribution and decrease moisture lost, by alternating the direction of mass transfer and uniformizing the movement of water through the system. However, during their assessment of this approach, Ekinci et al. (2004a) found that reversed directional airflow, with or without recirculation, lead to significant oxygen limitation and moisture retention, though they note that this may be due to the chosen operating conditions. Though some of the alternatives discussed above can be interesting for process control or optimization of certain factors, such as emissions reductions and energy optimization, the simplest and most straightforward option of continuous, unidirectional, and non-recirculated air flow seems to be the most certain alternative for efficient composting (Ekinci et al., 2004a). Indeed, the other configurations showed promise, but in every case other than this standard configuration, significant oxygen limitations were encountered, pointing to the greater need of optimization when considering such alternatives.

4.2.6 Sampling and analysis

The final consideration when designing composting experiments is determining the desired analyses and the sampling necessary to achieve these readings.

For analyses, the composting process generates three primary phases that can be pertinent to analyse: the compost (solid), the leachate (liquid), and emissions (gas). The quality of compost is the most analysed aspect in composting literature, with basic assessments of organic matter, total carbon, nutrient (N and P) content, moisture content, pH and electrical conductivity (EC) being extremely common. Further analyses also include heavy metals, organic toxins, microbial ecology, and the presence of humic and fulvic substances. When evaluated, leachates generally tend to go through the same tests as the compost.

For process emissions, which is the second most analysed aspect of composting, the main chemical species of interest include: CO_2, CH_4, NH_3, N_2O, and O_2, given their role as markers of aerobic degradation and nitrogen loss, as well as dimethyl sulfide and H_2S for odour quantification. The main sampling tools for gases used throughout composting literature include dedicated gas analyzers, chemical traps, such as NaOH for CO_2 and boric or sulfuric acid for NH_3, gas chromatography, and multi gas analysis (photoacoustic or FTIR spectroscopy).

Regarding sampling, the number of sampling locations and the frequency of sampling can vary significantly and is dependent on the size, operation, and objective of the experiments. For example, for temperature sampling, Smårs et al. (2001) sampled the temperature at 17 locations throughout their 200 L composting reactor, compared to the 100 L reactor and single sampling location of Chen et al. (2020b). Indeed, works focusing on spatial and temporal distributions of composting variables require significant sampling, given the dynamic and heterogeneous nature of the composting environment.

4.3 The proposed system design and experimental plan

4.3.1 Objective of the experimental plan

The purpose of the proposed system design and plan was to the provide the necessary information to validate the pathways for nitrogen transformation and loss from the composting environment, as well as greenhouse gas emissions. The intent was to then be able to use this information in the calibration and validation of the composting models developed later in this dissertation. To achieve this, focus was placed on being capable of quantifying emission profiles, as well as solid and liquid compositions. This information could then serve to determine the composting kinetics, as well as ammonification, de/nitrification rates, and microbial growth rates, with the aim of being capable to determine the individual contribution of the various transformation pathways to the global balance.

4.3.2 Laboratory-scale reactor

For this project, given the focus on evaluating pathways for nutrient transformation and greenhouse gas emissions, the laboratory-scale was prioritized, though ensuring as much similarity with larger processes was desired. Having two reactors that could serve as duplicates was also preferred over one larger reactor, given the inherent variability in composting experiments and the desire to achieve replicability, as highlighted earlier through the works of Lashermes et al. (2012) and Baptista et al. (2012). In this case, two 15 L vessels with a working volume of approximately 10 L were chosen. Therefore, a controlled temperature difference (CTD) setup was chosen, given that Mason and Milke (2005) identified it as being the most effective at mirroring full-scale operation and that the designed reactors had a SA:V ratio of 20, which is approximately three times higher than full-scale processes (Mason and Milke, 2005). In this case, insulation of the reactors is assured by submerging the reactors in a water bath. The temperature near the center of the reactors and inside the bath is measured using K-type thermocouples, and a constant temperature difference of 1 °C is maintained between the water bath and the reactor with the lowest temperature. This would ensure that the system would experience a slight cooling, but without losing too much heat due to its size and higher SA:V ratio. Figure 4.2 presents the 3D rendering of the reactors, while Figure 4.3 shows a front view of the installed system in the laboratory.

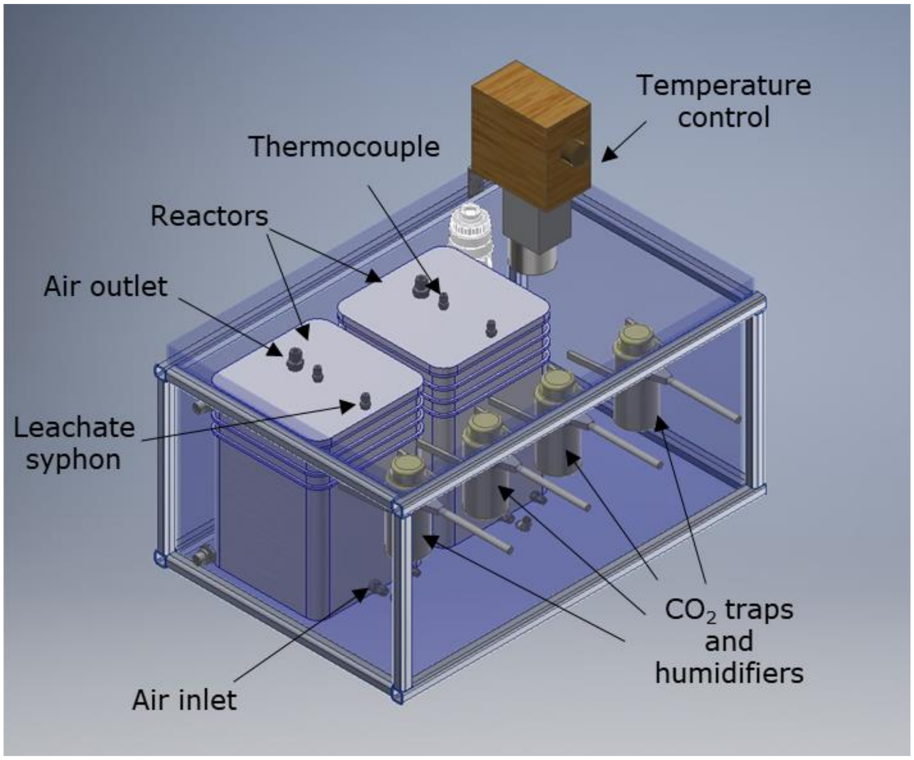


Figure 4.2 3D rendering of the experimental composting system.

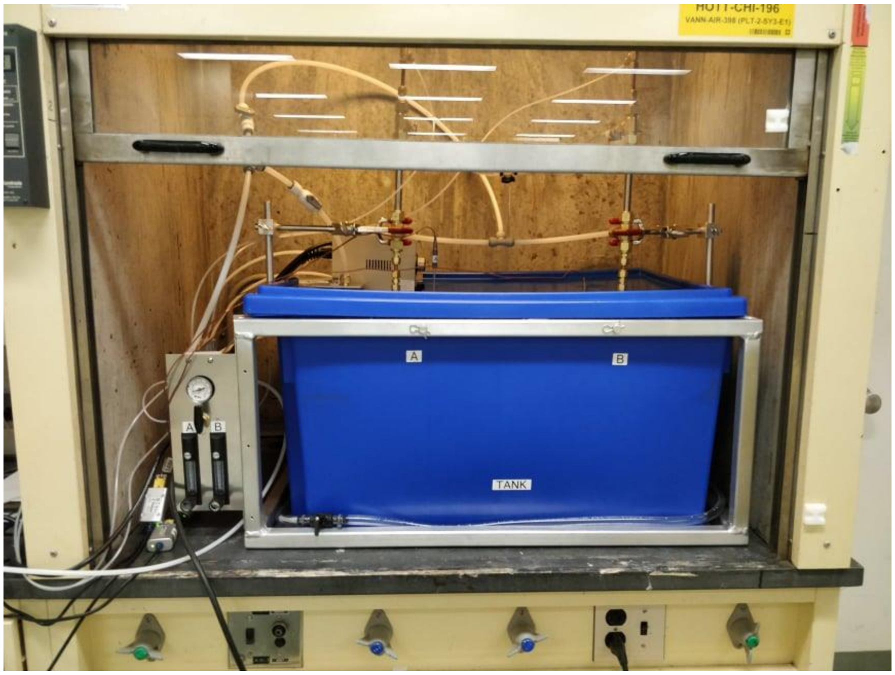


Figure 4.3 Composting setup in the laboratory.

Inside the reactors, the substrate is seated on a metallic, perforated, plate, slightly elevated from the bottom of the reactor, as shown in Figure 4.1 (a). This plate serves both as a diffusor for aeration, which is pushed through the bottom of the reactor, and a barrier to collect leachate in the bottom of the reactors; the leachate then being siphoned out through a syringe.

Regarding aeration, a continuous air flow of 0.5 L min^{-1} kg OM^{-1} was chosen, given the range presented in section 4.2.4. Before entering the reactors, the air is passed through a CO_2 trap, using a 4% NaOH solution, followed by a humidifier (bubbled in water) held within the water bath. The removal of CO_2 is to ensure that the CO_2 measurements at the exit of the system are representative of the CO_2 produced by biodegradation, i.e., without including CO_2 in the air feed, while the humidification aims to guarantee a more stable moisture content, given that the laboratory air supply is dry.

Mixing is undertaken in a periodic manner, with frequencies being dependent on the experiments. The mixing is done manually by removing the contents of the reactor into another bucket, mixing inside this bucket, and then putting the matter back into the reactor. Given the CTD reactors, other than momentary heat loss during the mixing, heat loss overall is limited, given that the water bath can be maintained at the same temperature as before the mixing and heats the contents rapidly.

4.3.3 Storage and preparation of substrates

Aside from selecting the desired substrates, which is purely dependent on the objective of the experiments, storage and preparation of composting substrates is extremely important. Synthetic substrates can be made in the laboratory, with “synthetic” options ranging from dog food (Chang et al., 2005; Nakasaki and Ohtaki, 2002; Schloss et al., 2000; VanderGheynst et al., 1997a) to mixes of any wide variety of substances to ensure any variety of compositions or characteristics. To ensure comparability between composting trials, freezing of a large amount of initial substrate is recommended; preferably by freezing into smaller lots that can be unthawed when needed. Multiple freeze-thaw cycles are to be avoided, given that it can alter the state of the substrates, reducing comparability and reproducibility. However, Trémier (2004) demonstrated that the freezing of organic matter had a small effect on moisture content, organic matter, chemical oxygen demand, total carbon and Total Kjeldahl Nitrogen (TKN), generally inferior to 5% over periods of more than one year. When thawing organic matter, it is recommended to thaw it at 4 °C for 48 hours, followed by bringing the substrate/bulking agent to ambient temperature over a few hours (< 6h) before launching experiments.

Following selection and storage, preparation is of utmost importance, especially when working at smaller scales, notably at laboratory-scale. Maintaining physical similarities is necessary and can be challenging when working with organic waste and bulking agents that will naturally be oversized in a system with an operating volume of 10 L, as noted in section 4.2.3. In this case, the substrate would be ground and sieved to obtain a range of approximately 2 to 4 mm, with bulking agents being ground to about 4 mm in size.

4.3.4 Sampling and analysis

The proposed goal of the experiments was to provide a complete and comprehensive following of nutrients and gaseous emissions during composting. Therefore, having frequent sampling of solids and liquids (leachate), alongside continuous emissions monitoring, was primordial. For a 30-day experimental trial, the solid and liquid sampling would be undertaken on days 0, 2, 4, 6, 8, 10, 12, 16, 20, 25, and 30. The following would be measured for every sampling point:

4.3.4.1 Solid samples (compost)

For solid samples, **moisture content** would be measured by drying a 10 g sample at 110 °C for 24 hours. The difference in weight between the fresh and dried samples would represent the amount of water within them, following eq. 4.1:

$$\mathrm{MC} = \frac{\text{Wet weight} - \text{Dry weight}}{\text{Wet weight}} \times 100 \tag{4.1}$$

To ensure accurate measurements, a larger sampling mass would be preferable. However, given the frequency of sampling and the limited amount of matter in the reactors (about 7 kg each), sampling more than 10 g for moisture would lead to too significant mass loss.

Following this drying, multiple tests would be undertaken on the residual dry fraction. 5 g of the dried sample would be ground at 0.5 mm and a two-step loss-on-ignition (LOI) approach would be applied (Wang et al., 2012). In the first step, the sample would be calcinated in a muffle furnace at 375 °C for 17 hours to determine **organic matter content**, as described in eq. 4.2. This would then be followed by a subsequent combustion at 800 °C for 12 hours to estimate **total inorganic carbon (TIC)** through equation 4.3.

$$\mathrm{OM}\ (\%) = \frac{\text{Dry weight} - \text{Weight}_{375\,°\mathrm{C}}}{\text{Dry weight}} \times 100 \tag{4.2}$$

$$\mathrm{TIC}\ (\%) = \left(\frac{\text{Weight}_{375\,°\mathrm{C}} - \text{Weight}_{800\,°\mathrm{C}}}{\text{Weight}_{105\,°\mathrm{C}}}\right) \times 0.273 \times 100 \tag{4.3}$$

Where the 0.273 in eq. 4.3 is a conversion constant applied to convert mass of CO_2 to mass of carbon (Wang et al., 2012).

Total organic carbon (TOC), which is the sum of carbon from organic species (proteins, lignins, lipids, carbohydrates, organic acids, etc.) would also be measured. Organic carbon provided through compost amendment is of great agricultural and environmental value as a way of replenishing soil organic carbon (SOC) contents in topsoils, which is primordial to ensuring a strong soil food web and soil health (Habteweld et al., 2020). Total organic carbon would be measured through the Walkley-Black chromic acid wet oxidation method, the most commonly used method throughout the field. The protocol for this method (FAO, 2019; Schumacher, 2002) calls for the addition of 10 mL 1 N (0.163 M) potassium dichromate ($K_2Cr_2O_2$) and 20 mL concentrated (≥ 96%) H_2SO_4 to between 0.5 and 1g of substrate/compost. If significant amounts of Cl^- are expected in the sample, then Cl^- can be removed by adding Ag_2SO_4 to the digestion acid to precipitate the chloride. The solution is then swirled while being heated to 135 °C (important to not go above 150 °C because the acid dichromate solution decomposes) for approximatively half a minute, though heating is often deemed unnecessary, with the heat generated from the exothermic reaction being sufficient. The solution is then cooled before adding 200 mL of deionized water to halt the reaction. Two blanks (without any compost sample) must be run to standardize the 0.4 N $FeSO_4$ solution, or H_3PO_4 can be added to the solution after cooling to help eliminate interferences from ferric (Fe^{3+}) iron. The digested solution is then titrated with Ferroin (ortho-phenanthroline ferrous complex) indicator (3 or 4 drops) and 0.4 N $FeSO_4$. The Ferroin solution is made by dissolving 1.485 g O-phenanthroline monohydrate and 0.695 g of ferrous sulphate in approximately 80 mL of deionised water, which is then diluted to 100 mL and stored away from light. As the titrated solution approaches the end point, the solution will become greenish and transition to a dark green. The addition of $FeSO_4$ will then transition the solution sharply from blue-green to reddish-brown-grey. If the endpoint is exceeded, 0.5 or 1 mL of potassium dichromate can be added, and the titration can be tried again. If over 8 mL of the initial 10 mL of $K_2Cr_2O_2$ have been consumed, a smaller compost sample must be used. The chemical reaction undertaken by this process is presented in eq. 4.4, while equation 4.5 presents the determination of organic carbon, considering that 1 mL of 1N dichromate is equivalent to 3 mg of carbon.

$$2\,\mathrm{Cr_2O_7^{2-}} + 3\mathrm{C} + 16\mathrm{H^+} \rightarrow 4\mathrm{Cr^{3+}} + 8\mathrm{H_2O} + 3\mathrm{CO_2} \tag{4.4}$$

$$\text{Total organic carbon (\%)} = \frac{3\left(1 - \mathrm{V_{FeSO_4,titration}}/\mathrm{V_{FeSO_4,blank}}\right)}{\text{dry sample weight}} \tag{4.5}$$

Where $\mathrm{V_{FeSO_4,titration}}$ is the volume of $FeSO_4$ used during the sample titration (mL), $\mathrm{V_{FeSO_4,blank}}$ is the volume used in the blank titration (mL), and dry sample weight is in g.

Total Kjeldahl nitrogen (TKN), which represent the sum of organic nitrogen, ammonia-nitrogen, and ammonium-nitrogen, is one of the most commonly used regulatory markers for waste management and organic fertilizer/soil amendment application. Pertaining to the model development for this thesis, having these nitrogen fractions is necessary to follow the complete nitrogen balance, as has been partially undertaken in the activated sludge models (ASMs) (Henze et al., 2000) and in a few composting models (Oudart et al., 2015; Sole-Mauri et al., 2007; Trémier, 2004), as will be discussed in detail in chapter 5.

TKN would be measured through Hach test kits, following the traditional EPA (US Environmental Protection Agency) digestion methodology (EPA method 351.2, revision 2.0). This method consists in a digestion of the sample in concentrated sulfuric acid, starting at 160 °C for one hour, followed by a digestion at 380 °C for half an hour. The TKN reading would then be done using a Hach TKN test kit (TNT880) following a filtration to remove residual solid particles.

Given the focus on having a complete understanding of the state of nitrogen throughout the process, **ammonia, ammonium, nitrate, and nitrite** would also be measured, using Hach kits (TNT832 for ammonium, TNT835 for nitrate, and TNT840 for nitrite) following the above digestion. Therefore, with these measurements and those of TKN, we could calculate the **total nitrogen (TN)** and **organic nitrogen**:

$$\text{Organic nitrogen} = \mathrm{TKN} - \left(\mathrm{NH_{4,nitrogen}} + \mathrm{NH_{3,nitrogen}}\right) \tag{4.6}$$

$$\text{Total nitrogen} = \text{TKN} + \text{NO}_{3,\text{nitrogen}} + \text{NO}_{2,\text{nitrogen}} \tag{4.7}$$

The **pH** and **electrical conductivity (EC)**, which are measures of acidity/alkalinity and salinity, respectively, would be measured using a 1:10 soil/distilled water (w/V) extract and would be stirred for 1h and then centrifuged at 10 000 g for 5 minutes. A pH and EC meter (in this case, a Fisher accumet Basic (AB200) benchtop meter) would then be used to determine the pH and EC of the supernatant. The value of these measurements is twofold: firstly, both measurements are important to evaluate the quality of compost, given that plants and soils can be sensitive to both these factors, and maintaining a balance is very important to avoid environmental harm, such as soil acidification and erosion (Walling and Vaneeckhaute, 2021a). Secondly, pH can be a good indicator of decomposition, given the production and consumption of various organic acids, which leads to a characteristic pH profile, as described in chapter 1. Therefore, from a modelling standpoint, being able to follow these factors, especially pH, can be of interest.

The **germination index (GI)**, a measurement commonly used throughout the composting field and which is an estimate of the amount of time it takes for seed germination to occur, alongside the root length, would also be measured. In the composting context, the germination index can be particularly interesting given that it can help quantify and qualify maturation, given the wide variety of changes during this step that may not be easily observed otherwise. Experimental measurements would be undertaken using *Brassica napus* (Rapeseed) seeds, following their use in prior works (Luo et al., 2013; Shen et al., 2011). The seeds would be distributed over filter paper in petri dishes, about 1 cm apart, and moistened with 8 mL of compost extract. The samples would be incubated at 25 °C for three days. Following this incubation, the number of germinating seeds and their root length would be measured, using distilled water as a control. The GI would then be calculated as follows (eq. 4.6):

$$\text{GI}(\%) = \frac{\text{Seed germination }(\%) \times \text{Root length of treatment}}{\text{Seed germination of control }(\%) \times \text{Root length of control}} \times 100 \tag{4.8}$$

The final solid analysis would be to determine **humic substances**, mainly made up of **humic and fulvic acids**, which are indicators of maturation during composting. Indeed, humic substances are the principal components of soil organic matter and play a major role in the agricultural and environmental benefits of compost application (Klučáková, 2018). Humic acid is a macromolecular substance made of up series of polymer polycondensates with different molecular weights, while fulvic acid contains compounds with smaller molecular weights and high oxidation levels (Zhou et al., 2014b). Indeed, humic acid contains approximately 40-60% carbon, 30-50% oxygen, 4-5% hydrogen, 1-4% nitrogen, 1-2% sulfur, and 0-0.3% phosphorus, whereas fulvic acid contains lower mass fractions of everything except oxygen (Gaffney et al., 1996). Generally, as composting progresses and maturity increases, compost shifts from a high fulvic acid and low humic acid content to one with a significantly higher humic acid content (Zhou et al., 2014b). Given the importance of humic substances in soil organic matter, making up over 60% of the latter (Canellas et al., 2015), and their various functional groups, including phenols, carboxylic acids, quinones, enolics, and ethers (Amir et al., 2010; Zhou et al., 2014b), humic substances are attributed a wide variety of benefits. These benefits include agronomic benefits, such as enhanced plant growth, water and nutrient retention, disease suppression, as well as environmental benefits such as decreasing the risks of eutrophication (Guo et al., 2019).

Though unlikely to be of use for the model development undertaken in this thesis, such information could be of great use for future modelling endeavours, given that, as noted in chapter 2, modelling of composting maturation is greatly lacking.

The most commonly referenced protocol in the reviewed literature is the one presented in Huang et al. (2006) and adapted by Zhou et al. (2014a), and is based on the fact that humic acids are soluble in alkaline solutions and insoluble in acidic solutions, while fulvic acids are soluble at any pH (Simpson et al., 2002). The protocol calls for a 1:10 dry solid/solution (m/V) extract using a proportional mix of 0.1 M $Na_4P_2O_7*10H_2O$ and 0.1 M NaOH to be shaken at room temperature for 24 hours and centrifuged at 25 931 g for 20 minutes, repeating this step three times in total. Following the centrifugation, the supernatant contains the humic substances. The supernatant is then left to stand overnight with a pH adjusted to 1.0, after which another centrifugation at 25 931 g for 20 minutes is undertaken. The precipitates of this centrifugation contain the humic acids, while the supernatant contains the fulvic acids. Humic acids are then washed with 0.05 M HCl several times and the pH is adjusted to 7.0. The fractions are then lyophilized to obtain the solid mass, which are then used to analyse the TOC through the Walkley-Black method presented earlier.

4.3.4.2 Liquid samples (leachate)

Any leachate obtained (if any) would be extracted during every sampling and would go through the same evaluation as the solid samples, without the drying for moisture content or the need for extractions and digestions. Given the solubility of NH_4^+, NO_3^-, and PO_4^{3-}, assessing the amount produced during composting and lost through leaching is necessary to have a complete nitrogen and phosphorus balance.

4.3.4.3 Gaseous samples (emissions)

Quantification of emissions is very important for this thesis, given the role of nitrogenous emissions in the transformation and loss of nitrogen during composting, as well as the important environmental impact of NH_3 and N_2O. The initial design and experimental plan used a micro-GC (Agilent 990 Micro GC system) to undertake this analysis, providing quantification for CO_2, CH_4, NH_3, N_2O, and O_2 of the outlet with automated sampling every 20 minutes. However, due to the impacts of the COVID-19 pandemic, the micro-GC was received following 8 months of delays, while the gases needed for calibration were unavailable into the fall of 2021. This in turn forced the validation of the comprehensive model to be undertaken based on a dataset from the literature, as discussed in the following chapter.

4.4 Conclusion

Throughout this chapter, the basics of composting experimentation have been explored, going over various types of composting systems, the different experimental scales, methods used to ensure similarity between experimental and real processes, the multitude of operating conditions to consider, how process control can be applied on these systems, and commonly used sampling and analysis methods. This was followed by the presentation of the groundwork that was laid during this thesis to allow for a thorough assessment of greenhouse gas emissions and nutrient transformation and loss during the composting process. This foundation includes the design and construction of two composting reactors, a storage and preparation strategy for substrate, and the planned sampling and analysis of solid, liquid, and gas fractions.

Chapter 5: A comprehensive model to predict nutrient transformation and GHG emissions during composting

5.1 Introduction

As noted in the first chapters of this thesis, despite the many potential benefits of composting, the process often suffers from significant nutrient loss. Indeed, nitrogen losses can be upwards of 90% of initial nitrogen (N) (Eghball et al., 1997), with common N losses being between 20 and 70% (Eghball et al., 1997; Li et al., 2017; Lim et al., 2017; Martins and Dewes, 1992; Ogunwande et al., 2008; Steiner et al., 2010; Witter and Lopez-Real, 1988), generally through the emission of ammonia (NH_3), nitrous oxide (N_2O), and nitrogen gas (N_2). Similarly, phosphorous (P) losses through leaching can be considerable, with some studies finding losses of around 30% (Tiquia et al., 2002). This loss can considerably hamper and even counteract the benefits of resource recycling through composting, leading to a decreased agronomic value and contributing to an undesirable environmental impact. The environmental impact can be of great detriment to the process, given that composting is often viewed as one of the most environmentally sound ways of treating and valorizing organic wastes. Indeed, through the emission of powerful greenhouse gases and the release of nutrients to soils and waters, sub-optimal composting can contribute to global warming, eutrophication, soil acidification and erosion, and loss of biodiversity (Walling and Vaneeckhaute, 2020b; Walling and Vaneeckhaute, 2021a).

The complexity of nutrient loss during composting stems from the multiple factors that contribute to it. As noted in previous chapters, these factors include temperature, aeration, moisture content, and pH. For example, process temperature has been identified as the most important factor contributing to ammonia (NH_3) emissions, with NH_3 emissions being twice as high at 67 °C as compared to 55 °C (Eklind et al., 2007; Pagans et al., 2006), while also being a primary contributor to emission of other GHGs, such as CO_2, CH_4, and N_2O (Beck-Friis et al., 2001; Cui et al., 2019; Czepiel et al., 1996; Ermolaev et al., 2015; Hellmann et al., 1997; Sánchez-Monedero et al., 2010; Sommer and Møller, 2000). For moisture, its contribution to the development of anaerobic zones in the environment makes it the most important factor determining CH_4 emissions (Ermolaev et al., 2019; Xu et al., 2020), while it has also been found to be among the main factors influencing N_2O emissions through the regulation of denitrification

(Ermolaev et al., 2019; Wang et al., 2013a; Xu et al., 2020; Yang et al., 2019). Aeration regulates the mass transfer through the process, providing both oxygen to the environment, which decreases both CH_4 and N_2O emissions, while also increasing ammonia volatilization (Oliveira et al., 2018; Shen et al., 2011). Finally, as described in chapter 1, pH also plays a key role in ammonia loss by driving volatilization, especially when the pH exceeds 7 (DeLaune et al., 2004; Ekinci et al., 2000).

The issue, as detailed in chapters 1 and 2, is that all these factors are interrelated during the composting process. Therefore, efficient optimization of composting to produce a valuable and attractive compost while limiting nutrient loss and greenhouse gas emissions can be best achieved through mathematical modelling, considering all of these interdependencies. Chapter 2 detailed how, despite considerable work on composting modelling, only very few have, mostly superficially, explored nutrient loss and transformation during composting (Bonifacio et al., 2017a; Bonifacio et al., 2017b; Oudart et al., 2015; Vasiliadou et al., 2015; Vlyssides et al., 2009). Without considering the full picture of nutrient transformation and loss, an important aspect of emissions and environmental impact assessment of composting is lacking.

Therefore, given the lack of mechanistic and comprehensive GHG and nutrient modelling for composting, this chapter explores the development of a novel composting model capable of predicting GHG emissions and nutrient transformation and loss during the process. Section 5.2 presents the materials and methods used to develop the model, while section 5.3 presents the results of this development and calibration.

5.2 Materials and methods

5.2.1 Model description

The model was created in MATLAB from the foundation of the Activated Sludge Models (ASMs) (Henze et al., 2000), similarly to Trémier's (2004) composting model, and is designed to represent an in-vessel composting system (reactor). However, to accurately represent the composting context, significant modifications needed to be made to this foundation.

Biological processes considered by the model include hydrolysis of entrapped organics, aerobic and anoxic growth of microbial fractions on the substrates, assimilative nitrate reduction to ammonia, decay of microorganisms, ammonification, immobilization, volatilization, the full nitrification and denitrification pathways, and phosphorus solubilization. Regarding microbial fractionation, despite the complex fractionations used by some authors and discussed in chapter 2, such as those of Kaiser (1996) and Sole-Mauri et al. (2007), because of the similarity in kinetic parameters between thermophiles and mesophiles, and actinomycetes and fungi presented in Sole-Mauri et al. (2007), the choice has been made to include only bacterial and fungal fractions. Figures 5.1 and 5.2 provide an overview of the biological processes included in the model.

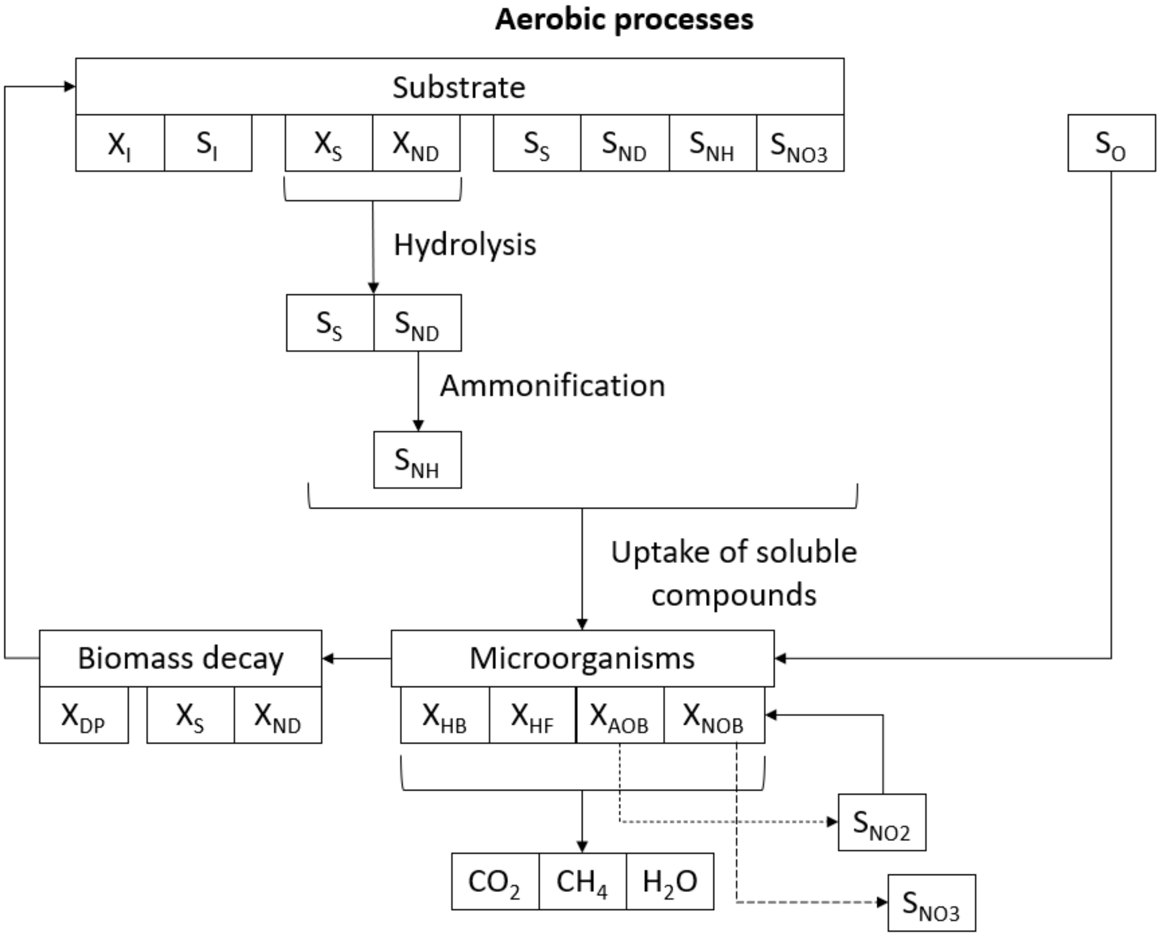


Figure 5.1 Schematic representation of the aerobic growth processes of the model. Symbols detailed in Table 5.1.

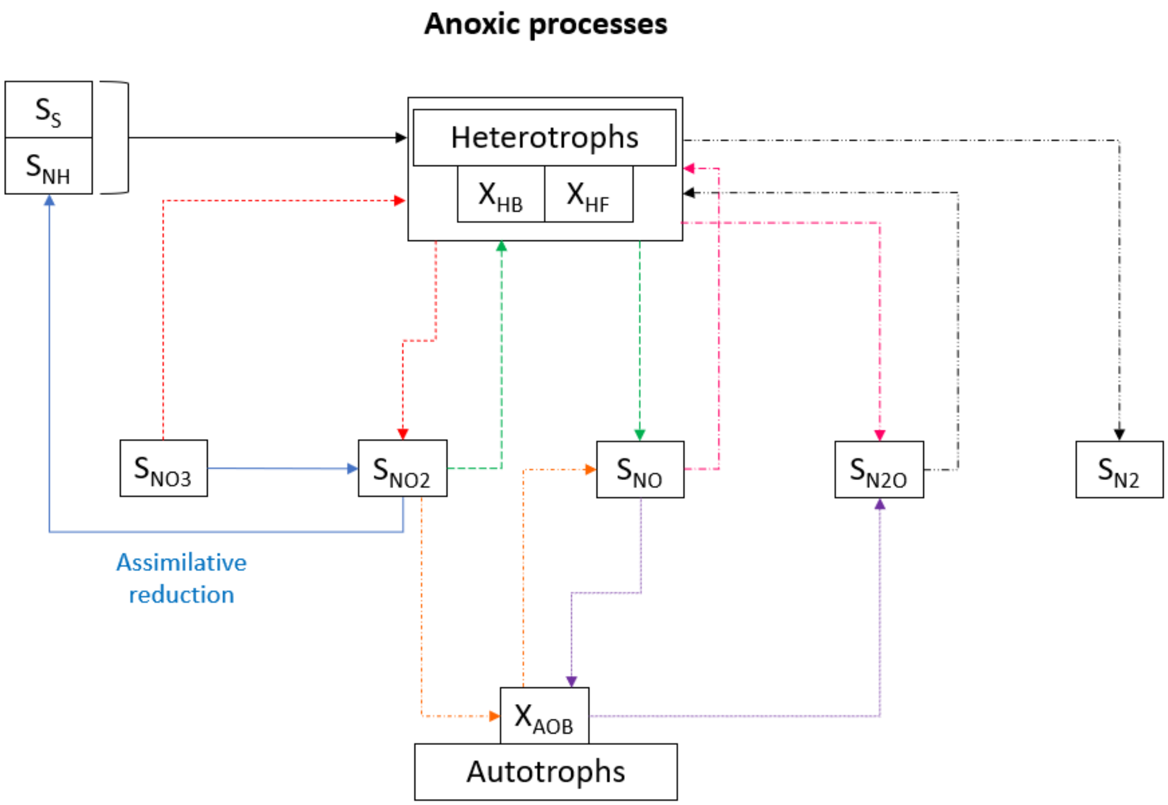


Figure 5.2 Schematic representation of the anoxic growth processes of the model. Symbols detailed in Table 5.1.

5.2.2 Model development

Table 5.1 presents the various substrate fractions used in the model.

Table 5.1 Substrate and product fractionations used in the model. All terms in the table are concentrations, with TOC standing for Total Organic Carbon.

Symbol	Description	Units
S_I	Soluble inert organic matter	g TOC/m^3
S_S	Soluble biodegradable substrate	g TOC/m^3
X_I	Particulate inert organic matter	g TOC/m^3
X_S	Particulate biodegradable substrate	g TOC/m^3
X_{HB}	Active heterotrophic bacteria biomass	g TOC/m^3
X_{HF}	Active heterotrophic fungi biomass	g TOC/m^3
X_{AOB}	Autotrophic ammonia oxidizing biomass	g TOC/m^3
X_{NOB}	Autotrophic nitric oxidizing biomass	g TOC/m^3
X_{DP}	Particulate decay products	g TOC/m^3
S_O	Oxygen (O_2)	g O_2/m^3
S_{NO3}	Nitrate-nitrogen	g N/m^3
S_{NO2}	Nitrite-nitrogen	g N/m^3
S_{NO}	Nitric oxide-nitrogen	g N/m^3
S_{N2O}	Nitrous oxide-nitrogen	g N/m^3
S_{N2}	Dinitrogen-nitrogen	g N/m^3
S_{NH}	Ammonia-nitrogen	g N/m^3

S_{ND}	Soluble biodegradable organic nitrogen	g N/m^3
X_{ND}	Particulate biodegradable organic nitrogen	g N/m^3
S_{alk}	Alkalinity	g HCO_3^-/m^3

A plethora of further detailed information on the model is provided in the appendices of this dissertation: Appendix C presents the full Petersen matrix, which describes the system of biochemical reactions used by the model; Appendix E is a list of base parameters used before model validation and calibration, mainly stemming from the literature; and Appendix F presents the continuity check for the model, both on a COD and TOC basis.

5.2.2.1 Microbial growth and substrate degradation

The model considers three main biological processes: hydrolysis of particulate compounds, microbial uptake, and microbial decay. Four microbial fractions are included: heterotrophic bacteria (X_{HB}) and fungi (X_{HF}), autotrophic ammonia (X_{AOB}) and nitric (X_{NOB}) oxidizing bacteria. The mechanisms for the growth of X_{AOB} and X_{NOB} will be detailed in the section on nitrogen (5.2.2.3).

For hydrolysis of particulate substrate, which has generally been identified as the rate-limiting step of composting (Jolanun et al., 2005; Sole-Mauri et al., 2007; Wang and Witarsa, 2016), with further confirmation provided in chapters 3 and 7 of this thesis, the process rate is described by a Michaelis-Menten kinetic equation undertaken by the heterotrophs (eq. 5.1 for bacteria and 5.2 for fungi). In these equations, the terms between brackets allow for consideration of hydrolysis fueled by both aerobic and anoxic growth.

$$R_{h,HB} = k_{h,HB}(T, MC)\frac{X_S/X_{HB}}{K_{X,HB} + (X_S/X_{HB})}\left[\left(\frac{S_O}{K_O + S_O}\right) + \eta_g\left(\frac{K_O}{K_O + S_O}\right)\left(\frac{\sum S_{NO_X}}{K_{NO_3} + \sum S_{NO_X}}\right)\right]X_{HB} \quad (5.1)$$

$$R_{h,HF} = k_{h,HF}(T, MC)\frac{X_S/X_{HF}}{K_{X,HF} + (X_S/X_{HF})}\left[\left(\frac{S_O}{K_O + S_O}\right) + \eta_g\left(\frac{K_O}{K_O + S_O}\right)\left(\frac{\sum S_{NO_X}}{K_{NO_3} + \sum S_{NO_X}}\right)\right]X_{HF} \quad (5.2)$$

Where $R_{H,i}$ is the overall rate of hydrolysis (kg TOC/m^3.day), $k_{h,i}(T, MC)$ is the temperature and moisture corrected rate of hydrolysis (kg TOC/kg.day), as described in eq. 5.3. The temperature correction is undertaken using the cardinal temperature (Rosso) model (Rosso et al., 1995; Rosso et al., 1993), and the moisture correction is that of Haug

(1993), chosen based on the work undertaken in chapter 3. $K_{i,j}$ is the half-saturation coefficient (kg slowly degradable TOC/kg cell TOC), with K_O being given a value of 2%, based on the works of Haug (1993) and Richard et al. (2006), and η_g is the anoxic hydrolysis discount (-).

$$k_h(T, MC) = k_{h,max} * \frac{(T - T_{max})(T - T_{min})^2}{(T_{opt} - T_{min})[(T_{opt} - T_{min})(T - T_{opt}) - (T_{opt} - T_{max})(T_{opt} + T_{min} - 2T)]} * \frac{1}{\exp(-17.684MC + 7.0622) + 1} \qquad (5.3)$$

Where $k_{h,max}$ is a degradation rate measured at optimal conditions (kg/kg.day), T is the temperature (°C), T_{max} is set to 71.6 °C, T_{min} is set to 5 °C, and T_{opt} is set to 58.6 °C, following the work of Richard and Walker (2006). MC is the moisture content, expressed as a fraction between 0 and 1.

Soluble organic matter is then used for microbial growth through uptake which can be effectively represented by Monod kinetics, with supplemental considerations for oxygen, ammonium, and alkalinity/pH limitations, as shown in eqs. 5.4 and 5.5. These processes occur in aerobic conditions, while anoxic growth (through denitrification) is also possible and detailed further in section 5.2.2.3.

$$R_{U,HB} = \mu_{H,BH}\left(\frac{S_S}{K_S + S_S}\right)\left(\frac{S_O}{+S_O}\right)\left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk} + S_{alk}}\right)X_{HB} \qquad (5.4)$$

$$R_{U,HF} = \mu_{H,HF}\left(\frac{S_S}{K_S + S_S}\right)\left(\frac{S_O}{K_O + S_O}\right)\left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk} + S_{alk}}\right)X_{HF} \qquad (5.5)$$

Where $R_{U,i}$ is the overall growth rate of bacteria/fungi (kg cell TOC/m^3.d) and $\mu_{H,i}$ are the uninhibited growth rates of bacteria/fungi (day^{-1}).

Finally, decay, which decreases biomass and releases soluble and particulate matter back into the environment, is represented using a first-order (Herbert (1958)) model, as expressed in eq. 5.6.

$$R_{X,i} = b_i X_i \qquad (5.6)$$

Where $R_{X,i}$ is the rate of biomass decay (kg cell biomass/m^3.day) and b_i is the microbial death rate (day^{-1}).

5.2.2.2 Carbon emissions

CO_2 emissions are modelled using commonly implemented conversion factors based on oxygen consumption, while CH_4 emissions are determined based on moisture content. During composting, the majority of carbon emissions are expected to be in the form of CO_2, though poorly aerated or mixed systems can form anaerobic pockets leading to important CH_4 emissions (Walling and Vaneeckhaute, 2020b). Some amount of methane production is normal, though it is often assumed that these emissions get oxidized in aerobic layers further out in the system.

CO_2 emissions are determined based on the oxygen consumption by using a stoichiometric yield (eq. 5.8):

$$\mathrm{R_{CO_2} = Y_{CO_2} S_{O,consumed}} \tag{5.8}$$

Where $\mathrm{R_{CO_2}}$ is the rate of CO_2 emissions (kg CO_2/m^3.day), $\mathrm{Y_{CO_2}}$ is the stoichiometric yield of O_2 to CO_2, which has a value of 1.375 kg CO_2/kg O_2 (2 moles of O_2 consumed (32 g) per mole of CO_2 produced (44 g)).

For CH_4 emissions, the amount of CH_4 emitted is determined based on a ratio between CH_4 and CO_2 emissions, based on moisture content. The expression for this ratio of carbon emissions is shown in eq. 5.9 and was obtained empirically, with the work presented in detail in chapter 7. CH_4 emissions are then determined following eq. 5.10.

$$\%\mathrm{CH_4} = \begin{cases} \exp(-16.6771 + 0.274338 * MC) & \text{for MC} \leq 70 \\ 20 \text{ for MC} > 70 \end{cases} \tag{5.9}$$

$$\mathrm{R_{CH_4}} = \frac{\mathrm{R_{CO_2}}}{100 - \%\mathrm{CH_4}} \%\mathrm{CH_4} \tag{5.10}$$

Where $\%\mathrm{CH_4}$ is the percentage of carbon emissions as CH_4 (%) and $\mathrm{R_{CH_4}}$ is the rate of CH_4 emissions (kg CH_4/m^3.day).

Regarding the impact of anaerobic degradation on the growth of bacterial fraction, the model does not consider a separate pathway to the one mentioned in section 5.4.2.1 for microbial growth. The impact of anaerobic zones is already taken into consideration through the oxygen and moisture limitations applied through eq. 5.3. However, regarding the mass balance on substrates, it is important to consider the removal of carbon through CH_4 from the soluble fraction. Simply put, the model considers soluble carbon removal through anaerobic biodegradation, but this biodegradation is not directly linked to microbial growth, given the influence of moisture and oxygen correction.

5.2.2.3 Nitrogen transformation and transfer

Composting literature has seen limited work on nitrogen transformation, the main works being those of Oudart et al. (2015) and Bonifacio et al. (2017a; 2017b). However, these models lack the full pathway for nitrogen transformation and loss, presenting an important limitation. Nevertheless, there are some models for activated sludge treatment that have focused on similar problems. Two of these prominent models are those of Hiatt and Grady (2008) and Ni et al. (2011), both of which are extensions to the ASMs and therefore present a good opportunity for integration in this composting model.

As mentioned, the aim of this model is to represent the full nitrogen transformation pathway, which is achieved through modelling of ammonification and mineralization, volatilization, assimilative reduction, nitrification, and denitrification.

Ammonification and mineralization are represented by net ammonification, which is the sum of both. Net ammonification is denoted by a first-order equation in which biodegradable organic nitrogen is converted to soluble ammonia by heterotrophs (eq. 5.11).

$$\mathrm{R_{NH} = k_{a,HB} S_{ND} X_{HB} + k_{a,HF} S_{ND} X_{HF}} \tag{5.11}$$

Where $\mathrm{R_{NH}}$ is the rate of ammonification (kg NH_4^+/m^3.day) and $\mathrm{k_{a,i}}$ is the ammonification rate coefficient (m^3/kg TOC.day).

Ammonium is also used by autotrophic ammonia oxidizing ($\mathrm{X_{AOB}}$) and nitric oxidizing bacteria ($\mathrm{X_{NOB}}$), converting it to nitrite and then nitrate, respectively. These processes are expressed through eqs. 5.12 and 5.13.

$$\mathrm{R_{AOB} = \mu_{AOB} \left(\frac{S_{FA}}{K_{FA} + S_{FA} + \frac{S_{FA}^2}{K_{I8FA}}} \right) \left(\frac{S_O}{K_{O,A} + S_O} \right) \left(\frac{K_{IFNA}}{K_{IFNA} + S_{FNA}} \right) \left(\frac{S_{alk}}{K_{alk} + S_{alk}} \right) X_{AOB}} \tag{5.12}$$

$$R_{NOB} = \mu_{NOB}\left(\frac{S_{FNA}}{K_{FNA} + S_{FNA} + \frac{S_{FNA}^2}{K_{I9FNA}}}\right)\left(\frac{S_O}{K_{O,A} + S_O}\right)\left(\frac{K_{I8FNA}}{K_{I8FNA} + S_{FNA}}\right)\left(\frac{S_{alk}}{K_{alk} + S_{alk}}\right)X_{NOB} \quad (5.13)$$

Where $R_{AOB/NOB}$ are the overall growth rates of ammonia/nitric oxidizing bacteria (kg cell TOC/m^3.day), $\mu_{AOB/NOB}$ are the uninhibited growth rates of ammonia/nitric oxidizing bacteria (day^1), S_{FA} is the concentration of free ammonia (kg N/m^3), K_{FA} is the half saturation coefficient for free ammonia (kg N/m^3), and K_{I8FA} is the inhibition coefficient for free ammonia (kg N/m^3). In eq. 5.13, S_{FNA} is the concentration of free nitrous acid (kg N/m^3), K_{FNA} is the half saturation coefficient for free nitrous acid (kg N/m^3), and K_{I9FNA} and K_{I8FNA} are inhibition coefficients for free nitrous acid (kg N/m^3).

The aerobic growth of ammonia and nitric oxidizing bacteria are restricted by the amount of free ammonia (AOB) and free nitrous acid (NOB), following the Andrews (1968) equation (first term between parentheses in eqs. 5.12 and 5.13). High levels of free nitrous acid also inhibit both reactions. Indeed, to better represent these processes, Hiatt and Grady (2008) proposed using free ammonia (FA) and free nitrous acid (FNA) as substrates, both being dependent on the temperature and pH, these equations being based on the work of Anthonisen et al. (1976) (note that there is a transcription error in the work of Hiatt and Grady). The equations used to describe the concentration of these species in the environment are given in eqs. 5.14 and 5.15.

$$S_{FA} = S_{NH}\frac{10^{pH}}{\exp\left(\frac{6.344}{273 + T}\right) + 10^{pH}} \quad (5.14)$$

$$S_{FNA} = S_{NO_2}\frac{1}{\exp\left(\frac{-2.300}{273 + T}\right) + 10^{pH}} \quad (5.15)$$

The nitrate and nitrite produced by the autotrophic bacteria can then be used by the heterotrophic organisms for nitrification and denitrification, implemented through the following pathways, starting with a simplification to reduce the size of the following equations (eq. 5.16):

$$A = \left[\mu_{H,HB}\eta_i X_{HB} + \mu_{H,HF}\eta_i X_{HF}\right] \quad (5.16)$$

Where η_i is the growth factor of heterotrophs on the specific substrate compared to aerobic conditions (-).

- Growth on NO3 (NO_3^- reduction to NO_2^-)

$$R_{NO_2} = A\left(\frac{S_S}{K_S + S_S}\right)\left(\frac{K_O}{K_O + S_O}\right)\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk} + S_{alk}}\right) \tag{5.17}$$

- Growth on NO2 (NO_2^- reduction to NO)

$$R_{NO} = A\left(\frac{S_S}{K_S + S_S}\right)\left(\frac{K_O}{K_O + S_O}\right)\left(\frac{S_{NO_2}}{K_{NO_2} + S_{NO_2}}\right)\left(\frac{K_{I3NO}}{K_{I3NO} + S_{NO}}\right)\left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk} + S_{alk}}\right) \tag{5.18}$$

- Growth on NO (NO reduction to N_2O)

$$R_{N_2O} = A\left(\frac{S_S}{K_{S5} + S_S}\right)\left(\frac{K_O}{K_O + S_O}\right)\left(\frac{S_{NO}}{K_{NO} + S_{NO} + S_{NO}^2/K_{I4NO}}\right)\left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk} + S_{alk}}\right) \tag{5.19}$$

- Growth on N_2O (N_2O reduction to N)

$$R_{N_2} = A\left(\frac{S_S}{K_{S5} + S_S}\right)\left(\frac{K_O}{K_O + S_O}\right)\left(\frac{S_{N_2O}}{K_{N_2O} + S_{N_2O}}\right)\left(\frac{K_{I5NO}}{K_{I5NO} + S_{NO}}\right)\left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk} + S_{alk}}\right) \tag{5.20}$$

Where R_{NO_2}, R_{NO}, R_{N_2O}, and R_{N_2} are the rates of production of nitrite, nitric oxide, nitrous oxide, and dinitrogen (kg N/m^3.day). K_{NO_3}, K_{NO_2}, K_{NO}, and K_{N_2O}, are all expressed in kg N/m^3. K_{I3NO}, K_{I4NO}, and K_{I5NO} are nitric oxide inhibition coefficients, given values of 5E-4 kg/m^3, 3E-4 kg/m^3, and 7.5E-5 kg/m^3, respectively, based on Hiatt and Grady (2008).

Ammonia oxidizing bacteria have also been demonstrated as being important contributors to N_2O production (Fu et al., 2020; Jiang and Bakken, 1999), a previously neglected aspect that was amended in Ni et al.'s (2011) activated sludge model. Autotrophic denitrification is represented with the following equations (eqs. 5.21 and 5.22), where AOBs reduce NO_2 to NO and finally N_2O:

$$R_{AOB,NO} = \mu_{AOB}\eta_{AOB}\left(\frac{S_{NO_2}}{K_{NO_2} + S_{NO_2}}\right)\left(\frac{K_O}{K_O + S_O}\right)X_{AOB} \tag{5.21}$$

$$R_{AOB,N_2O} = \mu_{AOB}\eta_{AOB}\left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right)\left(\frac{K_O}{K_O + S_O}\right)X_{AOB} \tag{5.22}$$

Where $R_{AOB,NO}$ and R_{AOB,N_2O} are the rate of nitric oxide and nitrous oxide production from AOBs (kg N/m^3.day).

Ammonium can also be lost as ammonia through volatilization, especially at higher pHs. The equilibrium between ammonium and ammonia is given by eq. 5.23, with Henry's law (eq. 5.24) being used to calculate the amount of NH_3 in the gaseous state based on the concentration of NH_4^+ in the environment.

$$\mathrm{NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-} \tag{5.23}$$

$$\mathrm{NH_{3(g)}} = \mathrm{SFA} \cdot \frac{\mathrm{K_H^{pc}}}{\mathrm{RT}} \tag{5.24}$$

Where $\mathrm{K_H^{pc}}$ is Henry's constant, R is the gas constant, and T is the temperature. Two choices are available regarding the temperature to use in eq. 5.24: (1) using the temperature of the pile/reactor or (2) the ambient temperature. Conceptually, pile/reactor temperature would make the most sense. However, Oudart et al. (2015) obtained better results using ambient temperature than pile temperature, hypothesizing that this method considers condensation at the pile surface. Though, it is important to note that they were studying a windrow system.

Gaseous NH_3 is then carried away from the system through convection, driven by aeration. The volatilization process can therefore be described following eq. 5.25.

$$\frac{\mathrm{dNH_3}}{\mathrm{dt}} = \frac{\mathrm{G \cdot NH_{3(g)}}}{\mathrm{V\varepsilon\rho_a(T)}} \tag{5.25}$$

Where G is the mass air flow (kg dry air/s), V is the volume of compost (m^3), ε is the porosity of the pile, and $\rho_a(T)$ is the density of air (kg/m^3), the expression of which can be found in eq. 5.31.

Finally, assimilative nitrate reduction to ammonia completes the nitrogen transformation pathways considered in this model. In situations where microorganisms are lacking ammonia, they can convert nitrate (eq. 5.26) and nitrite (eq. 5.27) into NH_4^+ through the following pathways:

$$\mathrm{R_{ANRN}} = 1.2 \cdot \mathrm{i_{XB}} \left(\frac{\mathrm{S_{NO_3}}}{\mathrm{K_{6NO_3}} + \mathrm{S_{NO_3}}}\right)\left(\frac{\mathrm{K_{INH}}}{\mathrm{K_{INH}} + \mathrm{S_{NH}}}\right)\left(\frac{\mathrm{K_{I6NO_2}}}{\mathrm{K_{I6NO_2}} + \mathrm{S_{NO_2}}}\right) \left(\sum_{i=1}^{13} \mathrm{R_i} - \mathrm{R_{21}} - \mathrm{R_{22}}\right) \tag{5.26}$$

$$\mathrm{R_{ANRA}} = 1.2 \cdot \mathrm{i_{XB}} \left(\frac{\mathrm{S_{NO_2}}}{\mathrm{K_{7NO_2}} + \mathrm{S_{NO_2}}}\right)\left(\frac{\mathrm{K_{INH}}}{\mathrm{K_{INH}} + \mathrm{S_{NH}}}\right)\left(\sum_{i=1}^{13} \mathrm{R_i} - \mathrm{R_{21}} - \mathrm{R_{22}}\right) \tag{5.27}$$

Where $\mathrm{R_{ANRN}}$ and $\mathrm{R_{ANRA}}$ are the production rates of nitrate and ammonium, respectively, from assimilative reduction (kg N/m^3.day), $\mathrm{i_{XB}}$ is the nitrogen content of active biomass (kg N/kg cell TOC). The reaction rates (Ri) refer to the reactions listed in the Petersen matrix.

5.2.2.4 Phosphorus transformation and transfer

In biological systems such as composting, phosphorus is mainly transformed through either phosphate solubilizing microorganisms (PSMs) or polyphosphate accumulating organisms (PAOs). Regarding PSMs, these organisms release compounds capable of causing the transformation of labile P to soluble P by decreasing the pH of the environment, most often through the release of metabolic products (acids, ions, etc.) (Estrada-Bonilla et al., 2017; Kumar and Singh, 2001; Wei et al., 2017; Wei et al., 2018a; Wei et al., 2018b). Therefore, the characteristic pH curve associated to many composting operations, with a decrease in pH early on during the process due to the release of short-chained organic acids, as discussed in chapter 1, is the main pathway responsible for P transformation during composting. For PAOs, which are organisms capable of accumulating large amounts of P and are commonly used for enhanced biological phosphorus removal during wastewater treatment, their presence in the composting environment has yet to be demonstrated. For this reason, consideration of PAOs is not included in the present model. However, some research has investigated the potential of inoculating compost with PAOs to enhance P transformation and long-term availability (Wei et al., 2017). Though not included in this model, the addition of a PAO fraction to the model will be necessary if such a step is undertaken and can base itself on the work of the ASM2(d) (Henze et al., 2000), which both seek to improve P-modelling capability of the base ASM.

To the best of our knowledge, only the models of Vlyssides et al. (2009) and Vasiliadou et al. (2015), which was built upon the prior, have considered phosphorus during composting. These models are based on the assumption that P is released in soluble form by hydrolysis of particulate P, which is then consumed by the general biomass. Though not considering the pH of the environment, which plays an important role in P solubilization, the lack of pH modelling capabilities in the composting field has made this the most straightforward pathway to modelling phosphorus and has demonstrated strong results in both works. Therefore, the pathway to model P transformation in this model follows the same basis, as presented in eq. 5.28, based on the work of Vlyssides et al. (2009).

$$\frac{dP_L}{dt} = k_h(T)X_S P_{X_S} - \left(\mu_{H,HB}X_{BH} + \mu_{H,HF}X_{HF}\right)P_{X_H} + \left(b_{HB}X_{H,HB} + b_{HF}X_{H,HF}\right)P_{X_H} \qquad (5.28)$$

Where P_{X_S} is the phosphorus content of particulate matter and P_{X_H} is the phosphorus content of biomass. The first term on the left of eq. 5.28 describes the production of soluble phosphorus through the hydrolysis of the particulate matter. The second term represents the consumption of soluble phosphorus by the biomass during growth, while the third term describes the release of soluble phosphorus during biomass decay.

5.2.2.5 Mass transfer

Mass transfer in the model is accounted for by global mass balances on many of the compounds, assuming the system to be a homogenous environment. Despite the complex and heterogenous nature of composting in reality, this assumption has managed to provide accurate results without requiring complex mathematics and computation, as detailed in chapter 2. The balances for water and oxygen are presented in eqs. 5.29 and 5.30 below (Higgins and Walker, 2001):

$$\frac{dH_2O}{dt} = \frac{G\left(H_s(T_a) - H_s(T)\right) - y_{H_2O} \cdot {}^{dS}/_{dt} - \dot{m}_{leaching}}{\rho_{DM} V} \qquad (5.29)$$

$$\frac{dS_O}{dt} = \frac{G\left(X_{O_2,in} - X_{O_2,in}\right) - y_{O_2} \cdot {}^{dS}/_{dt}}{V\varepsilon\rho_a(T)} \qquad (5.30)$$

Where H_2O is the concentration of water in the substrate (kg H_2O/kg dry matter), G is the mass airflow (kg dry air/s), H_s is the saturated humidity of the air (kg H2O/kg dry air), T and T_a are the temperature of the system and the ambient temperature (°C), respectively, y_{H_2O} is the metabolic production of water (kg H_2O/kg TOC consumed), ρ_{DM} is the density of dry matter (kg/m^3), and V is the volume (m^3). In eq. 5.30, $X_{O_2,in}$ is the oxygen contents of dry air entering the system (kg O_2/kg dry air), ε is the porosity of the bed (-), and $\rho_a(T)$ is the density of the air (kg/m^3) at the temperature of the composting environment, estimated using eq. 5.31. The latter equation is determined by regressing air density as a function of temperature between the ranges of 0 and 100 °C.

$$\rho_a(T) = 1.2832\exp(-0.003T) \qquad (5.31)$$

Similar balances are used for the other gaseous compounds followed by the model, such as CO_2, CH_4, NH_3 and N_2O.

Leaching is also another pathway for mass loss during the process, though the literature has shown very variable results for leaching. Indeed, the review by Roy et al. (2018) identified ranges of leachate production varying between 4 and 400 m^3 at industrial composting sites treating between 1000 and 1500 tons of waste per day. Furthermore, nutrient content of leachate is highly variable, ranging upwards of three orders of magnitude (Krogmann and Woyczechowski, 2000). Therefore, to accurately estimate losses from leaching, a complex leaching module would have to be integrated, which exceeds the scope of this work. However, to consider leaching in the model and its impact on mass balances, leaching and nutrient and carbon concentrations of leachate have been included as user inputs in the model.

5.2.2.5 Heat transfer

Heat transfer throughout the system is represented by the following energy balance (eq. 5.32), following the general balance presented in chapter 2:

$$\frac{\mathrm{dT}}{\mathrm{dt}} = \frac{\mathrm{G}(\mathrm{H_i} - \mathrm{H_0}) - \mathrm{UA}(\mathrm{T} - \mathrm{T_a}) - \mathrm{G}\Delta\big(\mathrm{H_s}(\mathrm{T}) - \mathrm{H_s}(\mathrm{T_a})\big) - \Delta \mathrm{H_S}\, {}^{\mathrm{dO_2}}/_{\mathrm{dt}}}{\mathrm{mc}} \tag{5.32}$$

Equation 5.32 considers the main pathways for heat transfer. The first term on the right is for convection (sensible heat), the second is for conduction through the reactor wall, the third is for evaporation (latent heat), and the final is biological heat generation. This model assumes radiation to be negligible and does not consider the spatial variability of temperature and heat transfer throughout the system. The parameters and variables of equation 5.32 are as follows: m is the mass of the substrate (kg), c is the heat capacity of the substrate (kJ kg^{-1} °C^{-1}), T is the temperature (°C), G is the airflow through the system (kg s^{-1}), $\mathrm{H_i}$ and $\mathrm{H_0}$ are the enthalpies of the gas at the inlet and outlet of the system (kJ/kg), U is a global heat transfer coefficient (kW m^{-2} °C^{-1}), A is the area of the system (m^2), $\mathrm{T_a}$ is the ambient temperature (°C), and $\Delta\mathrm{H_S}$ is the biological heat generation coefficient (kJ/kg O_2 consumed).

5.2.3 Numerical solution

The model was programmed in MATLAB. Currently, two versions of the model exist, (1) one using a finite differences resolution approach, and another (2) using MATLAB's ODE (ordinary differential equation) solver (ode15s). The reason for having both versions is that the model using finite differences is much easier to approach and to understand for a user, with every relationship, definition, equation, and process being explicit, easily identifiable, and contained within the same file. However, unlike an ODE solver, this method is not flexible, meaning that processing times can be long, increasing significantly as the timestep decreases or the process duration increases. For general use, seeking to model a few alternatives, this was not a problem. However, an important part of the calibration of this model was to be undertaken through a Monte Carlo assessment, requiring tens of thousands of iterations, as will be discussed in section 5.2.4. Furthermore, such assessments would be pertinent to evaluate model sensitivity whenever evaluating or recalibrating the model. Therefore, the resolution time for the model had to be decreased from a few minutes to a few seconds per run.

This was achieved using an ODE solver, which can apply a variety of methods to solve systems of ordinary differential equations based on their initial conditions. In the case of the solver used for this model, ode15s, the method is a variable-step and variable-order solver. The main advantage over the finite difference approach, focusing on processing time, is the variable-step nature of the solver, which allows the solver to adjust the time step throughout the process. This means that, when variables are varying rapidly, the solver can use smaller time steps to capture this variation, while using larger time steps when variables are unchanging. In a composting context, this relates to very small-time steps during the early stages of the process, when organic matter is being consumed, microorganisms are growing, and nitrogen is being transformed, followed by much larger time steps during cooling and curing. Transitioning to this approach managed to decrease the resolution time to what was desired for iterative solving, lowering it from about four minutes per run to two seconds per run, for a 50-day process duration. However, this was accompanied by a decrease in the approachability of the model, transitioning from a singular .m file to five separate files, each calling on one-another. As such, the ODE model is much less accessible and understandable for users, particularly those who are not familiar with MATLAB's nomenclature. Issues facing usability will be discussed 5.3.4 and throughout chapter 6.

5.2.4 Model calibration and validation

With a model of this size and complexity, with 24 variables and 75 parameters, calibration is crucial, while also being the primary challenge to its use. This challenge is especially important given the great variability witnessed during composting, with many of the parameters associated to biological aspects, such as degradation rates, yield factors, etc., being highly variable based on the context. Indeed, as was noted in chapter 4, the review of Baptista et al. (2012) found that kinetic parameters reported at the laboratory-scale ranged upwards of 3900%, compared to the variation of 300% observed at full-scale operations. However, as was broached in chapter 2 (section 2.5.5), prior sensitivity analyses have provided some consistent support for the importance of maximum growth and hydrolysis rates ($\mu_i s$ and $k_i s$ throughout this model), death rate constants ($b_i s$ in the model), yields and consumption rates ($Y_i s$ in the model), and the biological heat generation coefficient (ΔH_S in the model), which can serve as an initial and restrained scope for calibration.

Therefore, when approaching the calibration of this model, priority was given to these parameters, while seeking to set as many parameters as possible based on literature and prior work. Where possible, theoretical factors have been used, such as stoichiometric yields, in the aim of facilitating the calibration of the most important parameters, while also seeking to limit the dependence of the model on parameters that would require recalibration for different uses. Appendix E provides the values of parameters taken from prior works and the literature, as well as certain that can be determined theoretically.

A schematic representation of the calibration and validation process used for the development of this model is presented in Figures 5.3 through 5.5. The first step, shown in Figure 5.3, consisted in identifying which parameters were the most important to achieve consistently low errors on outputs. To do this, it was firstly necessary to have a calibration dataset. Once again, this was one of the primary purposes of the planned experiments, which had to be delayed due to COVID-19. As such, the literature was searched for a relevant dataset. This proved to be difficult to find, given a lack in data reporting and/or balances that were either incomplete or erroneous, as well as the specific needs of this composting model, focusing on nitrogen, alongside all the other, traditional, process variables. In the end, the experimental dataset that was chosen for the model was that of Guo et al. (2016), given that it presented the most thorough follow-up of nitrogen, tracking NH_4^+-N, NO_2^--N, NO_3^--N, and TKN throughout the entirety of their 50 day composting trials. Though this does not track the full extent of nitrogen that this model was designed for, notably missing out on gaseous emissions, it is the best dataset that could be found. From here, the process of setting as many of the parameters as possible before initiating a more focused calibration began. This was done by varying all model parameters through a large Monte Carlo simulation, aiming at covering a wide range of parameter combinations. The Monte Carlo run consisted of 100,000 model iterations, with all parameters randomized within a set range, which is presented in Appendix D. Following the full Monte Carlo run, the error between model outputs and calibration dataset was determined, calculating both the Root Mean Squared Error (RMSE) and the Normalized RMSE (NRMSE), following eqs. 5.33 and 5.34.

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(y_{\,\mathrm{model,i}} - y_{\mathrm{exp,i}}\right)^2}{n}} \tag{5.33}$$

$$\mathrm{NRMSE} = \frac{\mathrm{RMSE}}{y_{\mathrm{max}} - y_{\mathrm{min}}} \times 100 \tag{5.34}$$

Based on the information available in the calibration dataset, errors were calculated for temperature, moisture content, NH_4-N, NO_3-N, TKN, dry matter, and biodegradable organic matter loss (BOM_{loss}). The goal here was not to identify specific parameter values, but to instead determine if certain parameter ranges led to consistently accurate results, as well as to see if the model appeared to be unsensitive to certain parameters. From the RMSEs and NRMSEs obtained for each of the assessed variables and for every iteration, the sets of parameters which led to an error below 10%, or the lowest error plus 10% (in case the lowest was higher or lower than 10%) were compiled. This was then followed by a basic but informative analysis of some statistics of this low error dataset, such as the mean, the standard deviation, the variance, as well as minimum and maximum values. Through these statistics, we could see which parameters should be targeted for a more focused calibration in step 2, though evaluation of statistic significance will only come later, once the model is properly calibrated and validated. For example, considering that all parameters are positive, if the mean and standard deviation were equivalent and at the midpoint of the parameter range used for the Monte Carlo, we could infer that the parameter was likely to be less significant to the evaluated variable. Conversely, if a parameter was given a large range in the Monte Carlo, but if a parameter in the low error sets only contained small standard deviation and variance, it would stand to reason that this parameter has an impact on model outputs. For example, during the Monte Carlo, the biological heat generation coefficient (ΔH_S) could range between 0 and 20,000 kJ/kg O_2 consumed, while the half-saturation coefficient for autotrophs (K_{OA}) was varied between 0 and 1 g O_2/m^3. When looking at the parameters within the low error dataset for temperature, ΔH_S had a mean of 17852 kJ/kg O_2 and a standard deviation of 1784 kJ/kg O_2, with a minimum value of 15180 kJ/kg O_2. This was viewed as being indicative that the calibrated value of ΔH_S was likely to be within this range, a range which would serve as for the more targeted Monte Carlo that would follow in step 2. Conversely, K_{OA} had a mean of 0.45, a standard deviation of 0.41, a minimum of 0.008, and a maximum of 0.98, emphasizing that its value had little impact on temperature in the model. This process was done for every assessed output, as well as for the outputs together, seeking to identify which parameters the second step should focus on, as well as setting certain parameters.

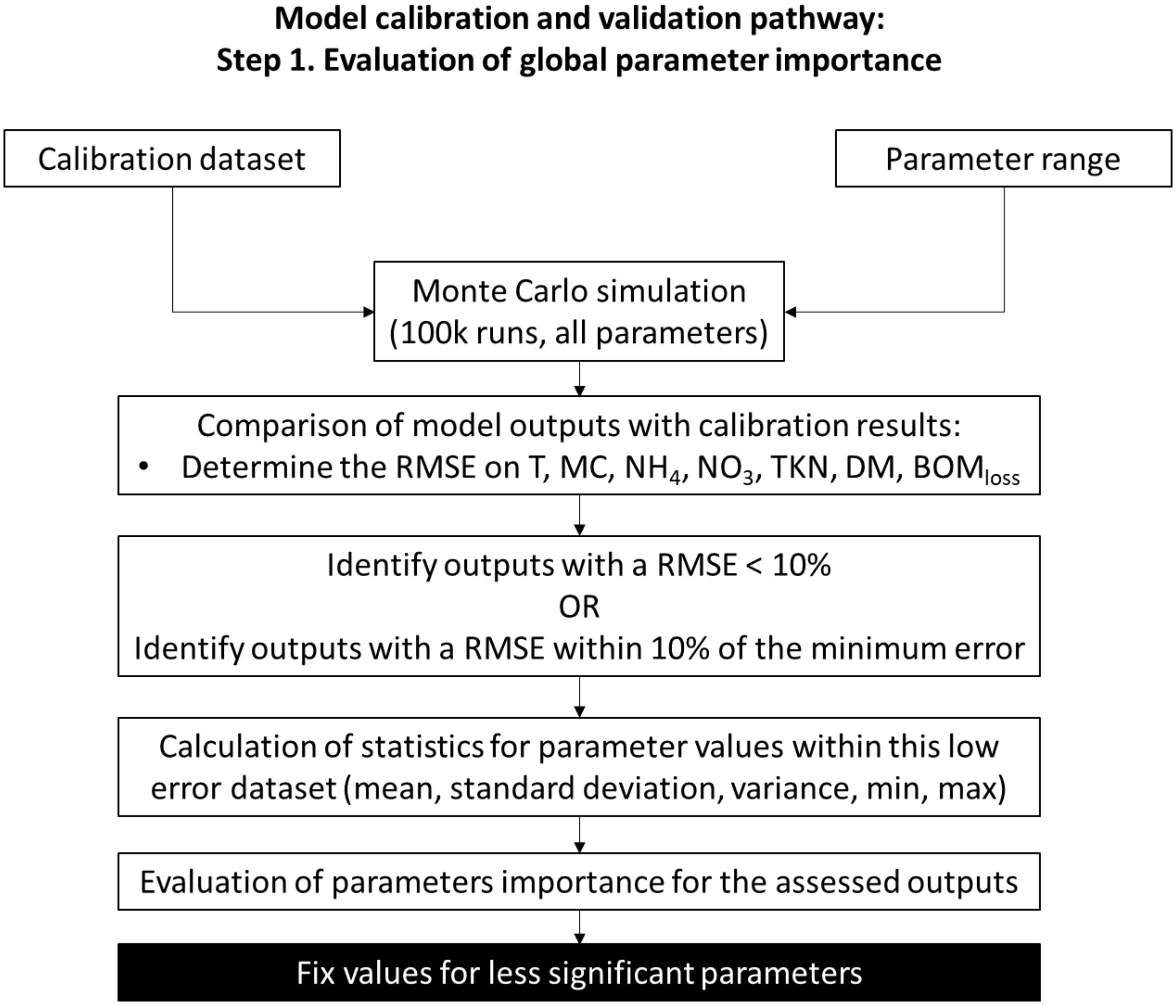


Figure 5.3 Pathway used for the first step of the model calibration and validation, seeking to evaluate the impact of all parameters on select model outputs based on a large Monte Carlo simulation.

This first step was then followed by a more concerted calibration, the pathway for which is shown in Figure 5.4, aiming to produce a calibrated model. In this step, Monte Carlo simulations were used once again, this time with 10,000 simulations by attempt. A similar pathway to step 1 was taken, calculating (N)RMSEs, identifying a low error dataset, and calculating parameter statistics. Two situations would then present themselves: (1) either an iteration in the low error dataset would provide a model that would meet our target (general error < 10%); or (2) none of the solutions would provide a calibration with an acceptable error. In the latter case, the parameter range of the Monte Carlo would be modified, restarting the process. If a model provided acceptable error, it could still be evaluated for further optimization.

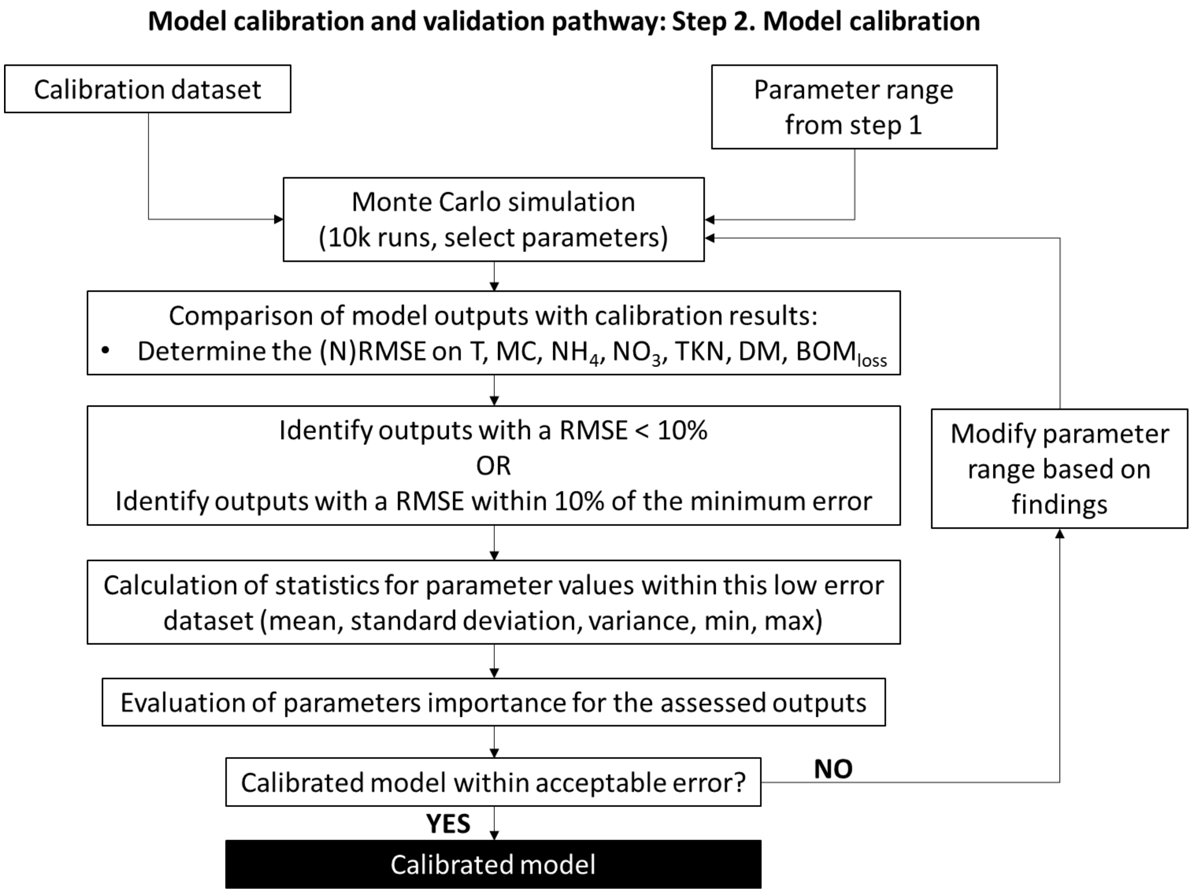


Figure 5.4 Pathway used for the second step of the model calibration and validation, seeking to calibrate the model based on a Monte Carlo simulation. Given the reduced number of parameters varied at this stage, the number of iterations can be greatly decreased.

The final step of this process, schematized in Figure 5.5, is the validation of the model, where the results of the calibrated model are compared with those of a validation dataset. This comparison includes both quantitative and qualitative assessments, including the RMSE and NRMSE, as presented earlier, as well as a visual quality of fit (shape of profiles, presence or absence of key features). This can result in either a calibrated model validated for one or more situations, depending on the validation set, or a calibration that does not adequately meet the requirements of the validation set, therefore not being valid for the evaluated situation(s). In the case where the calibration does not meet the validation criteria, the culprit is likely to be either at the model/process level, where the pathways and/or assumptions used by the model are incapable of representing reality, or due to a calibration that might not capture the full extent of the situation.

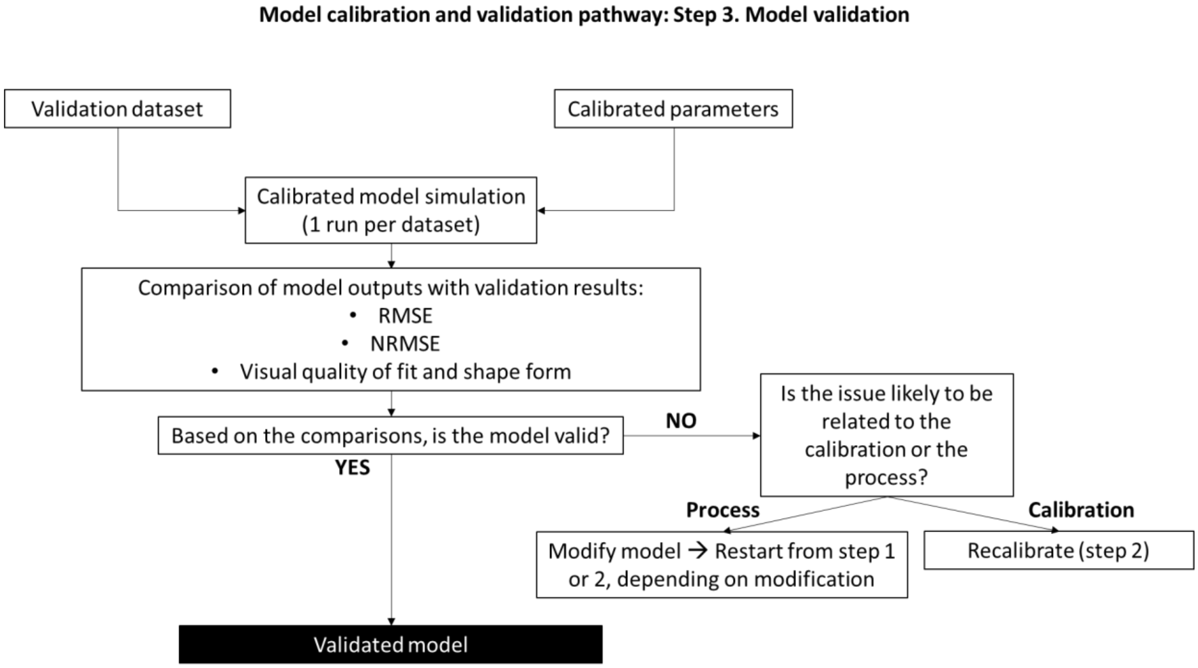


Figure 5.5 Pathway used for the final step: model validation. This step uses the calibrated parameters determined in step 2 and compares the outputs with a validation dataset.

Once again, given the issues faced due to COVID-19 on the experimental front, the choice was made to undertake calibration and validation with the same dataset (that of Guo et al. (2016)). Though this is not ideal, given the risk of overfitting the model by designing it for a singular dataset, it sets the way for the model to be fully calibrated and validated with novel experiments once the reactors are operational and high-quality and extensive data can be obtained. Furthermore, the author stresses that the purpose of this whole process is to validate that the developed model is capable of representing the composting process and nitrogen transformation from a fundamental perspective. If the model manages to represent the experimental data of Guo et al. (2016), then it will be interpreted as an indication that the pathways used to model composting and presented throughout section 5.2.2 are indeed capable of providing predictive insight into the process, though nothing should be inferred as to a "general" calibration or a validation of the model for any other case based on this specific case. Nevertheless, due to the efforts made in undertaking this calibration and validation, the tools are now available to quickly and easily calibrate and validate the model with any future, more robust, dataset.

5.3 Results

5.3.1 Step 1: Identification of key parameters

Following the first Monte Carlo simulation, with 100,000 runs of the model with 40 randomized parameters, the ranges of which are presented in Appendix D, the following information on parameters were identified, with key parameters for each evaluated output being presented in Table 5.2.

Table 5.2 Parameters identified as main influencers on particular outputs through the Monte Carlo simulation of step 1.

Outputs	Key parameters	minimum NRMSE
Temperature	$\Delta H_s, \mu_{AOB}, K_S, K_{NO_3}, K_{FNA}, K_{I14FNA}, \eta_{NO}, b_{HB}$	10.9%
Moisture	$\Delta H_s, \mu_{HB}, K_S, K_{I6NO2}, K_{N_2O}, \eta_H, b_{HB}$	20.5%
NH_4-N	$\mu_{HB}, K_{S5}, K_{NH}, K_X, K_{I14FNA}, \eta_H, b_{HB}, b_{NOB}$	13.1%
NO_3-N	$K_{OH}, b_{AOB}, K_{I6NO_2}, K_{I4FA}, b_{HB}, K_{I14FNA}, \eta_Y$	17.1%
TKN	$\mu_{HB}, \mu_{NOB}, K_{S5}, K_{OH}, K_{N_2O}, K_X, \eta_Y, \eta_{NO_2}, b_{HB}, k_{a,HB}$	10.2%
BOM_{loss}	$\mu_{HB}, K_s, K_{S5}, K_{OH}, K_{NO}, K_{N_2O}, K_X, \eta_{NO_2}, b_{HB},$	9.2%

Considering the information presented in Table 5.2, we see a good concordance with what was reported in past composting model sensitivity assessments, as detailed in chapter 2. Notably, the importance and predominance of growth rates ($\mu_{HB}, \mu_{AOB}, \mu_{NOB}$), decay rates ($b_{HB}, b_{AOB}, b_{NOB}$), the biological heat generation coefficient (ΔH_s), certain half-saturation and inhibition coefficients, particularly for substrate (K_S, K_{S5}), (free) ammonia (K_{NH}, K_{FA}, K_{I4FA}), nitrous acid (K_{FNA}, K_{I15FNA}), oxygen (K_{OH}), and anoxic growth adjustments ($\eta_H, \eta_{NO_2}, \eta_{NO}, \eta_Y$).

From here, of the 40 parameters that were varied, 30 (the parameters that did not appear particularly significant or that had a very constrained range) were fixed, while the remaining 10 were the initial focus of the following step. These 10 parameters included: μ_{HB}, K_S, K_{S5}, $K_{OH}, k_{H,HB}, k_{a,HB}, \Delta H_s, b_{HB}, b_{AOB}, b_{NOB}$. Another factor of note from step 1 was that, based on the minimum error (NRMSE) achieved for each output, presented in Table 5.2, there appeared to be a potential decoupling with moisture, when compared to the other outputs. Indeed, with an NRMSE of approximately 10% for minimum temperature and BOM_{loss}, one would expect moisture to be near the same error range, given that both these factors are the two main contributors to moisture in the system, though this was not the case. This will be explored in more detail in the following sections.

5.3.2 Step 2: Model calibration

From the results of section 5.3.1, step 2 was initiated with Monte Carlo simulations of 10,000 runs using the new parameter ranges. At this point, issues with the model calibration became evident, mainly due to the non-identifiability of the model. Indeed, for a model to be identifiable, the true values of the parameters can be obtained following significant observations, meaning that a specific parametrization will lead to a unique outcome. Conversely, in the case of a non-identifiable model, multiple parametrizations can produce equivalent outcomes, meaning that it is not possible to determine the true value of the parameters. A model not being identifiable is not inherently bad, but the extent to which the developed model is non-identifiable greatly exceeded the author's expectations.

For example, Table 5.3 provides the range of certain of the key parameters that led to nearly equivalent model outputs, highlighting this gross unidentifiability.

Table 5.3 Parameter ranges producing equivalent model outputs, highlighting the non-identifiability of the developed model.

Parameter	Range
μ_{HB}	7.7-26.0
μ_{AOB}	3.4-28.2
μ_{NOB}	9.4-27.4
K_S	15.6-97.0
b_{AOB}	0.006-0.277
b_{NOB}	0.02-0.49
$k_{H,HB}$	1.6-4.4
$k_{a,HB}$	0.018-0.07
ΔH_s	5967.0-16247.3

Beyond the issue of identifiability, which made it difficult to identify an effective calibration, it appeared that, as stated in section 5.3.1, certain parts of the model might be decoupled from one-another. Indeed, following strenuous attempts to calibrate the model through the Monte Carlo simulations, it became clear that certain outputs could not be optimized together. A notable rift became apparent between the carbon/organic matter outputs, such as BOM_{loss} and dry matter, as well as temperature, with the nitrogen outputs (TKN, NH_4-N, NO_3-N). When optimizing the prior, it was impossible to get the latter within an acceptable range of error.

Given the significant time spent on the calibration, which did not lead to a conclusive result that would allow to move to the 3rd step (validation), the author decided to focus on the evaluation of individual components within the model to try and pinpoint what areas might be causing issues. This evaluation process had two aims: (1) verifying that the model components (heat balance, mass balances, biological module) were capable of providing the desired profiles, and (2) investigate how the parametrization of these different calibrations compared to try and identify what areas of the model were not working. The results of this process are presented in the following subsection (5.3.3).

5.3.3 Model component validation and identification of problem areas

Many of the model outputs managed to match up with the experimental results, as presented in Figure 5.6. Individually, a NRMSE of 8.1% was obtained for BOM_{loss}, 6.4% for dry matter, 12.0% for temperature, 9.1% for moisture, 17.3% for NO_3-N, and 17.9% for NH_4-N. For temperature, despite many experimental points being above the modelling curve, it is important to note that the consistent three-point patterns (highlighted on the figure) are due to mixing events, which this model did not seek to simulate. Therefore, following the lower end of the experimental profile, as is shown in Figure 5.6, is what would be expected without turning, which is what the model represents. From the various profiles, we can note a generally good capacity to accurately represent these aspects of the composting experiments. There are some deviations, such as the model underpredicting the maximum BOM loss, but it is very difficult to know what is the fault of the model versus what might be an error from data uncertainty, especially given that some assumptions had to be made regarding starting fractionations. Overall, the profiles are largely agreeable, with what may appear to be large errors being due to the scaling of the plots, such as the estimate for moisture at t = 3 days, which seems to be a significant overestimation, but is only about 3% higher than the real value. However, purely from a visual standpoint, there is one behaviour that is not desired. For NH_4-N, the model predicts a much higher production of ammonium than the experimental data, despite being spot on for the rest of the profile, which also explains why it has the highest NRMSE of the evaluated outputs.

From here, given that the individual processes could be mostly adequately represented, it became pertinent to look at the value of the parameters that produced each of these outputs, which should highlight areas of “conflict” in the model. Table 5.4 presents an overview of the main differences, highlighting only the situations that were different from the “norm”. Surprisingly, there were many similarities throughout, something which was unexpected given the difficulty in obtaining an overall accurate simulation. Looking through the table, we can see that many areas are similar between outputs, particularly for temperature (T), moisture content (MC), and dry matter (DM), which will be what the others shall be compared to when we say if they are lower or higher for certain parameters. From this information, we can paint a picture of what is happening within the current model structure.

Starting with TKN: it is the most obvious area of issue in the model, though whether this is due to the model itself or an issue with the experimental dataset or data reporting is unclear. Indeed, from Table 5.4, we can see that, for TKN to be accurate, it requires a low growth rate (μ_{HB}), a high half-saturation coefficient for soluble substrate (K_S), a low hydrolysis rate ($k_{H,HB}$), and a low heat generation coefficient (ΔH_s), basically meaning that it requires nearly no biodegradation. Indeed, the low growth rate, hydrolysis rate, and heat generation, coupled with the high half-saturation coefficient, is a recipe for nothing, from a composting perspective. Given this behaviour, and prior investigations not finding anything wrong, more time will be spent trying to understand this source of error.

When looking at the other outputs, the situations are much more understandable. BOM_{loss} favored a low decay rate for NOBs, which makes sense given that a low death rate results in more degradation through a longer lifespan of organisms. However, the reason that this targeted NOBs specifically, and not the other two microbial fractions (they were lower, but not out of the range of the others), is not completely clear. It is potentially because of the role NOBs play in producing NO_3-N in the system, which is the gateway for all of the subsequent anoxic processes, which make up a non-negligible part of the degradation.

For NO_3-N to achieve a comparable modelling result to the experimental ones, a low growth rate of NOBs was needed, alongside high half-saturation coefficients for ammonium and oxygen (K_{NH} and K_{OH}), a low anoxic yield factor (η_g), and low decay coefficients for both AOBs and NOBs. This can be interpreted as indicating that the anoxic pathways implemented in the model are too aggressive at consuming the nitrate fraction, which would be limited by having a low η_g and a high K_{NH} and K_{OH}. Furthermore, a decrease in the rate of decay of both AOBs and NOBs would also lead to higher NO_3-N concentrations; AOBs producing the NO_2 which the NOBs require for NO_3 production. The only area of uncertainty on this aspect is the low NOB growth rate (μ_{NOB}), though the author speculates that this is to ensure that the growth in NOB fraction happens after the primary consumption of NH_4, when more nitrogen substrate is available, as is traditionally observed during composting.

Regarding the other nitrogen fraction that was assessed, NH_4-N is also expressing a similar issue as NO_3-N, being consumed too rapidly. Indeed, in this case, this is highlighted by a need for high half-saturation coefficients on substrate, ammonium-nitrogen, and oxygen, all of which will decrease the rate of degradation, while favoring a low half-saturation coefficient for oxygen in the AOB process, which is a primary generator of NO_2 in the system, which can then be reduced to ammonia through the assimilative reduction pathway. This is also further highlighted by the significantly higher (600%) assimilative nitrate reduction coefficient than in the other calibrations. However, there is the particularity of the timeliness of this all, as the need for a high ΔH_s indicates that this calibration also favors maintaining high temperatures to allow for volatilization, once NH_4-N concentrations have peaked.

Based on the information discussed above and identified in Table 5.4, it will be pertinent to modify the model to try and account for this. A summary of the current interpretation of the situation and the changes that should be brought accordingly is provided below:

- TKN is aberrantly wrong and requires a full assessment. The only way the model can currently meet the experimental dataset is by assuming barely any composting happens.
- Both NO_3-N and NH_4-N are being consumed too aggressively in the calibrations that accurately predict temperature, BOM_{loss}, dry matter, and moisture. This explains why we seem to either get accurate carbon/organic matter outputs or nitrogen outputs, but not both together.
- However, the issue is that decreasing degradation to favor NO_3-N and NH_4-N would also decrease BOM_{loss}, temperature, and dry matter, while also impacting moisture content.
- It is possible that decreasing the anoxic pathways will allow for continued aerobic degradation, while putting less stress on the nitrogen fractions. However, until a comprehensive dataset that follows all forms of nitrogen is available, it will not be possible to validate this.

- Conversely, what may appear as a penchant towards decreasing consumption of these fractions (NO_3 and NH_4) might also indicate that the processes producing them are not aggressive enough, and therefore tend to lag the consumption of carbon substrate.

This will all be assessed in the near future to try and assuage these issues.

Table 5.4 Key differences in calibrations that allowed to obtain an accurate prediction for each output.

	BOM_{loss}	**T**	**MC**	**TKN**	**DM**	**NO_3-N**	**NH_4-N**
Growth rates	-	-	-	low μ_{HB}	-	low μ_{NOB}	-
Half-saturation coeffs.	-	-	-	high K_S	-	high K_{NH}, K_{OH}	high K_S, K_{NH}, K_{OH} low K_{OA}
Inhibition coeffs.	-	-	-	-	-	-	-
Anoxic adjustment factors	-	-	-	-	-	low η_y	low η_y
Decay coefficients	low b_{NOB}	-	-	-	-	low b_{AOB}, b_{NOB}	-
Hydrolysis	-	-	-	low $k_{H,HB}$	-	-	-
Ammonification	-	-	-	-	-	-	high $k_{a,HB}$
Biological heat	-	-	-	low ΔH_s	-	-	high ΔH_s
Assimilative nitrate reduction	-	-	-	-	-	-	high AR

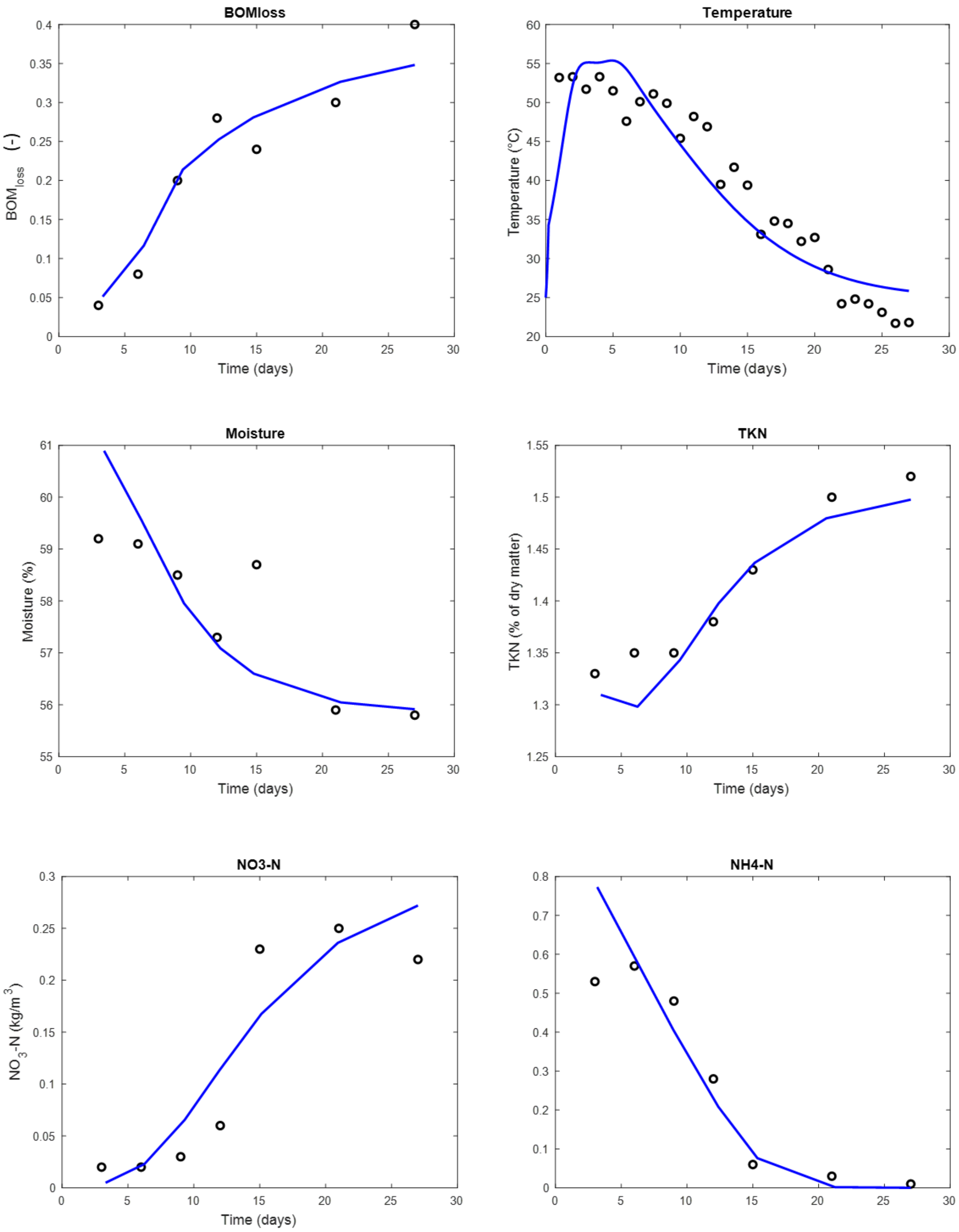


Figure 5.6 Comparison of model outputs and experimental results for calibrations seeking to optimize each output individually.

5.3.4 Limitations and perspectives

The model in its current form obviously suffers from significant issues limiting its use, as well as serious doubt as to its validity, given the lack of necessary high-quality data that the author had planned on having to calibrate and validate the model. However, the development process of this model provided many valuable lessons about how composting modelling should be approached, how the continued development of this model will be undertaken moving forward, as well as being an invaluable source of knowledge, while also identifying limitations of this model:

- Though the model is based on the widely used activated sludge models (ASMs), as was the prior composting model of Trémier (2004), the author highly cautions against using this basis for composting models in the future. The main issue with the ASMs is that the fractionations are not particularly intuitive to work with and understand, especially in the case of a composting model, which focuses on carbon/organic matter. Indeed, the ASMs are built on a chemical oxygen demand (COD) basis, which works fine when dealing with wastewaters, but adds unnecessary complexity in the case of solid waste such as compost. Though the development of this composting model was done on both a COD and TOC basis, certain nonsensicalities come through, such as the loss of carbon as CO_2 technically being accounted for in the S_O (oxygen) consumption (see Petersen matrix in Appendix C for details). Developing the model from the ground-up and integrating aspects of the ASMs would likely have provided a smoother experience for the author, as well as a more approachable model. To address some of these issues, works such as that of Takács and Vanrolleghem (2006) can serve as inspiration to represent the elemental balance, notably on carbon, in a much clearer fashion than what is currently implemented.
- In a similar vein, the fractionation used by the model, though simpler than many that have been used in the past and similar to that of the ASMs, remains very impractical in a composting setting. Knowledge most commonly available on a composting site generally include moisture content, organic matter, and C/N ratio (Alberta Environment and Parks, 2018). Therefore, attempting to split the substrate into soluble and particulate biodegradable and inert fractions, among multiple microbial fractions, will not be normally available or meaningful to most users.

- The main contributors to the size of the model and the large number of parameters are the half-saturation and inhibition coefficients, which play a role in every biological rate included in the model. These are also the main reason that the model is non-identifiable. Transitioning away from these limitation terms should greatly improve the usability and identifiability of the model. Some will obviously be necessary, but it is likely that, at the moment, many serve a limited purpose and mainly bloat the model.
- On a positive note, the heat balance appears to work very well, consistently being among the most accurate model subsets. No change would be recommended on this front.
- The water balance also appears to produce desirable profiles, though it tends to be either over or under reactive (i.e., good shape, but not over the desired range). Once the proper data is available, it should not be difficult to verify and adjust.
- Despite the comments on the complexity of the model and its multiple fractionations, it does provide a great tool to follow carbon and nitrogen during the process. Obviously, value will only come from this when the model is adequately calibrated and validated, but it has the potential to offer a great instrument to understand the dynamics taking place during the process, such as being able to identify rate-limiting steps, quantify the transformation between fractions dynamically, and explore a variety of process and operating modifications. This being said, extensive understanding of composting, modelling, and this particular model structure will be necessary to achieve this.

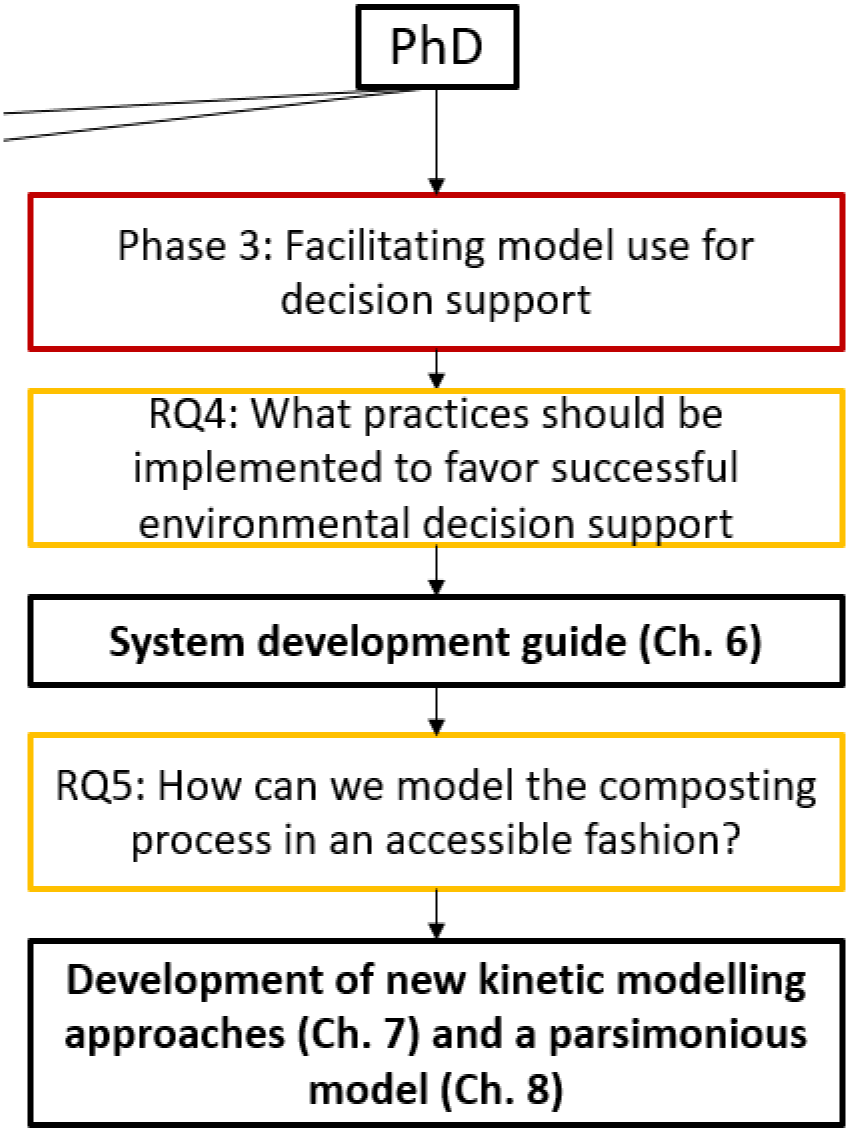
These lessons shall be applied in the following phase of this Ph.D., which focuses on the development of usable, accessible, and accurate composting models.

5.4 Conclusion

Throughout this chapter, a novel comprehensive deterministic and mechanistic composting model focusing on nutrient (particularly nitrogen) transformation and loss, and greenhouse gas emissions was developed. The model is based on a sound theoretical foundation through a robust representation of microbial biodegradation pathways, heat transfer, and mass transfer. Following an extensive attempt at calibrating and validating the model through Monte Carlo methods, greatly hampered by the lack of expected experimental data due to COVID-19, the developed model remains in need of a proper calibration and validation on a strong dataset. However, significant effort was put to ensure that this process will move smoothly in the future, with the appropriate methodology and tools in place to undertake such an evaluation rapidly. Nevertheless, the evaluation of the model highlighted certain flaws that the author will seek to address in the future, notably relating to model identifiability, as well as an overly complex structure which greatly limits its potential user-base. Despite these issues and this chapter not concluding in the way the author had envisioned when starting this process (i.e., with a functional, calibrated, and validated model), the development of this model and the work undertaken throughout this chapter presents an incredible development of knowledge and learning, both for the author and for the field of composting modelling. Continuity on this project will be ensured by the experimental work developed in chapter 4, which should provide an answer to most of the questions raised throughout this chapter, while clear paths for model evaluation and improvement have been highlighted in sections 5.3.3 and 5.3.4. This development process highlighted many questions that the author felt were important to address, particularly regarding the development of usable and approachable composting models. Therefore, following the work undertaken up to this point, the third phase of this Ph.D. was envisioned, which aimed at answering two questions: (1) What modelling practices should be implemented to favor successful environmental decision-making and system design? And (2) How can we model the composting process in both a simple and generalizable fashion?

Phase 3

Facilitating the use of models for successful environmental decision support



Chapter 6: Developing successful environmental decision support systems: challenges and best practices

6.1 Résumé

Les outils d'aide à la décision sont appliqués depuis plus de 40 ans dans le domaine de l’environnement. Cependant, la majorité de ces outils ne trouvent pas d'utilisation ou tombent hors d'usage rapidement. Dans le but d'aider à la conception et au développement de systèmes d'aide à la décision pratiques et efficaces, cette revue examine la littérature existante, à la fois centrée sur les outils d’aide à la décision environnementale et dans des domaines plus larges liés à la prise de décision, pour mettre en évidence certains des défis les plus importants qui influencent le succès et la convivialité de ces systèmes. Au total, 13 défis majeurs auxquels est confronté le développement de ces outils ont été identifiés et plus de 60 recommandations et meilleures pratiques ont été fournies pour relever ces défis. Bien que ce chapitre se concentre principalement sur les systèmes d'aide à la décision environnementale, la majorité des informations et des conclusions mises en évidence sont applicables au développement de systèmes d'aide à la décision dans n'importe quel domaine.

Mots clés : Système d’aide à la décision environnementale ; prise de décision ; évaluation ; défis ; parties prenantes ; meilleures pratiques

3.2 Abstract

Environmental decision support systems (EDSSs), or DSS applied in the environmental field, have been developed for over 40 years now. However, most of these tools fail to find use or fall out of use quickly. In the aim of aiding in the conception and development of practical and successful decision support systems, i.e., systems that can lead to positive outcomes, this review looks over the existing literature, both EDSS-centric and from broader decision-related fields, to highlight some of the most important challenges influencing the success and usability of these systems. In all, 13 major challenges facing EDSS development were identified and over 60 recommendations and best practices were provided to address these challenges. Though this chapter is mainly focused on environmental decision support systems, most of the highlighted information and conclusions are applicable to the development of decision support systems in any field.

Keywords: Environmental decision support system; decision-making; evaluation; development challenges; stakeholders; best practices

6.3 Introduction

In the previous two phases of this thesis, focus has been placed on consolidating, developing, and applying fundamental knowledge on composting modelling to produce a highly comprehensive composting model. Though the model detailed in chapter 5 presents a potentially interesting tool to evaluate and understand what can be happening during the composting process, as noted, it suffers from its complexity. Indeed, to be able to use it to its fullest extent and to understand its results and their meaning in the clearest of manners, extensive knowledge on the fundamentals of composting, including biological degradation, heat transfer, and mass transfer, and how this is modelled, is necessary, without even considering the issue of identifiability. As such, other than for research or in the hands of well-trained experts in the field, it seems unlikely that the work that has gone into developing this knowledge would be usable to a wider audience. Making the tool accessible to as many actors in the composting and environmental fields as possible is therefore of great importance and value. Indeed, if this knowledge could be placed in the hands of decision-makers, industrials, researchers, and composting operators, the benefits of the work undertaken thus far could be felt on a much greater scale and the impact of this PhD project would be greatly increased. As such, this third and final phase of this dissertation will aim at facilitating the use of the knowledge developed thus far, seeking to make it usable to a large group of actors.

The first step in this process is to determine how to actually achieve this goal. Indeed, there is significant work on modelling, particularly environmental modelling, and how to approach model design, uncertainty, etc., but guidance on making these models usable, particularly to decision-makers, is surprisingly lacking. Indeed, decision-making scenarios are far more complex than simple optimization cases, and are becoming ever more common in waste management and environmental fields. In these particular cases, the current context of ever tightening environmental regulations, increasing focus on sustainable development, and the pressure to transition towards circular economies, has placed decision-makers in situations where they must make choices that will have a long and lasting impact on their communities. Such decisions often require a compromise around social, economic, technical, and environmental issues, with numerous alternatives and various sources of uncertainty to be considered (French and Geldermann, 2005; Liu et al., 2008; Matthies et al., 2007; Reichert et al., 2015). This renders the decision-making process highly complex, and, as such, simply applying mathematical models is not enough to address these situations. Indeed, such situations call for the use of specialized tools, known as decision support systems (DSSs), to help address them.

DSSs are developed to assist decision-makers in dealing with situations where there are multiple potential solutions to a problem and none is objectively better than the others; the selection of an alternative being based on the p of the decision-makers (subjective) (Buchanan et al., 1998; Saaty, 2008). These systems are not simply models, assessments or decision trees, for example, but are instead systems having the capacity to aid in structuring and resolving contested problems, while also increasing the transparency of decision-making, providing users with a better understanding of the problem situation and promoting learning (McIntosh et al., 2011). Therefore, DSSs deal with unique challenges related to the decision-making process that are not experienced in traditional model or system design.

In environmental fields, EDSSs have been present since the 1980’s (e.g. Johnson, 1986; Maeda, 1984; Rossman, 1980). Examples include systems aiding in assessing environmental management and site selection (Carrick and Ostendorf, 2007; Massei et al., 2014; Negahban et al., 1995; Rahman et al., 2012), waste collection routes (Rada et al., 2013), water quality management alternatives (Assaf and Saadeh, 2008), water and waste treatment alternatives (Bertanza et al., 2016; Castillo et al., 2017; Comas et al., 2004; Latawiec et al., 2017; San Martin et al., 2017), resource management (Dong et al., 2013; Naz et al., 2017), environmental impact of agriculture (Horn et al., 2003; Nicholson et al., 2013; Oliver et al., 2012; Passuello et al., 2012), and energy planning (Hobbs and Meier, 2012; Kumar et al., 2017; Sánchez-Lozano et al., 2013; Trivyza et al., 2018). However, even nearing 40 years of development and growth in this field, a majority of EDSSs have failed to reach the market or to provide their expected outcomes (French and Geldermann, 2005; Hamouda et al., 2009; Mysiak et al., 2005; Newman et al., 2017; Poch et al., 2017; Reiter et al., 2018; Uran and Janssen, 2003; Zasada et al., 2017). Indeed, the works of Uran and Janssen (2003), Hamouda et al. (2009) and Poch et al. (2017) have all arrived to the similar conclusions that “although there have been many [E]DSSs developed over the past years, few appear on the market as useful products” (Hamouda et al., 2009), or, as Poch et al. (2017) state: “wide and generalized use of deployed EDSSs has not been observed”. These remarks have been further supported by the recent reviews of Zasada et al. (2017) and Reiter et al. (2018), finding “limited evidence […] on the success of [E]DSSs in practice” (Zasada et al., 2017). Regarding outcomes, Mysiak et al. (2005) also noted that, in many cases, EDSSs have stopped being used once decision-makers understood the decision process or that decision-makers arrived to different conclusions than the system, representing a significant waste in resources to develop these tools.

Where this becomes important for this thesis is that the integration of composting models within EDSSs could provide a unique pathway to valorize and use these models, as will be further discussed in the perspectives and conclusion section of the dissertation. However, to achieve this integration, it is important to know and understand if these models should have specific design considerations, given that it is very unlikely a model such as the one developed in chapter 5 could be integrated and used in such a system.

Currently, there exists no widespread guide or standard for the production of EDSSs and the development of these systems is plagued with challenges and potential pitfalls. McIntosh et al. (2011) identified four main challenge areas for EDSSs through a workshop with 24 EDSS development professionals and provided some best practices with the aim of improving EDSS development practices. These challenge areas include: (1) engagement challenges, (2) adoption challenges, (3) business, cost, and technology challenges, and (4) evaluation challenges. Following in this vein, a study by Merritt et al. (2017) identified 33 factors influencing the success of modelling projects based on an analysis of 15 water resource modelling projects. These included factors related to project management, project actors, stakeholder engagement, model/system development, model evaluation, contextual factors, and model use. Following a survey of the model developers, the authors concluded that good relations between the development team and end users, strong model validation and having developers with the proper skills and understanding were the factors most associated with a successful outcome.

Other than these few studies, there has been little interest in identifying success factors for EDSS developers and providing them with the guidance necessary to produce successful systems. Despite the work undertaken by McIntosh et al. (2011) and Merritt et al. (2017), an extensive review of the literature is lacking, although of high interest to provide guidance towards the development of robust and successful EDSSs.

Given that a majority of EDSSs fail to find use and the lack of general guides for their development, a review of the literature was undertaken to identify the challenges facing EDSS development and to determine the key factors that promote the success of these systems, in the aim of assisting developers to produce higher quality systems. This review aims at answering two research questions: 1) what challenges lead to the failed long-term and practical use of EDSSs? and 2) what practices can we implement to address these challenges and promote system success? Though a deviation from the composting specific nature of the previous chapters, the intention of chapter 6 is twofold. Firstly, as mentioned, understanding how models interact with decision-makers, notably through these decision support systems, and what designers should be aware of is of great importance to achieve the objective of the third phase of this PhD. Secondly, while undertaking this work, it became evident that the field of environmental modelling and decision-making could greatly benefit from a more thorough, comprehensive, and consolidated guide, similarly to what was observed and done in chapter 2.

This chapter is divided as follows: section 6.4 presents the review's methodology, which is followed by the identified challenges in section 6.5. Section 6.6 provides an analysis and discussion of these challenges, the impacts they can have on the quality of an EDSS, the practices that can be used to mitigate these issues, followed by the recommendations that have been identified for EDSS development. In section 6.7, we discuss the importance of EDSS evaluation during the development process and provide a list of evaluation criteria based on our review of evaluation-specific literature. Finally, section 6.8 provides a summary of our work and some concluding remarks.

6.4 Review methodology

To carry out this review, the Web of Science database was used as the primary tool to identify relevant publications, while Google Scholar was used to complete the search for potential non-inventoried works (pre 1990's). White papers were the primary source of information, though grey literature (reports and books) had to be considered for some of the seminal works on decision support (only 7-8% of reviewed works, i.e., 32 of the total reviewed works, 16 of which are referenced in this paper). Only published works were considered, with all but two being in the English language. Publications ranging from 1960 to 2019 have been investigated, though a majority (97%) of the works used in the review range from 1980 to 2018.

This was undertaken in multiple steps. Firstly, an initial identification and review of EDSSs was done using various combinations of the search terms: "environmental", "waste", "water", "land management", "environmental management", "decision support system", "multi-criteria", "rule-base" and "expert system". Though this was the starting point for this work, the information gleaned from papers that detailed the development and use of EDSSs was generally less informative than we would have hoped. Therefore, this was followed by a review of development guides and success factors for EDSSs, using the keywords: “environmental decision support”, “develop*”, “guide”, “challenges”, “failure” and “success”. These searches were then complemented with general searches for more case-specific information, looking to gather information from other fields that might be pertinent and transferable for EDSS development. These searches usually involved dropping the environment specific search terms and resulted in literature form a variety of fields, such as requirements engineering, social sciences and operational research.

In total, the general search on EDSSs resulted in 20,421 articles on Web of Science, while the search for development guides and success factors led to 1,260 results. Given the massive number of results for the first search, this one was limited to highly cited papers (180). The second search provided more pertinent results and was more manageable, so it remained unaltered. These results were then screened using their titles, abstracts, and keywords to determine their relevance, with 316 articles being retained for further review. Articles were deemed relevant when they pertained to the development or evaluation of a decision support system applied to environmental applications and not simply the application of a decision support method or assessment, the latter making up a majority of the identified literature. Google Scholar was then used to identify or retrieve 87 seminal or highly pertinent articles that were not identified during the initial retrieval but during the review, notably for works prior to 1990. Overall, 405 papers were consulted, 231 of which are referenced in this chapter.

6.5 Identification of challenges facing EDSS development and use

During the review process, any information on potential factors that influenced the success of EDSSs and models was noted. These were then aggregated into three major categories: stakeholder-oriented, model-oriented, and system-oriented challenges. The breakdown of these categories can be found in Table 6.1. In all, a list of 13 challenges that can influence the quality and success of an EDSS was compiled. The first category, stakeholder-oriented challenges, refers to the factors that are either directly related to stakeholder participation, such as identification and prioritization, or to understanding their needs and expected outcomes. Model-oriented challenges refer to considerations that pertain to the selection and implementation of the models within the system (with noted focus on decision methods/models), whereas system-oriented challenges relate to system design considerations, usually pertaining to how the system meets the needs of the stakeholders.

Table 6.1 Challenges and considerations influencing the end-quality and success of EDSSs identified from the literature.

Challenge type	**Description**
Stakeholder-oriented	1. Identifying stakeholders (Arnott and Pervan, 2005; Lautenbach et al., 2009; McIntosh et al., 2011; Zasada et al., 2017) 2. Prioritizing stakeholder influence and participation (Abelein and Paech, 2015; Bano and Zowghi, 2015; Basco-Carrera et al., 2017; Black et al., 2014; Horne et al., 2016; Jakeman et al., 2006; Krueger et al., 2012; McIntosh et al., 2011; Voinov and Bousquet, 2010; Voinov et al., 2016) 3. Establishing a strong relationship between developers and stakeholders (McIntosh et al., 2011; Merritt et al., 2017; Oliver et al., 2012; Uran and Janssen, 2003; van Delden et al., 2011) 4. Eliciting the problem situation (McIntosh et al., 2005; Merritt et al., 2017; Sojda et al., 2012)
Model-oriented	1. Understanding the type of decision to be supported (Sojda et al., 2012) 2. Selecting a decision support method (Arroyo and Molinos-Senante, 2018; Bertanza et al., 2016; Huang et al., 2011; Massei et al., 2014; McIntosh et al., 2005; Pick and Weatherholt, 2013; Ren et al., 2017; Vitorino de Souza Melare et al., 2017) 3. Determining the simplicity of the models (Hajkowicz, 2008; Janssen, 2001; Olson et al., 1995) 4. Dealing with uncertainty (Ascough et al., 2008; Aulinas et al., 2011; De Kort and Booij, 2007; Hepting, 2007; Jakeman and Letcher, 2003; Kryszkiewicz, 1998; Matott et al., 2009; Pesonen et al., 1998; Reichert and Borsuk, 2005; Uusitalo et al., 2015; Yan et al., 2003) 5. Dealing with variable results (Belton and Gear, 1985; Bertanza et al., 2016; Olson et al., 1995; Ren et al., 2017)
System-oriented	1. Providing pertinent queries and results (Liu et al., 2008; Merritt et al., 2017; Uran and Janssen, 2003) 2. Communicating/understanding how the results have been achieved and their limitations (Bertanza et al., 2016; Licitra et al., 2017; Liu et al., 2008; Rudin, 2018) 3. Producing a user-friendly system (Hamouda et al., 2009; Van Meensel et al., 2012) 4. Determining appropriate system restrictiveness (Bertanza et al., 2016; Chaudhry et al., 1996; McIntosh et al., 2005; Parikh et al., 2001; Rhee and Rao, 2008; Van Meensel et al., 2012)

6.6 Analysis and discussion of factors influencing success and best practices

Section 6.6 will provide a description of the challenges presented in Table 6.1, as well as the methods that can be used to limit their impact and to promote project success.

6.6.1 Stakeholder-oriented challenges

The first major type of challenge explored is stakeholder-oriented challenges. These challenges are primarily centered around acquiring a full understanding of why the system is being developed (for whom and for what purpose?) and ensuring that the tool, from a conceptual standpoint, meets the requirements of the users.

6.6.1.1 Identifying stakeholders

The first challenge is the identification of stakeholders, i.e., people or organisations that have an impact on the development or use of the tool. Indeed, some researchers have shown some very concerning trends in this respect. For example, a review of DSSs by Arnott and Pervan (2005) noted that, out of over 1000 articles reviewed between 1990 and 2003, 58.6% were unclear as to the primary user of their tool. This trend remaining high in the following decade (2004-2010), with 52.3% being unclear on the primary user (Arnott and Pervan, 2014). More recently, Zasada et al. (2017) reviewed the use of EDSSs for landscape and environmental management and found that, of the 29 projects they reviewed, more than 10% failed to involve the stakeholders in any way, while the review of DSS for natural hazards risk reduction by Newman et al. (2017) found that 22% of reviewed projects did not explicitly outline the end users.

This trend of poor user involvement is distressing seeing how the beneficial influence of stakeholders on system's success has been widely reported throughout the literature (Abelein and Paech, 2015; Bano and Zowghi, 2015; Black et al., 2014; Díez and McIntosh, 2009; Hajkowicz, 2008; Horne et al., 2016; Merritt et al., 2017; Pacheco and Tovar, 2007; Tsouvalis and Waterton, 2012; van der Most et al., 2018; Voinov and Bousquet, 2010; Voinov and Gaddis, 2008). Indeed, user participation was identified as the best predictor of success for the pre-implementation phase of information system development by Díez and McIntosh (2009) and stakeholder engagement was found to be amongst the highest rated success factors by Merritt et al. (2017), second only to proper problem elicitation (see section 6.6.1.4). This is in large part due to stakeholders having the knowledge and experience necessary to guide the development of a DSS, while also providing feedback that, when implemented, tends to increase their adoption of the tool (Jakeman et al., 2006; Tsouvalis and Waterton, 2012; Voinov and Bousquet, 2010).

Therefore, stakeholder identification is a necessary and primordial step for EDSS design, though its implementation remains tedious and consistent results are uncertain (Jepsen and Eskerod, 2009; Pacheco and Garcia, 2012; Pacheco and Tovar, 2007). Many of the proposed methods revolve around inventorying stakeholders into predetermined taxonomies through either interviews or workshops (e.g. Alexander, 2005; Kotir et al., 2017; Krupa, 2016; Leventon et al., 2016; Pacheco and Garcia, 2012; Sharp et al., 1999), while determining the number and span of stakeholders can still remain a major challenge (the balance between "breadth" and "depth" of engagement, as stated by Gregory et al. (2012)). Typologies pertaining to stakeholder analyses have been provided by Reed et al. (2009) and Black et al. (2014), while the latter present various methods for stakeholder identification and analysis. These include using methods such as focus groups, snow-ball sampling, semi-structured interviews, and expert opinion to identify stakeholders. They note however that these methods do have their limits, particularly being subject to the development team's bias during selection and requiring that the stakeholders and developers be aware of a wide-range of potential stakeholders. Alexander (2005) also explored the use of stakeholder taxonomies, i.e. classifications based on their role and relation to the project, that can be used to identify gaps in the coverage provided by stakeholders.

6.6.1.2 Prioritizing stakeholder influence and participation

Multiple researchers have recommended that stakeholders should be directly engaged and have a hand in developing the entirety of the system, from initial scoping to final evaluation (van Delden et al., 2011; Voinov and Gaddis, 2008; Voinov et al., 2016; Wu et al., 2016). Wu et al. (2016) also noted that stakeholders will become more knowledgeable about the situation and the system over time, improving the quality of feedback as the project progresses. Regarding the degree of involvement, it has been recommended that stakeholders be allowed to challenge the development of every aspect of the system (including the models) and that their feedback be integrated into the design, leading them to develop a "sense of ownership" that makes them more likely to accept the suggested results (van Delden et al., 2011; Voinov and Bousquet, 2010; Voinov and Gaddis, 2008). There is however a noted dilemma between being inclusive and selecting only a limited number of stakeholders who will likely have an influence on the system development (Reed et al., 2009), potentially marginalizing certain groups (Chambers, 1997), as well as mitigating potential problems arising from their involvement, such as a resistance to change, unrealistic expectations, miscommunications and disagreements as to the end goal, and disagreements as to the level of influence the stakeholders should have (Bano and Zowghi, 2015).

Given the importance of stakeholder involvement, it is paramount to properly define the roles and responsibilities of stakeholders within the project. To start this process, developers should aim at categorizing their stakeholders. The classification of stakeholders can generally be undertaken in one of two manners, either through analytical or reconstructive categorization (Bryson, 2004; Reed et al., 2009). Analytical categorizations are top-down methods which usually use matrices (such as the interest-influence matrices) and Venn diagrams to classify stakeholders. These methods can be useful to identify which stakeholders should be solicited based on their influence and interest in the project (those with the highest combined interest and influence should be targeted). However, these methods can let developer bias seep through, as well as leading to the marginalization of non-influential stakeholders. On the other hand, reconstructive methods are bottom-up approaches in which stakeholders can either categorize themselves or be categorized based on how their discourse fits with that of the others. This limits the influence that the developers have on the categorization, which can allow for a wider-ranging discussion and can reduce the impact of the developers' biases, but it can also lead to conflicting or incomplete categorization. Recent methods aiming to promote stakeholder identification and participatory development have also been proposed by Krupa (2016) and Basco-Carrera et al. (2017) respectively.

Following identification and categorization, it can be pertinent to identify the relationships between stakeholders. The group dynamics that arise between stakeholders can be complex, ranging from cooperative to conflicting, and must be managed to ensure efficiency. Conflict between stakeholders can be useful to bring to light certain contentious areas surrounding the development of the tool, however, when these conflicts overshadow the development process, it is necessary to work towards mitigating or resolving them. In this case, traditional conflict resolution methods such as providing a neutral ground for discussion and "negotiation" can be used, while professional facilitation might be necessary if the conflict becomes unmanageable (Grimble and Wellard, 1997; Voinov and Bousquet, 2010). Reed et al. (2009) also provide an overview of methods for investigating the relationship between stakeholders.

These methods include actor-linkage matrices, social network analysis and knowledge mapping, though we will not explore these in this paper and highly recommend that readers consult Reed et al.'s (2009) work.

6.6.1.3 Establishing a strong relationship between developers and stakeholders

Once stakeholders have been identified and their role in the project has been determined, it is necessary that developers establish and cultivate a strong relationship with them (Merritt et al., 2017). The quality of this relationship is often defined by the trust between participants and is usually brought about through transparency and credibility (Voinov et al., 2016).

Credibility is often cited as one of the main factors necessary for system uptake (Aumann, 2011; van Delden et al., 2011; Voinov et al., 2016). It is important to note that, in this context, credibility does not refer to the validity of the system or its models, but refers instead to the believability that the system can provide the expected outcome (Saunders-Newton and Scott, 2001). Credibility can stem from a few areas, including stakeholder involvement, and model and data credibility. For credibility that arises from stakeholder involvement, the main recommendation is to ensure that a diverse and representative range of stakeholders take part in the project development as early as possible, notably for problem elicitation, and all the way through the selection of models and approaches. Whereas stakeholder involvement is necessary for general system credibility, a more specific credibility is required for the models used by the system. For credibility to be achieved, transparency is necessary. To favor transparency, Liu et al. (2008) and McIntosh et al. (2011) recommend that developers be open and honest about the limitations of their system and note that they should highlight weaknesses and areas requiring improvement. Transparency is also achieved through developing a system whose logic can be followed. It is therefore of utmost importance that the stakeholders are clear on how the system operates, that is, how the models operate, where the data comes from and how the recommendations are provided.

A practical example of this in the environmental modelling field is the work of Wieland and Gutzler (2014) who used a "white box" approach to develop simple models that aimed at maximizing user understanding and transparency. The method they propose is stakeholder driven and allows for interactive simulation and development by stakeholders. They found that their simple interactive model developed through this method still had good accuracy and could then be used as a starting point for optimization and uncertainty analysis, all the while gaining more credibility from stakeholders.

Overshadowing both the issues of transparency and credibility is the need for proper communication, seeing how, without it, the prior issues cannot be properly addressed. Both van Delden et al. (2011) and McIntosh et al. (2011) stress the importance of having people onboard the project that can work towards promoting good communication between developers and stakeholders. In McIntosh et al.'s (2011) case, they focus primarily on having a champion or representative within the "targeted organisations" to maximise responsiveness and adoption of the system. Though these "champions" are rarely mentioned in EDSS literature, a recent paper by Reiter et al. (2018) noted a significant beneficial impact on user/participant satisfaction when champions were involved when comparing two case studies, one with and one without champions. In terms of communication, van Delden et al. (2011) instead bring up the vitality of having a project architect(s) onboard. The role of the architect(s) is to ensure integration, communication and management of the stakeholders, the experts and the system designers. This role is extremely important given the disparity that can arise when participants of various fields come together for a project, while bringing their own unique, and often conflicting, jargon. Robertson and Robertson (2000) also explored a few ways to engage stakeholders and mitigate bad experiences, mostly focusing on ensuring good communication and minimizing conflict. They highlight the importance of providing stakeholders with feedback and recommend using a "fit criterion" for each requirement, that is, a quantifiable measure of the requirement. They believe this would bridge the communication gap that often plagues multidisciplinary teams and would demonstrate to the stakeholders that they are being listened to and that the project is advancing in the desired direction. It is also important that communication between developers and stakeholders go in both directions, all parties must be receptive to learning from one-another (Röckmann et al., 2012).

6.6.1.4 *Eliciting the problem situation*

The final stakeholder-oriented challenge that we present pertains to problem elicitation, the literature having shown a worrying gap in this regard (Merritt et al., 2017; Sojda et al., 2012). Sojda et al. (2012), in their review of 100 environmental decision modelling papers, determined that 40% of these papers did not directly identify the decision to be addressed, while Merritt et al. (2017) also noted some gaps in problem elicitation for the 15 EDSS projects they reviewed.

The first step of problem elicitation seeks to get an understanding of the problem statement and the objective of the project. This step focuses on understanding the current situation, identifying the driving forces affecting the situation and determining the objectives of the stakeholders, as well as any uncertainties they might have regarding these objectives (Dong et al., 2013). Dong et al. (2013) propose that developers use a “storyline” approach to scope out the boundaries of their project. These storylines focus on linking the driving forces to the objectives, with any gaps in the storyline representing gaps in knowledge or data that need to be filled in until a complete and coherent story is achieved (understanding of the problem domain). In writing out these storylines, developers and stakeholders are simultaneously contributing to the development of the baseline conceptual models for the system, which can then be supplemented with more precise details as the development advances. Similarly, Gregory et al. (2012) propose decision sketching, where multiple attempts at solving the problem are undertaken to clarify and structure the problem. A recent review on the implementation of problem structuring methods for decision-making was published by Marttunen et al. (2017). As highlighted by Black et al. (2014), the development of the conceptual models should happen in tandem with the determination of system requirements. It is also pertinent to view this step as a learning experience for both the developers and the stakeholders. Indeed, the developers will oftentimes not have a full understanding of the problem situation, whereas stakeholders will not be aware of the potential functionality of the models or tools (Voinov and Bousquet, 2010). Voinov and Bousquet (2010) also recommend that, if developers dispose of a previously created model that can be applied in the current situation, they can provide it to stakeholders. This allows the latter to get a better understanding of the model so that they can start proposing modifications and highlight potential issues early in the process.

The second step focuses more specifically on identifying the factors that stakeholders consider necessary for decision-making and it is oftentimes pertinent to supplement this list with the opinion of experts. The more challenging part is to determine how these decision criteria are represented, i.e., what information are they based on (qualitative vs quantitative, type of data, etc.).

Regarding elicitation of expert knowledge and opinion, a review by Krueger et al. (2012) explored the challenges faced by developers when integrating expert opinion in environmental modelling. Note here that experts refer to “anyone with relevant and extensive or in-depth experience in relation to a topic of interest” (Krueger et al., 2012), differentiating them from stakeholders who are parties or organisations that have an influence on the development, without necessarily being an expert. These considerations include determining the type of information (qualitative, quantitative, or conceptual) that is sought and selecting the method (direct vs indirect) and setting (individual vs group) of elicitation. They note that the setting can present particular challenges due to the dynamics that can arise in either scenario, both of which can lead to unwanted biases. Indeed, individual elicitation can be biased by the preconceived notions or opinions of the interviewer (Ayyub, 2001), whereas group elicitation can be dominated by individuals and can lead to over-emphasis on consensus (Knol et al., 2010) or even groupthink (Janis, 1972). Krueger et al. (2012) discuss various elicitation methods, such as interviews and questionnaires and how to deal with uncertainty, thus we highly recommend readers consult their work.

6.6.2 Model-oriented challenges

Moving on to the second category of challenges, we have model-oriented factors. As presented in Table 1, these challenges pertain to the considerations developers should have regarding the development and implementation of the system's models.

In the environmental modelling field, literature on the development of various types of models (e.g. data models, qualitative models, quantitative models and mathematical models) (Parker et al., 2002) is abundant. Seminal research on environmental modelling has provided well-known overviews and frameworks for integrated modelling and EDSS development (Argent, 2004; Argent et al., 2009; Jakeman and Letcher, 2003; Jakeman et al., 2006; Kelly et al., 2013; Laniak et al., 2013; Schmolke et al., 2010; van Delden et al., 2011), understanding of the inherent uncertainty and methods to mitigate the associated risks (Bastin et al., 2013; Kloprogge et al., 2011; Matott et al., 2009; Warmink et al., 2010), prioritization of stakeholder involvement in the modelling process (Voinov and Bousquet, 2010; Voinov and Gaddis, 2008; Voinov et al., 2016) and validation and evaluation of models (Augusiak et al., 2014; Bennett et al., 2013; Matthews et al., 2011). However, investigations of the challenges that decision-making models deal with are notably lacking, even in the previous EDSS-centric work undertaken by McIntosh et al. (2011) and Merritt et al. (2017). As such, we will seek to address this research gap by focusing section 4.2 on decision modelling. Notable focus will be placed on multi-criteria decision-making due to its importance for decision support, as will be described in sections 4.2.2 and 4.2.5.

6.6.2.1 Understanding the type of decision to be supported

Once the problem is properly elicited, it is important for developers to understand what type of decision the problem situation requires. The type of decision will have major repercussions on the design of the system and proper understanding of this early-on can help developers determine the needs of their project. For example, decision type can impact the level of control the user should have, the type and structure of the models to be implemented, and it can help to determine the system requirements (McIntosh et al., 2005).

Decisions are often classified into one of three categories: structured (puzzles), semi-structured (problems) and unstructured (messes) decisions (Gorry and Scott Morton, 1971; Pidd, 1997).

- Structured decisions (puzzles) are made on a regular basis with all necessary data being known or acquirable. The decision formulation and the decision solution are both “agreeable”, meaning that the decision process has a well-defined structure surrounding it and there exists a specific solution. Structured decisions usually follow established guidelines (e.g.: technical, organisational, regulatory) and can be integrated into any variety of technological media to either automate them or aid in the decision process. For these reasons, structured decisions are said to be *programmable*. Such “decisions” do not require the assistance of a decision support system.
- Unstructured decisions (messes) refer to novel decisions for complex situations, which are of higher consequence than structured decisions. Both the decision formulation and solution are considered “arguable”, meaning that there is a multitude of ways to frame the decision and each way of framing the situation has a variety of possible solutions. Therefore, unstructured decisions are considered as *non-programmable*.
- Semi-structured decisions (problems) fall in the middle of structured and unstructured decisions. The decision formulation is “agreeable”, but the decision solution is “arguable”. Consequently, there are a variety of potential solutions to the clearly defined problem.

Furthermore, the aim of decision support can be to aid in choosing a unique solution, to rank several alternatives or to develop a systemic way of making a repetitive decision (Gregory et al., 2012), as will be discussed in the following sub-sections. Therefore, properly understanding the type of decision can have important repercussions on system design. Semi-structured decisions are more complex, though the focus of the system should mostly be on solution generation and analysis, whereas unstructured decisions will also require assisting users with problem formulation. Further considerations are presented by Hamouda et al. (2009) who note that EDSSs should be developed for complex situations where on-hand expertise is not available, but warn against producing systems that are applied to overly specific situations, noting that, in these cases, the investment is rarely warranted.

6.6.2.2 Selecting a decision support method

Once the developers understand the situation at hand, attention should be given to selecting the proper decision support method. Of the EDSSs and environmental decision support literature that we reviewed, four main "decision support" methods were identified. These include: 1) knowledge-based (artificial intelligence) systems (e.g. Aulinas et al., 2011; Ceccaroni, 2001; Comas et al., 2004; Dutta et al., 2014; Dym, 1985; Finlay et al., 1988; Lukasheh et al., 2001), though these have become much less numerous since the early 2000's, 2) life cycle assessments (LCAs) (e.g. Balkema et al., 2001; den Boer et al., 2007; Kalbar et al., 2016; Latawiec et al., 2017; Pasqualino et al., 2009; Turner et al., 2016; Wielgosiński et al., 2017), 3) cost benefit analyses (CBAs) (e.g. Barbier et al., 1990; Molinos-Senante et al., 2012; Molinos-Senante et al., 2010; Pearce, 1988) and 4) multi-criteria decision-making (MCDM) methods (e.g. Balkema et al., 2001; Bertanza et al., 2016; Garrido-Baserba et al., 2016; Hamouda et al., 2012; Kalbar et al., 2016; Lohri et al., 2013; Makropoulos et al., 2008; Mendes, 1994; Rahman et al., 2012; San Martin et al., 2017), echoing the results of the review of Karmperis et al. (2013) for EDSSs applied to solid waste management.

With respect to the knowledge-based approaches, these systems provide decision support, unlike LCAs and CBAs, but face major issues with their implementation. Expert-systems or rule-based systems are intended to emulate the human decision-making process, either through the use of a ruleset (conditional rules) or machine learning processes. As such, the time and effort required to develop these systems is very high and they tend to be limited in application due to their rigidity (Pick and Weatherholt, 2013). Furthermore, even when their implementation proves successful, they will likely end-up being labeled as “black boxes” (Licitra et al., 2017), which can limit the appeal and use of these systems, as will be discussed later in section 4.3.2. However, it would appear that we should be seeing a resurgence in knowledge-based approach due to machine learning methods, based on their advent for decision support in various fields (e.g. Dutta et al., 2014; Horng et al., 2017; Sharma and Virmani, 2017). It is also possible to complement a knowledge-base with MCDM methods, as was done by Castillo et al. (2017) in their EDSS for wastewater treatment selection.

Regarding life cycle assessments and cost-benefit analyses, their inadequacies stem from the fact that they are not actual decision support methods but are instead evaluation methods. LCAs and CBAs offer an evaluation of the costs or environmental impact of a scenario and can be very useful tools for project/problem assessment. However, these methods are reductionist and do not consider the complexity of decision-making, simply distilling the problem down to an environmental or economic evaluation. These assessments can be useful when coupled with actual decision support methods (e.g. Angelo et al., 2017), but they are not intrinsic decision support methods.

During the past decade, MCDM methods have become increasingly popular as models for decision support for EDSSs, and with good reason. Multi-criteria decision-making seeks to address the subjective nature of decision-making by attributing a certain importance (i.e., weight) to each influencing decision criterion. It can therefore be used to rank a set of alternatives based on the preferences of the decision-makers. This is of obvious interest, and some could say necessity, for environmental decisions, seeing how they often require balancing complex considerations from multidisciplinary fields. It is for this reason that we recommend MCDM methods for actual decision support, whereas the other alternatives mentioned above have major shortcomings in this regard.

Given the important use of MCDM methods in environmental decision support and the need to properly implement these methods, we felt it best to highlight issues surrounding their use, seeing how they are hardly ever mentioned in environmental literature. There are two main categories of MCDM methods: multi-attribute decision-making (MADM) and multi-objective decision-making (MODM), also known as multi-objective optimization or vector optimization (Deb, 2014; Kumar et al., 2017). MADM methods consist in ranking a set of predetermined alternatives (scenarios), whereas MODM methods focus on determining an optimal solution, or a set of solutions, from a large or infinite set of alternatives using objective functions. Therefore, MADM methods are discrete in nature, comparatively to MODM methods which are continuous (Zavadskas et al., 2014). These methods can also be modified to take into consideration certain types of scenarios, such as group decision-making (e.g. Zendehdel et al., 2009) or uncertain (fuzzy) situations (e.g. An et al., 2018; Dursun, 2016; Haastrup et al., 1998; Jia et al., 2016; Karimi et al., 2011; Ruiz-Padillo et al., 2016; Zhang et al., 2011).

This is where the complexity starts to arise. Developers are presented with a wide variety of MCDM methods to choose from. For MADM methods, in environmental applications, AHP (Saaty, 1977, 1980, 2008) is by far the most popular of these methods, often followed interchangeably by MAUT (Fishburn, 1970; Huber, 1974; Raiffa and Keeney, 1975), PROMETHEE (Brans and Mareschal, 2005; Brans, 1982; Mareschal et al., 1984), ELECTRE (Benayoun et al., 1966) and TOPSIS (Hwang and Yoon, 1981) as has been consistently demonstrated by multiple literature reviews (Achillas et al., 2013; Cegan et al., 2017; Goulart Coelho et al., 2017; Herva and Roca, 2013; Huang et al., 2011; Kabir et al., 2014; Kumar et al., 2017; Mardani et al., 2015). Though all MADM methods, there are significant differences between how each method operates and can be categorized (pairwise, multi-attribute utility or value functions, outranking processes, distance to ideal point methods, etc.). For a full and in-depth look at the various MADM methods, extensive reviews have been undertaken by Vaidya and Kumar (2006) for AHP, Wallenius et al. (2008) for MAUT, Behzadian et al. (2010) for PROMETHEE, Behzadian et al. (2012) for TOPSIS and Govindan and Jepsen (2016) for ELECTRE. The same abundance of choice is applicable for MODM methods, such as choosing between weighed summations, the e-constraint approach, the genetic algorithm, or a variety of other methods (Cui et al., 2017; Gunantara, 2018).

Where the choice of MCDM can become problematic is the impact this choice can potentially have on the results provided by the system. As demonstrated in the reviews by Huang et al. (2011) and Vitorino de Souza Melare et al. (2017) and by Arroyo and Molinos-Senante (2018), there is little consensus as to which method of decision-support is appropriate for any given case. The issue here is that the use of different methods can lead to different results. For example, Ren et al. (2017) used three MCDM to evaluate a problem (best worst method, TOPSIS and sum weighted method), some of which provided conflicting rankings with one-another. The authors noted that "the ranking difference among the different MCDM methods often puzzles the decision-makers, and it is usually difficult for them to make decisions due to the inconsistency among these results." Furthermore, the inconsistency between the different MCDM methods becomes ever more pronounced as the number of alternatives to be ranked increases, as well as the amount of attributes to be considered (Olson et al., 1995).

Some studies have looked into how to counteract these problems and select MCDM methods (De Montis et al., 2000, 2004; Guarini et al., 2018; Myšiak, 2006; Triantaphyllou and Mann, 1989; Yeh, 2002; Zanakis et al., 1998). However, many have concluded that these differences between MCDM methods can be beneficial to the decision-makers, forcing them to look at the problem through various lenses and giving them a better understanding of the situation and thus the reason for choosing an alternative. For these reasons, a frequent recommendation is the implementation of multiple MCDM methods to solve a decision-making problem (Ananda and Herath, 2009; Buchholz et al., 2009; Guitouni and Martel, 1998; Hobbs and Meier, 2012; Kangas and Kangas, 2005; Løken, 2007; Mysiak et al., 2005; Wang et al., 2009). Realistically, however, the implementation of some of these methods, especially the pairwise MADM methods such as AHP, which requires comparing every alternative in sets of pairs, can be time intensive. Furthermore, requiring the user go through a few of them would not be a viable recommendation for certain EDSSs. However, systems that center on aiding with longer and more complex decision scenarios could potentially benefit from the implementation of multiple MCDM methods.

6.6.2.3 Determining the simplicity of the models

Though the recommendations of the previous section might not be as clear-cut as many of the others highlighted throughout this paper, there is one factor that can potentially help with the selection of a decision method, i.e., determining model simplicity, though this is not without its own challenges. Simplify the models too much and you run the risk of losing touch with reality, whereas complex models are generally more resource intensive to develop and implement, while also being harder for users to understand, decreasing transparency.

When it comes to MCDM methods, there are two major factors that contrast with one-another: efficiency versus quality. It has been noted that simple methods are often sufficient to provide adequate decision support and that using more complex models can decrease the efficiency of decision-makers (Hajkowicz, 2008; Janssen, 2001). In both cases, Janssen (2001) and Hajkowicz (2008) noted that proper problem framing and selection of the decision criteria were more important to the success of the process than the complexity or type of method chosen. Bojórquez-Tapia et al. (2005) also found that more complex methods were problematic with users, the latter stating that the pairwise method (AHP) was a black box and thus losing trust in the system and its results. However, the researchers also found that, for those who were receptive to it, the more complex method led to a better understanding of the decision process and thus an improvement in the quality of decision-making. This can be of great value seeing how providing users with a better understanding of their problem situation and transferring knowledge has been highlighted as one of the important reasons to use EDSSs (McIntosh et al., 2011). Therefore, the main focus of developers should be on developing and implementing the least complex methods and models that provide quality results, leading to an increase in transparency and user efficiency (Hajkowicz, 2008).

6.6.2.4 Dealing with uncertainty

The environmental situations we seek to address with EDSSs are often highly complex and dependent on knowledge from various fields. However, this knowledge tends to be incomplete and can present a high degree of uncertainty. This is an issue faced by all types of models, and the impact of uncertainty is further compounded by the complexity (integration of various models) often associated to EDSSs (Jakeman and Letcher, 2003).

Multiple types of uncertainties exist, Ascough et al. (2008) having categorized them into knowledge, variability, linguistic and decision-making uncertainties. These uncertainties can arise at various steps in the development process and can stem from variations (stochastic uncertainty) or a lack of knowledge (epistemic uncertainty) in the external factors (outside of the system boundaries), the data, the models, the parameters and the system (Refsgaard et al., 2007; Walker et al., 2003; Warmink et al., 2010).

There are multiple ways to deal with uncertainty in modelling and decision support, many of which are reviewed in the works of Morgan et al. (1992), Reichert and Borsuk (2005), Refsgaard et al. (2007), Matott et al. (2009), Uusitalo et al. (2015) and Voinov et al. (2016). These include error propagation equations, expert elicitation, Monte Carlo analysis, multiple model simulation, scenario analysis and sensitivity analysis, just to name a few. Given their prevalence in environmental modelling, we will refrain from discussing these methods further in this paper and recommend that readers consult these works. No matter the method that is elected, it is important to (1) identify and describe the uncertainties (type and source), (2) propagate (and generate) them through the models and (3) determine the output uncertainty (Guillaume et al., 2012; Jakeman et al., 2006; Voinov et al., 2016).

For long-forecast decisions or situations that have outcomes that are hard to estimate, Liu et al. (2008), Maier et al. (2016) and Hamilton et al. (2019) recommend the use of scenario analysis, in which a spectrum of likely scenarios is constructed and evaluated, providing a representative range of plausible alternatives. It has also been recommended to include stakeholders in the discussion about uncertainty, getting them to both comment on the outputs most important to them (and their associated uncertainty), all the while allowing them to learn about how uncertainty is dealt with in the system (Liu et al., 2008; Voinov and Gaddis, 2008).

Similar analyses can also be applied to MCDM methods. Mustajoki and Marttunen (2017), in their comparison of various software used for MCDM in environmental process planning, highlight how methods such as sensitivity analyses can be applied to the weighing of decision criteria to demonstrate how sensitive the rankings can be to variation, noting however that this adds an extra dimension to the analysis and thus complexifies the situation for decision-makers. A similar issue had been noted previously by Mahmoud et al. (2009) who highlighted that, in certain cases, uncertainty assessments could be overwhelming and distracting to decision-makers, especially the probabilistic approaches that can lead to more uncertainty on their part.

However, despite the fervent and growing interest in dealing with uncertainty, especially given the complexity of integrated modelling and decision support, McIntosh et al. (2011) noted that decision-makers were potentially not interested in uncertainty per se, but more so in the robustness of the various alternatives. As such, they refer to the case of Amann et al. (2011) who decided to approach this concept by assessing alternatives by using the worst (most conservative) conditions instead of using a range of conditions. In a way, these works seem to mirror the earlier recommendations of implementing scenario analysis instead of sensitivity analysis for decision-making.

6.6.2.5 Dealing with variable results

Another important consideration that is lacking in EDSS literature is the potential for variable results within a single MCDM method. This issue is at the heart of proper decision-making, seeing how, as mentioned earlier, decisions are subjective in nature and thus there is no objectively right answer. Therefore, it stands to reason that presenting the decision situation in various manners could lead to differing results.

Indeed, most MCDM methods are affected by a phenomenon known as rank-reversal (Belton and Gear, 1983). This phenomenon consists in a change of ordering obtained by

MCDM methods when non-optimal alternatives are either added to or removed from the ranking process. This is due to the impact that a new alternative can have on the normalization process that is employed by a majority of MCDM methods, and is thus believed to affect most of them (Wang and Triantaphyllou, 2008; Wang and Luo, 2009).

Furthermore, there are other factors that can directly impact the result obtained by MCDM methods. These include factors such as the splitting and asymmetry bias, where the division of a decision criterion into multiple criteria can either increase the weight of this decision factor in the former or decrease it in the latter (either more or less weight is given to multiple sub-factors than the “original” factor), therefore unbalancing the intended weighing (Hämäläinen and Alaja, 2008). The number of alternatives and the number of objectives considered by the model can also cause issues (Olson et al., 1995; Salo and Hämäläinen, 1997). By increasing these factors (independently or together), the normalisation procedure can be influenced, thus leading to variable rankings. Some of the hierarchical methods (such as AHP) are also subject to varying rankings based on where the criteria fall within the multi-level structure of the hierarchy, a criterion being attributed more weight if it is placed at a higher level in the hierarchy (Jacobi and Hobbs, 2007). All of these factors can lead to variable results based on how the decision method is applied, and though different decision-makers can arrive at different results, it is undesirable for the same method to produce different results for the same decision-maker.

Though the issues so far have been methodological in nature, there are also human factors that can be problematic for decision support. Researchers have demonstrated that environmental and social criteria tend to be weighed more importantly than economic or technical objectives (Gregory et al., 2012; Keeney, 2002; Marttunen et al., 2018). There are a few potential reasons behind this phenomenon; the first being that giving higher weight to social and environmental criteria is considered as being more socially (morally) acceptable than favoring economic benefits, while a second proposed reason is that the labeling of higher-level criteria might be too abstract when compared to well-defined criteria (Hämäläinen and Alaja, 2008; Stillwell et al., 1987). Another issue to deal with is the equalizing bias, which is the tendency for decision-makers to allocate weights equally (Jacobi and Hobbs, 2007; Montibeller and Von Winterfeldt, 2015).

Though these issues have mostly been relegated from EDSS literature, most likely due to a lack of awareness, a recent analysis by Marttunen et al. (2018) sought to shed some light on the presence of these biases on real-world environmental and energy related decision analysis. Their meta-analysis concluded that these issues are indeed present in environmental applications, noting the presence of the asymmetry bias and an understatement of economic criteria, but they did not find any support for the equalizing bias in these fields. To aid in overcoming these issues, a few recommendations were provided by Marttunen et al. (2018). These include building concise and symmetric hierarchies, using interactive and iterative weight elicitation procedures and training and educating participants to avoid biases.

Given the possibility of these various phenomena leading to variable results, the main recommendation that we can make is to properly evaluate and validate the system and the decision support method to ensure that it provides reliable results (see section 5). However, it is important to ensure that this validation is not an unwitting calibration of the system to reflect the preferences of the developers (Sojda, 2007). The main issue with these challenges is that the environmental literature on these subjects is grossly lacking. As such, knowledge on how prevalent these issues are in environmental decision support and recommendations on how to deal with them are missing.

6.6.3 System-oriented challenges

Finally, we have system-oriented challenges. These challenges will stem from design considerations that are important to ensure that the users can interact and get the most from the system, representing the nexus between stakeholder and model-oriented considerations.

6.6.3.1 Providing pertinent queries and results

The first system-oriented challenge we will explore is the importance of supporting decision-makers by providing them with pertinent queries and results. This challenge stems from the human nature of the decision-makers and their cognitive limitations. Factors that can influence decision-makers include decision fatigue, an overwhelming amount of information and preference for visual aids (Baumeister et al., 2018; Speier, 2006; Uran and Janssen, 2003).

These issues are especially prevalent in cases of multi-objective optimization and spatial decision support where numerous alternatives can be provided. A prime example of this was noted by Uran and Janssen (2003) who addressed the fact that, during the late 1990’s and early 2000’s, spatial DSSs (using GIS software) were not frequently used.

One of the major limiting factors that they identified was that the many solutions generated by these systems only served to confuse the decision-makers and thus reduced the functionality of the tools. This can play into the phenomenon of decision fatigue, where a decline in decision quality occurs following extensive decision-making (Baumeister et al., 2018). Therefore, DSSs should be designed, based on the feedback of decision-makers, to avoid unnecessary and superfluous decisions. This can involve a restriction in the amount of decision criteria, the number of alternatives presented and avoiding redundancies in information.

Presenting non-relevant information or information that is not directly available to be applied to the problem at hand will also have a noted effect on the efficiency and quality of the decision support. This has to do with the cognitive fit theory of Vessey (1991) that states that if the format in which the information is presented does not match with the task, added effort must be exerted by the decision-maker to convert the information into a form that is suitable for problem solving, thus decreasing the efficiency and potential quality of the decision process. This impact on system-aided decision-making was investigated by Speier and Morris (2003) and Speier (2006), both finding that the format in which information is presented to decision-makers had a noticeable impact on system use. Indeed, Speier (2006) noted that decision-makers were more confident when using tables instead of graphs when completing certain tasks, but despite this, graphs yielded more accurate and faster results. Pertinent work on visualization methods and tools for environmental modelling and decision support have been presented by Matthies et al. (2007), Lieske (2015) and Reichert et al. (2013), while a short ten step guideline for data visualization in scientific publications was proposed by Kelleher and Wagener (2011). Though the latter focuses more on interpretability and not on decision-making, many of the concepts presented in this work are still relevant to EDSS presentation.

6.6.3.2 Communicating/understanding how the results have been achieved and their limitations

Whereas we previously emphasized the need for transparency with stakeholders, this section is an extension of how the system itself should also reflect this transparency. If developers can provide access to the models, have them be easily interpretable and provide the conceptual paths the system uses to reach its recommendations, then they reduce the risk of having the system labeled as a black box.

For example, Bertanza et al. (2016) found that experts desire to have a complete understanding of how the system operates and arrives at its recommendations, labeling the system as a “black box” at the slightest lack of transparency. This label can have major repercussions on the willingness of users to use the system. A system or model will usually be a black box in two general cases: either the user does not have access to the model-base (i.e., the system is restrictive (see section 4.3.4)) or the system is dependent on a knowledgebase (machine learning).

No matter the case, Rudin (2018) argues that it is imperative to avoid black boxes, especially for high-stakes decision-making. She highlights the importance of having a system be interpretable instead of explainable, and this regardless of the validity of the models or system, noting that explanations often leave out a lot of information and are of limited help to users. Such an issue was recently brought up by Reiter et al. (2018) who found that, despite the validity of the EDSSs they evaluated, the projects faced the hurdle of having a clear causal link between the recommendations provided by the systems and the data used to inform these recommendations.

As with any model or system, EDSSs will be subject to certain limitations. Given the need for transparency highlighted earlier, it is imperative that the system can communicate its limitations. This can simply be achieved by providing users with the range of applicability of the models and data and making clear what assumptions have been made. This, as well as how many of the factors discussed throughout this paper were addressed, can be presented through a user guide.

6.6.3.3 Producing a user-friendly system

User-friendliness is at the heart of any system. Frequent recommendations for system and model-design include having tooltips to guide the user through the system, being efficient and easy to navigate, allowing for simple installation and updating. However, there are some issues that are EDSS-centric that may not be apparent to developers. For example, Hamouda et al. (2009) noted that requiring users to alternate between modules (different model-bases or functionalities) had a harmful impact on system usability. They also recommend that EDSSs intended for wide ranges of users be highly interactive, allowing the users to add or remove certain constraints or to monitor the decision process.

Accessibility of the end-product is also highly dependent on the use of an enticing graphic user interface. Indeed, Worm et al. (2010) highlight that, when models are applied in a

DSS, the distance between the models and the end-user increases. Therefore, the users will increasingly judge the system the more complex it is and base their appreciation on the quality of the user interface. It is therefore highly recommended to get graphic designers to contribute to this stage of the project, as well as respecting industry norms and standards of design, while involving the stakeholders.

A list of design concepts and functionalities for user interfaces for integrated modelling and assessment was compiled by Harrison et al. (2013) based on the findings of previous researchers. These recommendations include having a minimal model set-up and runtimes, allowing the users to undertake various analyses while constraining them to "realistic" ranges, offering multiple methods of result visualization, and allowing exporting of model outputs for subsequent use. Furthermore, we would also like to highlight that, since EDSSs are often used by policymakers and officials, having a system that can provide the users with reports of the recommendations and information could be very helpful.

6.6.3.4 Determining appropriate system restrictiveness

The last challenge that we will explore is determining the appropriate level of system restrictiveness; that is, the amount of control/access users should be given to interact with and modify the various components of the system. This can be especially complex when systems are aimed at users of varying knowledge levels and plays a key role in having a transparent system, which can then greatly influence the willingness of participants to use it.

Indeed, system restrictiveness, or perceived restrictiveness, has been demonstrated as having an important impact on the usability of DSSs. This can translate into either diminished user satisfaction or decreased efficiency. The consensus seems to be that decision-makers benefit from being allowed to experiment with the model-base, providing them with a better understanding of the factors influencing the decisions and of the system's functionality (Chaudhry et al., 1996; McIntosh et al., 2011; Parikh et al., 2001; Pfeiffer et al., 2014; Rhee and Rao, 2008; Voinov et al., 2016), Pfeiffer et al. (2014) even finding that users preferred a minimally restrictive but more complex and hard to use system compared to a more restrictive counterpart. However, from a design perspective, this can be problematic. Beyond the added resources (costs and training) necessary to make a system more open (Rhee and Rao, 2008), there is a disparity between the actual (absolute) and perceived restrictiveness of the system. Oftentimes, perceived restrictiveness is higher than the actual restrictiveness. This has been noted as leading to a decrease in the efficiency with which the system is used (Parikh et al., 2001; Pfeiffer et al., 2014; Wang and Benbasat, 2009). Nevertheless, work on restrictiveness in both general DSS and particularly EDSS literature is greatly lacking and deserves more research.

6.6.4. Recommendations for EDSS development

Based on our review, we have compiled a list of recommendations from the literature, as well as added our own recommendations based on some of the issues we highlighted, to address the challenges identified in section 3. These results are presented in Figures 1, 2 and 3.

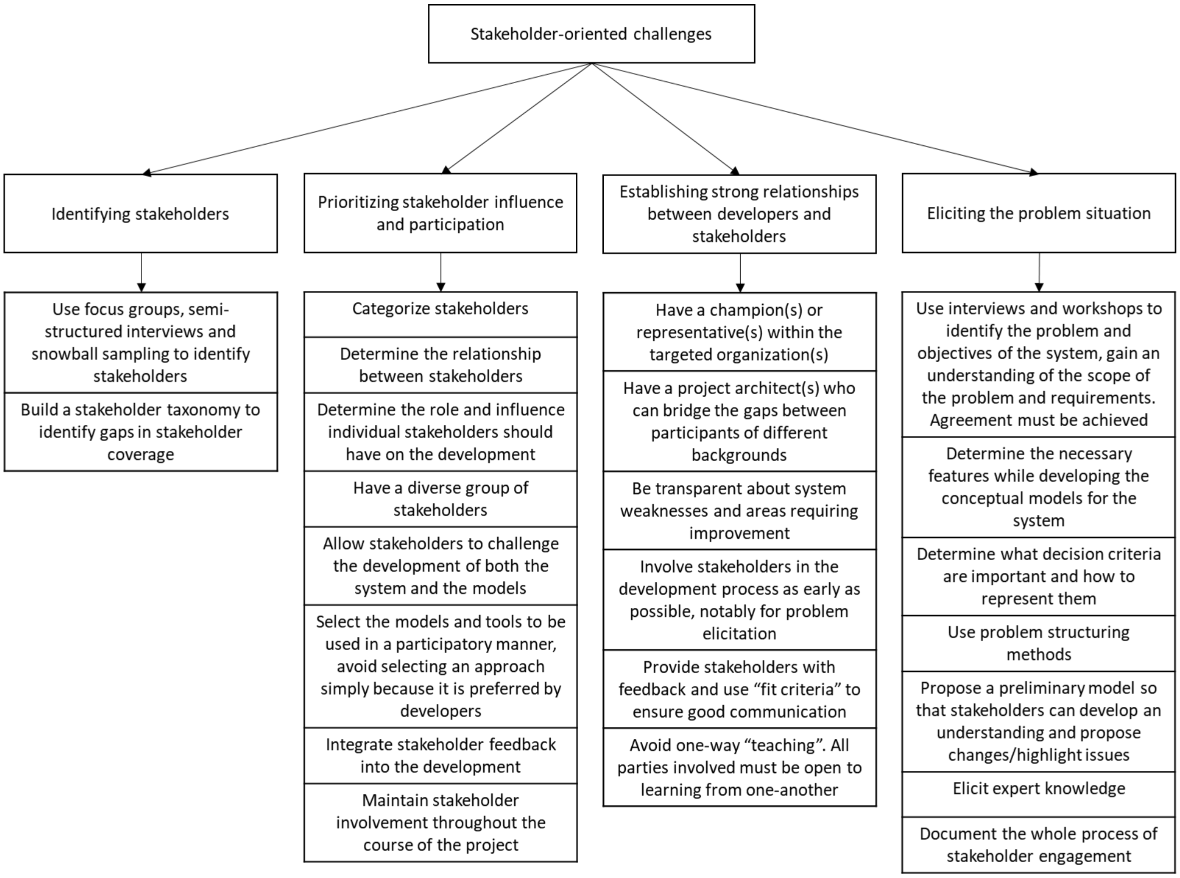


Figure 6.1 Recommendations to address stakeholder-oriented challenges.

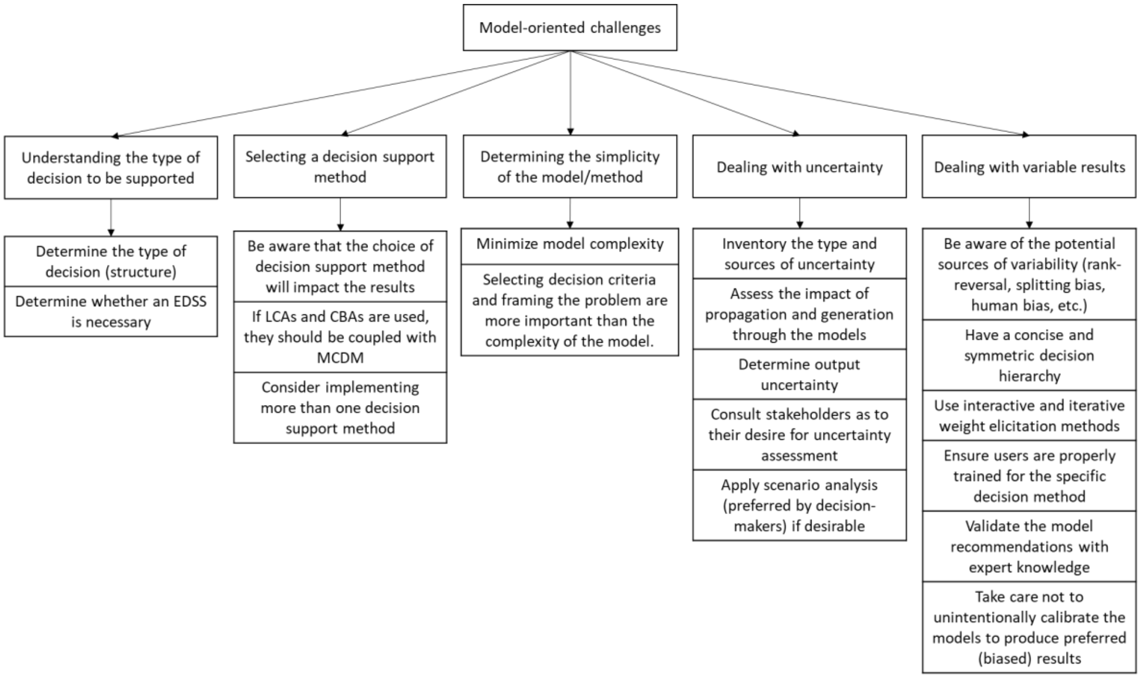


Figure 6.2 Recommendations to address model-oriented challenges.

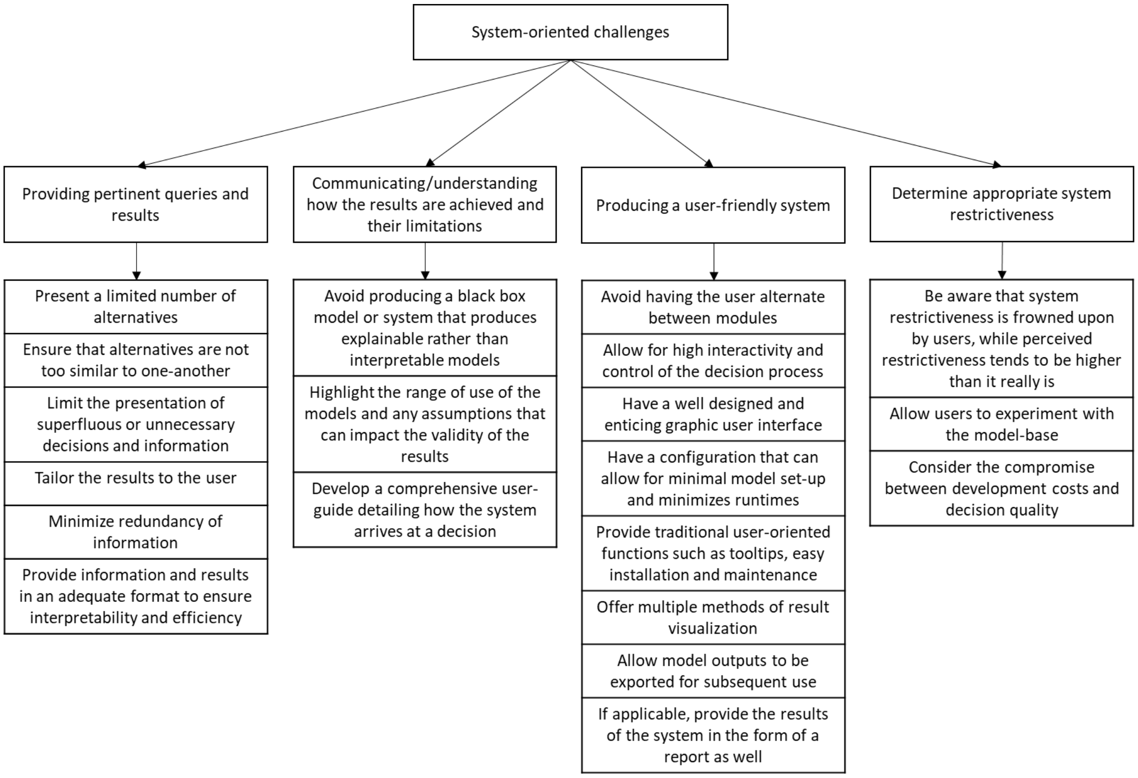


Figure 6.3 Recommendations to address system-oriented challenges.

6.7 Evaluation of EDSS

In the previous sections, we explored various challenges faced by EDSS developers and provided recommendations to address them. However, the impact of these challenges and the consequences of these recommendations can be hard to ascertain during the development process. As such, EDSS evaluation is an important step during the development process to promote project success and afterwards to gain valuable insight that can be applied to future endeavours. Yet, despite its importance, EDSS evaluation is rarely mentioned in the EDSS literature, with only a few studies on the subject (Inman et al., 2011; Sojda, 2004; Sojda, 2007) and being virtually absent in EDSSs that we examined (Ceccaroni, 2001; Chamberlain et al., 2014; Horn et al., 2003).

Multiple frameworks for DSS evaluation have been proposed over the years (Adelman, 1992; Boukhayma and ElManouar, 2015; Goeller, 1988; Hamilton et al., 2019; Inman et al., 2011; Jakeman et al., 2006; Khazanchi, 1991; Rhee and Rao, 2008), while empirical evaluation of EDSSs has also seen some interest (Sojda, 2004; Sojda, 2007). Despite these works, proper EDSS evaluation remains rare and, though these evaluation methodologies can be pertinent, the lack of clearly defined evaluation criteria appears to limit their application in a reliable manner. Certain evaluation criteria have been presented by Mysiak et al. (2005), Jakeman et al. (2006), McIntosh et al. (2011) and van Delden et al. (2011). These sources, as well as information gleaned from the previous sections, have been used to produce Figure 4.

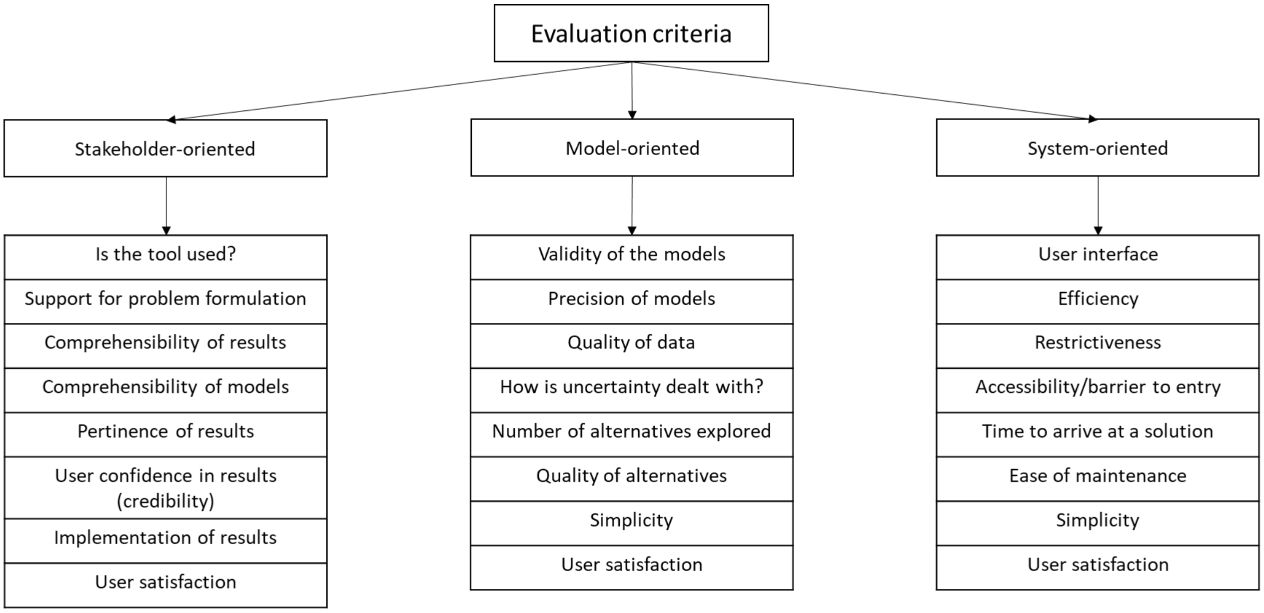


Figure 6.4 Evaluation criteria for EDSSs.

The stakeholder-oriented evaluation seeks to assess how the EDSS achieves the goals set out by the developers and the stakeholders early-on and validated throughout the design process. The most basic goal of the system is obviously to provide support for decision-makers. Other frequent goals for EDSSs, as for DSSs in general, are to increase organisational efficiency and raise awareness/understanding among decision-makers. Therefore, evaluation of the extent to which the EDSS has achieved its objectives should involve the users and stakeholders of the system. For the model-oriented evaluation, both the driving models (mathematical/knowledgebase) and the decision models used by the system are examined. This evaluation seeks to determine how valid these models are and how this can impact on the overall quality of the recommendations. The final category that we consider is the system-oriented evaluation, focusing primarily on the construction of the system and how its different components interact between each-other and with the user.

In all three categories, user-satisfaction is considered as an evaluation criterion, though it can be fickle. For example, in cases where the system provides users with a result that does not match their expectations, users will look unfavorably on the system (Potts et al., 2001), whereas the opposite can be true, regardless of the quality of the system (Rhee and Rao, 2008).

6.8 Conclusion

Following a review of the literature, a list of challenges faced by environmental decision support system developers was compiled. These challenges were categorized into stakeholder-oriented, model-oriented, and system-oriented challenges and recommendations on how to address them were presented. The aim of this paper was to supplement the work undertaken previously in this field by delving into areas that have seen little to no interest in EDSS literature, notably regarding proper decision modelling and decision theory, while updating and expanding existing knowledge on topics such as stakeholder engagement and system design. In all, 13 major challenges were identified and over 60 recommendations and best practices were provided to address these challenges.

Though environmentally focused decision support literature is rich in knowledge on modelling and system design, the limited interest (and seemingly awareness) of challenges facing decision-making are concerning. EDSSs are not simply environmental models, they have requirements that are unique to them and that deserve more attention within EDSS literature, as clearly highlighted throughout this review. Also, we cannot emphasize enough the importance of implementing a formal evaluation into the EDSS design process, both for its impact on the quality of the system and for the potential to gain invaluable knowledge for future projects.

Lastly, though we hope that this work can help provide guidance alongside the efforts of our predecessors, we believe that the production of high-quality EDSSs would greatly benefit from the creation of a detailed and formal framework to help developers with the challenges they face. Though our work has covered significant ground, it still barely scratches the surface of what the field needs. It stands to reason that this framework would far outreach the scope of a paper and should be in the form of a book or a report with the contribution of a variety of specialists from industry and academia.

Chapter 7: Novel simple approaches to modelling composting kinetics

7.1 Résumé

Durant les 40 dernières années, des modèles mathématiques ont été développés pour décrire le compostage, cherchant à faciliter sa mise en œuvre, son contrôle et son optimisation. En raison de la complexité du procédé, la capacité de simuler les cinétiques du compostage de manière simple et généralisable s'avère problématique. Ceci agit comme une limitation significative pour la prise de décision environnementale assistée par des modèles. Les modèles simples actuels ne sont pas généralisables, tandis que les modèles généralisables manquent de simplicité, nécessitant des informations sur de nombreuses variables, telles que la température, la teneur en humidité et la teneur en oxygène. Le but de ce travail est donc d'explorer l'utilisation de nouvelles approches de modélisation pour produire des modèles de compostage généralisables et simples qui ne nécessitent aucune de ces données, tout en fournissant une représentation plus précise de la biodégradation que les modèles simples actuels. Quatre méthodes de modélisation sont évaluées dans cette étude, toute basées sur une expression cinétique de premier ordre. Ces nouvelles approches de modélisation divisent la dégradation en trois phases distinctes et ne nécessitent que deux paramètres : une vitesse de dégradation et une estimation du rapport entre la durée des phases mésophiles et thermophile. Les modèles ont été évalués par leur erreur quadratique moyenne normalisée et validés sur trois ensembles de données indépendantes provenant de la littérature, couvrant un large éventail de types et de caractéristiques de déchets. Les nouvelles méthodes ont produit des erreurs variantes entre 1.13% et 6.32% et ont surpassé un modèle traditionnel de premier ordre dans tous les cas, ainsi que des modèles plus complexes dans certains cas. Les analyses de scénarios ont également démontré la résilience des approches proposées face à l'incertitude.

Mots clés : biodégradation aérobie; déchets organiques; boues d'épuration; déchets agricoles; déchets alimentaires; simulation

7.2 Abstract

Mathematical models have been developed over the past 40 years to describe the composting process, seeking to ease its implementation, control, and optimization. Due to the complex nature of composting, the ability to simulate the processes kinetics in a simple and generalizable manner has proven to be elusive, acting as a significant limitation to effective environmental, model-assisted, decision-making. Current simple models are ungeneralizable, while generalizable models lack simplicity, requiring information on many operating variables, such as temperature, moisture content, and oxygen content. The aim of this work is therefore to explore the use of novel modelling approaches to produce generalizable and simple composting models that do not require any of this data, while providing a more accurate representation of degradation than current simple models. Four modelling methods are assessed in this study, all based on a first-order kinetic expression. These novel modelling approaches split the degradation into three separate phases and only require two parameters: a degradation rate and an estimation of the ratio between the duration of the mesophilic and thermophilic phases. The models were assessed through their normalized root mean square error and validated over three independent datasets sourced from the literature, covering a wide range of waste types and characteristics. The novel methods achieved errors varying between 1.13% and 6.32% and outperformed a traditional first-order model in every case, as well as more complex models in certain cases. Scenario analyses also demonstrated the resilience of the proposed approaches to uncertainty.

Keywords: aerobic biodegradation; organic waste; sewage sludge; agricultural waste; food waste; simulation

7.3 Introduction

Given the transition towards sustainability and the expansion of circular economies, the ability to predict and optimize the outcomes of waste valorization processes, such as composting, is of primordial importance. These outcomes can include process duration, organic matter degradation, energy use, costs, environmental impact, among many others. Current composting models can indeed achieve many of these objectives, but they tend to be highly complex, requiring many interconnected equations and a large variety of parameters (Walling et al., 2020). This complexity may not be a problem for experts and highly technical work, but it can lend itself poorly to use by decision-makers, where the complex nature of these models can detract from efficient decision-making. Indeed, a recent critical review on the development of successful environmental decision support systems highlighted that model simplicity and flexibility are paramount to provide high quality decision aid (Walling and Vaneeckhaute, 2020a). This is notably due to simpler models favoring user understanding and transparency, two notions fundamental to decision-making (Hajkowicz, 2008; McIntosh et al., 2011; Wieland and Gutzler, 2014).

Regarding existing composting models, a plethora of mathematical models have been developed over the prior decades to help with the control and optimization of the composting process (Li et al., 2013; Mason, 2006; Walling et al., 2020). These models are often built around a kinetic biodegradation model, coupled with heat and mass balances to properly represent the composting environment (Walling et al., 2020). Indeed, heat and mass balances are generally required, unless experimental or in-field data are available for temperature, moisture content and oxygen content, given the impact of these variables on biodegradation (Li et al., 2013; Mason, 2006; Walling et al., 2020).

The simplest modelling approach used for composting thus far usually involves the use of a first-order kinetic expression with correction functions to adjust for the impact of different process limiting variables, as demonstrated in eq. 7.1 (Walling et al., 2020):

$$\mathrm{R_{degradation}} = -\frac{\mathrm{d[S_i]}}{\mathrm{dt}} = \mathrm{k_d f_T f_{MC} f_{O_2} [S_i]} \tag{7.1}$$

Where $\mathrm{R_{degradation}}$ is the rate of degradation (mass or concentration over time), $[\mathrm{S_i}]$ is the mass or concentration of biodegradable substrate, t is time, $\mathrm{k_d}$ is the (degradation/hydrolysis) rate constant (usually either at 20 °C or around 60 °C), and $\mathrm{f_T}$, $\mathrm{f_{MC}}$ and $\mathrm{f_{O_2}}$ are correction functions for temperature, moisture content and oxygen content (dimensionless), respectively (corrections can also be applied for pH, free airspace, and any other inhibiting variables).

The challenge with composting modelling is that the correction functions all vary as functions of time, given the change in these variables throughout the process. For example, common expressions used for these corrections include the cardinal temperature equation (eq. 7.2) (Rosso et al., 1995; Rosso et al., 1993), the Haug (1993) equation for moisture (eq. 7.3), and the Monod equation for oxygen (eq. 7.4):

$$\mathrm{f_T} = \frac{(\mathrm{T}-\mathrm{T_{max}})(\mathrm{T}-\mathrm{T_{min}})^2}{(\mathrm{T_{opt}}-\mathrm{T_{min}})\left[(\mathrm{T_{opt}}-\mathrm{T_{min}})(\mathrm{T}-\mathrm{T_{opt}})-(\mathrm{T_{opt}}-\mathrm{T_{max}})(\mathrm{T_{opt}}+\mathrm{T_{min}}-2\mathrm{T})\right]} \tag{7.2}$$

$$\mathrm{f_{MC}} = \frac{1}{\exp(-17.684\mathrm{MC}+7.0622)+1} \tag{7.3}$$

$$\mathrm{f_{O_2}} = \frac{\mathrm{O_2}}{\mathrm{O_2}+\mathrm{k_{O_2}}} \tag{7.4}$$

where T is the temperature, $\mathrm{T_{max}}$ is set to 71.6 °C, $\mathrm{T_{min}}$ is 5 °C, and $\mathrm{T_{opt}}$ is 58.6 °C (Richard and Walker, 2006), MC is the moisture content, ranging between 0 and 1, $\mathrm{O_2}$ is the oxygen content, expressed as a % v/v, and $\mathrm{k_{O_2}}$ is the oxygen half-saturation coefficient, given a value of 2% v/v following the works of Haug (1993) and Richard et al. (2006).

It is not rare to see correction functions being omitted if $\mathrm{k_d}$ is fit to the experimental data. Indeed, of the 209 models reviewed in chapter 2, 52% used first-order kinetics and 54% of the models did not implement correction functions. In many of these cases, eq. 7.1 can be integrated into a simple (inverse) exponential equation (Hamoda et al., 1998; Jolanun et al., 2005; Komilis, 2006; Nakasaki and Ohtaki, 2002; Qian et al., 2014). However, this can seriously limit the generalizability of such models, an aspect that can be very important when in a decision-making context. Ensuring the use of correction functions and general kinetic data, such as degradation rates at reference temperatures, allows for composting models to be as generalizable as possible, but also contributes to their complexity. Indeed, when correction functions are applied, eq. 7.1 must be solved by accounting for the time dependent nature of these functions, which limits its resolution to traditional numerical processes such as the finite differences approach, while requiring the necessary data for these correction functions.

Therefore, developing easily usable and generalizable composting models could provide a powerful tool for decision-makers, while addressing an important gap in composting modelling research, as identified in the most recent systematic review on the subject (Walling et al., 2020). This work therefore seeks to address this gap by focusing on two primary research questions: (1) how can the biodegradation of organic matter through composting be modelled without relying on correction functions, and (2) how do these approaches compare to the simplest existing composting models? It is therefore in this aim that novel simple modelling approaches to simulate the biodegradation of organic matter during composting are proposed and evaluated. The modelling approaches developed in this work are all based around the basic first-order equation (eq. 7.1) and seek to model the degradation process by circumventing the use of correction functions and temperature, moisture, and oxygen data, relying solely on degradation rates and process durations. In total, four methods are evaluated, with some methods having one or two different resolution approaches, resulting in the assessment of six different modelling approaches. These models were evaluated using three independent datasets taken from the literature and encompassing a wide range of feedstocks and operating conditions. The resulting outputs were then analyzed numerically using the normalized root mean square error (NRSME), as well as through scenario analyses to identify how the models react to various situations. Through this investigation, this work highlights the potential of novel simple mathematical modelling approaches for composting kinetics modelling.

This chapter is divided as follows: following the context, section 7.4 presents the materials and methods used to undertake this assessment, followed by a detailed presentation of the results and discussions around them in section 7.5, with concluding remarks being presented in section 7.6.

7.4 Methods

7.4.1 General assumptions

As detailed in the introduction, correction functions are a necessity to provide generalizable composting models that take into consideration the impact of the dynamic composting environment on the rate of biodegradation. One of the primary goals of this work is to develop and evaluate a modelling approach that could provide the benefits of correction functions, without requiring the modelling or data necessary to obtain these temperature, moisture, and oxygen corrections.

To achieve this, and considering the context for which these models are addressed, the following assumptions have been made: (1) it is assumed that the process is well operated, meaning that oxygen content is maintained above 10% and moisture content is maintained between 50 and 65% (Bertran et al., 2004; Haug, 2018; Richard et al., 2002; Tiquia et al., 1998). In well operated processes, oxygen and moisture content limitations are not very inhibitive, limiting growth (with respect to maximum degradation) by about 0 to 10% for each factor, within these ranges. As such, if it is assumed that the process operates within these ranges, constant correction coefficients for moisture and oxygen cannot be set. Based on the Haug (1993) moisture correction and the Monod oxygen correction, which have found strong support in the literature (Richard et al., 1999; Walling et al., 2020), these coefficients have been set at 0.9 for oxygen (c_{O_2}) and 0.95 for moisture content (c_{MC}). In cases where it is known that the process will operate outside these ranges, the correction coefficients can simply be changed accordingly, as dictated by the pertinent equations.

Regarding temperature, even well operated composting systems will see great variations in the temperature of the environment. This can lead to correction functions ranging in value from 0.2 (20% of maximum degradation) at 25 °C to 1 (100%) at 60 °C, as determined by the two most popular temperature correction functions, the cardinal temperature (Rosso et al., 1995; Rosso et al., 1993) and the Haug (1993) functions (Mason, 2008; Richard and Walker, 2006). In the continued aim of favoring simplicity, the authors therefore propose to consider these temperature corrections as step functions instead. Composting generally has a temperature profile with a consistent shape, heating up during the first few days of composting, reaching a thermophilic phase for a while and then cooling down during the passive phase of composting, as presented in Figure 1 (Abbasi et al., 2009; Tortarolo et al., 2008; Tortosa et al., 2017; Walling et al., 2019). Therefore, regarding temperature, the process can be split into three major phases: initial increase from mesophilic to thermophilic ranges, thermophilic composting, and the decrease back to mesophilic temperatures (as was seen in chapter 1) (Abbasi et al., 2009; Tortarolo et al., 2008; Tortosa et al., 2017; Walling et al., 2019). Consequently, the temperature correction could be expressed as a step function, with each step being a constant correction coefficient (c_{T_i}) representing an averaged temperature correction over these ranges, expressed as in eq. 7.5.

$$f_T \begin{cases} c_{T_1} & \text{if } 0 \leq t < t_1 \\ c_{T_2} & \text{if } t_1 \leq t < t_2 \\ c_{T_3} & \text{if } t_2 \leq t \end{cases} \tag{7.5}$$

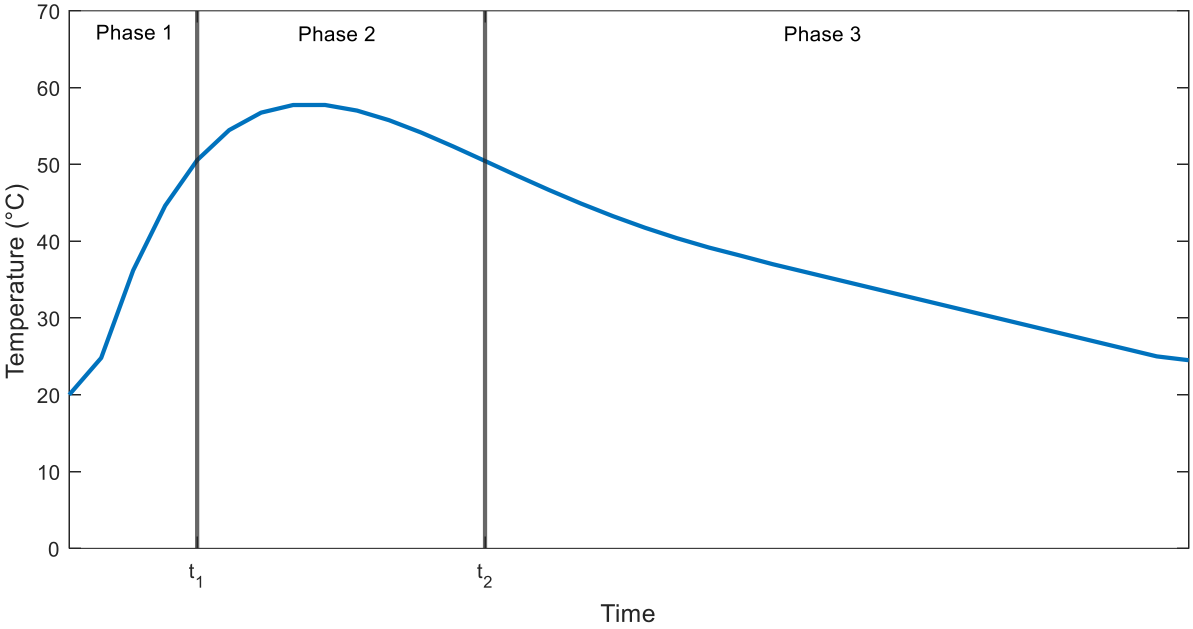


Figure 7.1 General composting temperature profile. Phase 1 represents the initial mesophilic phase of composting, while phase 2 represents the highly active thermophilic phase of the process. Phase 3 represents the passive phase of composting, where biodegradation slows down and returns to mesophilic ranges.

Therefore, using these assumptions and simplifications, the need for temperature, oxygen and moisture data can be removed, as will be described in section 7.4.2.

7.4.2 Modelling methods

An overview of the various proposed modelling approaches is presented in Table 7.1 and described below.

Table 7.1 Modelling approaches evaluated in this study.

Modelling method	**Description**	**Kinetic approaches**	**Required parameters**
Method 1a	First-order inverse exponential equation	average experimental k_d	k_d
Method 1b		optimized k_d	
Method 2a	First-order differential equation solved using finite differences	single averaged c_T	k_d
Method 2b		three phases $(c_{T,1}, c_{T,2}, c_{T,3})$	k_d, t_1, t_2
Method 3	Successive first-order inverse exponential equations fit to one-another	three phases $(c_{T,1}, c_{T,2}, c_{T,3})$	k_d, t_1, t_2
Method 4	Integrated first-order model with time dependent k_d	three phases $(c_{T,1}, c_{T,2}, c_{T,3})$	k_d, t_1, t_2

7.4.2.1 Method 1: Integrated first-order equation without time dependent k_d

Four different modelling methods were assessed in this study. Method 1 implements a traditional integrated form of the first-order equation (eq. 7.1) assuming a constant k_d:

$$S = S_0 \exp(-k_d t) \tag{7.6}$$

where S is the amount/concentration of biodegradable substrate at time t, S_0 is the initial amount/concentration of biodegradable substrate, t is the time, and k_d is the rate constant.

Two approaches were assessed for method 1: in one approach (method 1a), the average k_d of the entire process was determined based on experimental data, while in the other approach (method 1b), k_d was optimized to achieve the lowest error (discussed in section 7.4.3). The aim of both these approaches was to highlight potential differences in the accuracy of the first-order model, with the optimized k_d representing the best-case scenario, while the averaged k_d represents a more generalizable case. The approach with the optimized k_d also represents the error of the most accurate simple models that currently exist and will serve as an important comparison for the other methods.

7.4.2.2 Method 2: Finite differences

Method 2 applies the finite differences approach to a first-order equation implementing the correction coefficients. As in method 1, two approaches were also assessed for method 2. In the first approach (method 2a), a single averaged correction coefficient was used over the entire range. In the second approach (method 2b), the process was divided into three phases based on the temperature data, with each phase having a different, constant, temperature correction coefficient ($c_{T,i}$), as described previously. Though these methods are aimed at providing modelling solutions without the need for correction functions and their associated data, the authors chose to base the timing of each phase on experimental data to explore the potential accuracy of these methods, especially in comparison to an optimized first-order model (method 1). Results for applications of the models without basing the phase duration on experiments are presented in section 7.5.4.

7.4.2.3 Method 3: Successive first-order models

Method 3 takes the three-phase approach explored in method 2 and applies it with the integrated first-order equation for constant degradation rates (eq. 7.6). This method proposes to fit consecutive first-order models in series to maintain the simplicity of the first-order equation, while allowing for different kinetics over the various phases due to the different values of the temperature correction coefficient (c_T) for each phase. The resolution process is as follows:

The first phase of biodegradation is calculated by using eq. 7.7 with the correction coefficients for that phase (up to t_1). Then, a second exponential equation of the same form is used, with different values of correction coefficients. Given that during a subsequent phase only the degradation during this phase is of interest, this second equation must be fitted to have a starting time that provides the same degradation as the end of the previous phase, as described in eq. 7.8. Therefore, eq. 7.9 is solved for time and the degradation during the subsequent phase is calculated using eq. 7.10:

$$S = S_0 \exp\left(-k_d c_T c_{MC} c_{O_2} t\right) \tag{7.7}$$

$$\exp\left(-k_d c_{T,i} c_{MC,i} c_{O_2,i} t_i\right) = \exp\left(-k_d c_{T,i+1} c_{MC,i+1} c_{O_2,i+1} t_{i,i+1}\right) \tag{7.8}$$

$$t_{i,i+1} = \frac{c_{T,i} c_{MC,i} c_{O_2,i} t_i}{c_{T,i+1} c_{MC,i+1} c_{O_2,i+1}} \tag{7.9}$$

$$S = S_0 \exp\left(-k_d c_{T,i+1} c_{MC,i+1} c_{O_2,i+1}\left(t + t_{i,i+1}\right)\right) \tag{7.10}$$

where S is the amount/concentration of substrate at time t, S_0 is the initial amount/concentration of substrate, k_d is the rate constant, and $c_{T,i}, c_{MC,i}$, and $c_{O_2,i}$ are correction coefficients for the phase i (dimensionless).

This pathway is then repeated for every subsequent step of the process. Note that, in this specific case, t refers to the duration within a phase, and therefore resets to 0 at the beginning of each phase. The total composting time would therefore be a summation of the t of each phase, or t_1, t_2 and the t in phase 3.

7.4.2.4 Method 4: Integrated first-order model with time dependent k_d

The final method, method 4, uses the integrated form of eq. 7.1 by assuming that k_d is a step function over the different phases, each with their own constant correction coefficient (c_i), as expressed in eq. 7.11.

$$k_d \begin{cases} k_d c_1 & \text{if } 0 \le t < t_1 \\ k_d c_2 & \text{if } t_1 \le t < t_2 \\ k_d c_3 & \text{if } t_2 \le t \end{cases} \tag{7.11}$$

Assuming three phases, the integrated form of eq. 7.1 can be expressed as follows for the three different phases:

$$\text{Phase 1: } S = S_0 \exp(k_d(c_1 t_1)) \tag{7.10}$$

$$\text{Phase 2: } S = S_0 \exp(k_d(c_1 t_1 - c_2 t_2 + c_2 t_1)) \tag{7.11}$$

$$\text{Phase 3: } S = S_0 \exp(k_d(c_1 t_1 - c_2 t_2 + c_2 t_1 - c_3 t_3 + c_3 t_2)) \tag{7.12}$$

where S is the amount/concentration of substrate at time t, S_0 is the initial amount/concentration of substrate, k_d is the rate constant, and c_i are correction coefficients for the phase i (dimensionless), representing the production of corrections for temperature, moisture, and oxygen content.

7.4.3 Modelling assessment

The data used to undertake this modelling assessment was sourced from the works of Petric et al. (2012), Kulcu (2016), and Malamis et al. (2016). These works studied a wide range of feedstock types and operating conditions, providing a strong and independent dataset to verify the modelling approaches. Indeed, these works cover a range of size of 35 L to 4 m^3, with substrates including municipal solid waste, poultry manure, cattle manure, sheep manure, sewage sludge (primary and secondary), agricultural waste, sawdust, wheat straw, zeolite, and perlite. Of further pertinence to this study, temperature ranges between and within experimental sets were also highly variable, with ranges between 25 °C and 75 °C, with the lowest trial occurring between 25 °C and 55 °C, while the highest occurred between 45 °C and 75 °C. Initial substrate properties were also highly variable, contributing to the value of using these three datasets. Initial moisture content varied between 39 and 72%, initial organic matter varied between 62 and 87%, while initial C/N ratios were between 25 and 40. In total, 77 (11 trials x 7 models per trial) different simulations were undertaken for the initial assessment, with an added 91 simulations for the scenario analysis and 108 for the sensitivity analysis.

The quality of fit of the outputs of the models were compared quantitatively to the experimental results using a Normalized Root Mean Square Error (NRMSE) using eqs. 7.13 and 7.14:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(S_{model,i} - S_{exp,i}\right)^2}{n}} \tag{7.13}$$

$$\mathrm{NRMSE} = \frac{\mathrm{RMSE}}{S_0} \times 100 \tag{7.14}$$

where n is the amount of data points, $S_{model,i}$ is the amount of substrate predicted by the model at time i, $S_{exp,i}$ is the experimental value for substrate amount/concentration at time i, and S_0 is the initial quantity of substrate.

7.5 Results and discussion

7.5.1 Modelling results

7.5.1.1 Averaged NRMSEs over all the trials

The averaged NRMSEs for each method are presented in Table 7.2, with the results for each data set presented in Table 7.3. When looking at the averaged NRMSEs over all the trials in Table 7.2, one can start by noting that all the modelling approaches provide, on average, a low error, delivering accurate predictions for organic matter degradation over time. Indeed, the average NRMSE of the approaches assessed in this work varied from 1.86% to 4.98%, with the lowest and highest errors of individual trials being 1.13% and 11.98%, respectively.

Firstly, these results present a strong confirmation for the validity of first-order kinetic models to accurately represent biodegradation during the composting process. This has been a somewhat contentious area in the literature, with an important divide between modellers implementing first-order models (Das and Keener, 1997a; Ge et al., 2018; Zhang et al., 2010) vs Monod-type (Monod, Contois, Tessier) models (Kaiser, 1996; Sole-Mauri et al., 2007; Vidriales-Escobar et al., 2017). The main processes involved in microbial growth during composting are hydrolysis, cellular uptake, and cell death (Wang and Witarsa, 2016; Walling et al., 2020). For microorganisms to be able to absorb soluble substrates, these compounds must be made available for them. Though certain substrates (e.g., simple sugars) can be degraded easily, many of the substrates used in composting are complex and hard to degrade, such as (hemi)cellulose and lignin. Consequently, hydrolysis of these hard to degrade compounds has been believed to be the rate limiting step of the process, allowing for the accurate modelling of composting through first-order (hydrolysis) kinetics (Walling et al., 2020). Therefore, the results of this assessment seem to provide further confirmation that hydrolysis is the rate limiting process in the degradation of organic waste through composting (Jolanun et al., 2005; Sole-Mauri et al., 2007; Wang and Witarsa, 2016; Woodford, 2009).

Secondly, there are some interesting results regarding the relative performance of the models compared to one-another. One important comparison is method 1b, given that this represents the optimal case for simple models using a traditional first-order equation. Therefore, one of the main questions that this work sought to answer was whether the proposed alternative modelling approaches could outperform this commonly used method. From Table 7.2, it can be seen that the three novel modelling approaches managed to provide a lower average NRMSE than method 1b, though the NRMSE range of method 2b was comparable to method 1b, while that of methods 3 and 4 was notably lower. The only two methods that had a higher averaged percent error were the traditional first-order model using the averaged experimental $\mathrm{k_d}$ (method 1a; 4.15%) and the finite difference approach with an averaged correction coefficient (method 2a; 5.02%). These errors are likely more indicative of the errors to be expected if the models were generalized, given that they were based off general experimental degradation rates and not fit to case-specific data, which would be more likely of this kind of model application.

Of the novel modelling approaches, method 3, using the multiple first-order expression fitted to one-another in series, provided the lowest results (1.86%), though given experimental and data processing uncertainty, it appears to be on par with method 4 (integrated first-order equations with time dependent $\mathrm{k_d}$; 1.90% error). The finite differences approach using three different temperature correction coefficients for each of the three phases (method 2b) also provided a better performance than method 1b (2.61% vs 3.02%).

Table 7.2 Average NRMSE over all trials.

Modelling approach	NRMSE Range (%)	Average NRMSE (%)
Method 1a: averaged $\mathrm{k_d}$	1.94 – 8.84	4.15
Method 1b: optimized $\mathrm{k_d}$	1.86 – 6.38	3.02
Method 2a: averaged T coefficient	1.62 - 11.98	5.02
Method 2b: three phases	1.20 – 6.32	2.61
Method 3: three phases	1.13 – 3.56	1.86
Method 4: three phases	1.34 – 3.18	1.90

7.5.1.2 NRMSEs per trial

When looking at the results for each individual dataset, presented in Table 7.3, the findings mostly mirror those of Table 7.2. In the case of the data from Malamis et al. (2016), the same order is maintained, with methods 3 and 4 providing the most accurate models in every case, followed by method 2b, method 1b and then methods 1a and 2a. In the cases of data from Petric et al. (2012) and Kulcu (2016), method 2b has the lowest NRMSE in a few cases, though the results of methods 2b, 3 and 4 remain very similar. Beyond what was gleaned in section 7.5.1.1, an important takeaway of Table

7.3 is the consistently improved performance of the novel methods (2b, 3 and 4) when compared to the traditional models (methods 1a, 1b and 2a). In every trial, methods 1a and 2a are outperformed by the three proposed approaches, while method 1b, which represents the most accurate simple model currently available, is outperformed in all but two of the twelve trials.

Table 7.3 NRMSE of the individual datasets. Note that the "CF model" (correction function model) is described in section 3.1.4.

Dataset	**Modelling approach**	**NRMSE (%)**				
		Trial 1	**Trial 2**	**Trial 3**	**Trial 4**	**Average**
Malamis et al. (2016)	Method 1a	8.84	4.66	6.35	5.72	6.39
	Method 1b	6.38	3.40	4.36	4.54	4.67
	Method 2a	7.54	8.92	11.98	11.82	10.07
	Method 2b	3.17	5.00	6.32	3.41	4.48
	Method 3	3.56	1.13	1.34	2.28	2.08
	Method 4	3.18	1.64	2.41	1.97	2.3
	CF model	2.15	3.97	4.64	7.8	4.64
Kulcu (2016)	Method 1a	2.26	3.25	5.18	3.20	3.47
	Method 1b	2.11	1.87	3.13	2.01	2.28
	Method 2a	1.94	1.88	3.13	2.03	2.24
	Method 2b	1.29	1.2	2.32	1.67	1.62
	Method 3	1.38	1.25	2.4	1.43	1.62
	Method 4	1.35	1.34	2.31	1.44	1.61
Petric et al. (2012)	Method 1a	3.27	1.94	2.66		2.62
	Method 1b	2.24	1.86	2.11		2.07
	Method 2a	2.26	4.41	1.62		2.76
	Method 2b	1.88	1.56	1.82		1.75
	Method 3	2.14	1.59	1.97		1.90
	Method 4	2.12	1.63	1.62		1.79
	CF model	1.86	0.99	1.53		1.46

7.5.1.3 Numerical and visual quality of fit over different process durations

Further insight can be derived from looking at the profiles of the models compared to the experimental data, as presented in Figure 7.2, as well as a quantitative assessment of this in Table 7.4, which presents the average NRMSE of each modelling approach for three periods: days 1 to 5, 6 to 10 and 11 to the end (processes varying between 20- and 25-days, total). Both Table 7.4 and Figure 7.2 highlight the advantages of considering degradation in separate phases. In the simulations implementing methods 1, an overprediction of biodegradation during the beginning of the process can be noted, followed by an underestimation of degradation afterwards. This is to be expected, given the impact of using an invariable k_d, and reflects the reason the authors sought to explore these alternative modelling approaches. By using a constant degradation rate during the entire process, regardless of whether it is averaged or optimized, degradation will inevitably be over or underestimate at different locations. For example, if a maximum degradation rate is used (e.g., $k_d = k_{max}$, measured around 60°C), degradation outside of thermophilic stages, notably at the beginning of the process, will be greatly overestimated. Conversely, if a degradation rate at a lower reference temperature (e.g., k_d measured at 45°C) is used, then early degradation would be overestimated, while degradation during the thermophilic phase would be greatly underestimated. This latter case is what we observe in Figure 2 when looking at the results for method 1b.

Indeed, when looking at phase 1 (days 0 to 4), it can be noted that method 1b greatly overestimates degradation when compared to the other modelling approaches. This is confirmed towards the end of this period, when experimental data shows that degradation is around 32% of biodegradable organic matter (BOM), versus the 40% predicted by method 1b. The other three methods (2b, 3 and 4), which represent the novel approaches, are all closer to the real value, varying between 29 and 32%. Moving into phase 2, method 1b still overpredicts degradation early on, while quickly starting to underpredict it around day 7. During this same time period, the other three models continue to follow the experimental curve very well, with methods 2b and 4 being particularly close, while method 3 lags behind somewhat, though it is still much more accurate than method 1b. Thus far, between phases 1 and 2, the advantages of the variable degradation rate (achieved through the correction coefficients) is clear, allowing for inhibited degradation during phase 1, followed by unrestricted degradation during phase 2, better mirroring the reality of the process. This once again comes into play at the transition between phases 2 and 3, where the degradation becomes more inhibited again and progresses slower, though the benefit might be less obvious on this relatively small timeframe given that the majority of degradation has already happened in this case, and thus everything (models and experiments) converges towards about 80% of BOM degraded.

Comparatively, in methods 2b through 4, which all demonstrated similar behaviours, the error during the early phase of composting was decreased. In some cases, degradation was even underestimated, given the slightly inhibitive moisture and oxygen coefficients used ($c_{MC} = 0.95$, $c_{O_2} = 0.90$). For example, in the case of trial 2 of Petric et al. (2012), the error could be decreased from 1.56% to 1.41% by increasing oxygen and moisture coefficients to 1 during the second phase (a period of 4 days). This can always be considered and optimized by modellers, but given the interest in as simple a modelling approach as possible, the authors believe that the trade-off of using constant moisture and oxygen coefficients outweighs the small increase in error. Furthermore, in corroboration with the earlier findings, methods 3 and 4 generally outperformed the other methods, including method 2b.

Table 7.4 Average NRMSE during early, mid and late stages of composting.

Modelling approach	**Average NRMSE (%)**		
	Days 0 to 5	**Days 6 to 10**	**Days 11 to end**
Method 1a	2.98	5.30	3.93
Method 1b	3.89	3.17	2.16
Method 2a	3.84	3.29	1.70
Method 2b	1.97	2.12	2.68
Method 3	1.77	2.15	1.59
Method 4	1.74	2.21	1.59

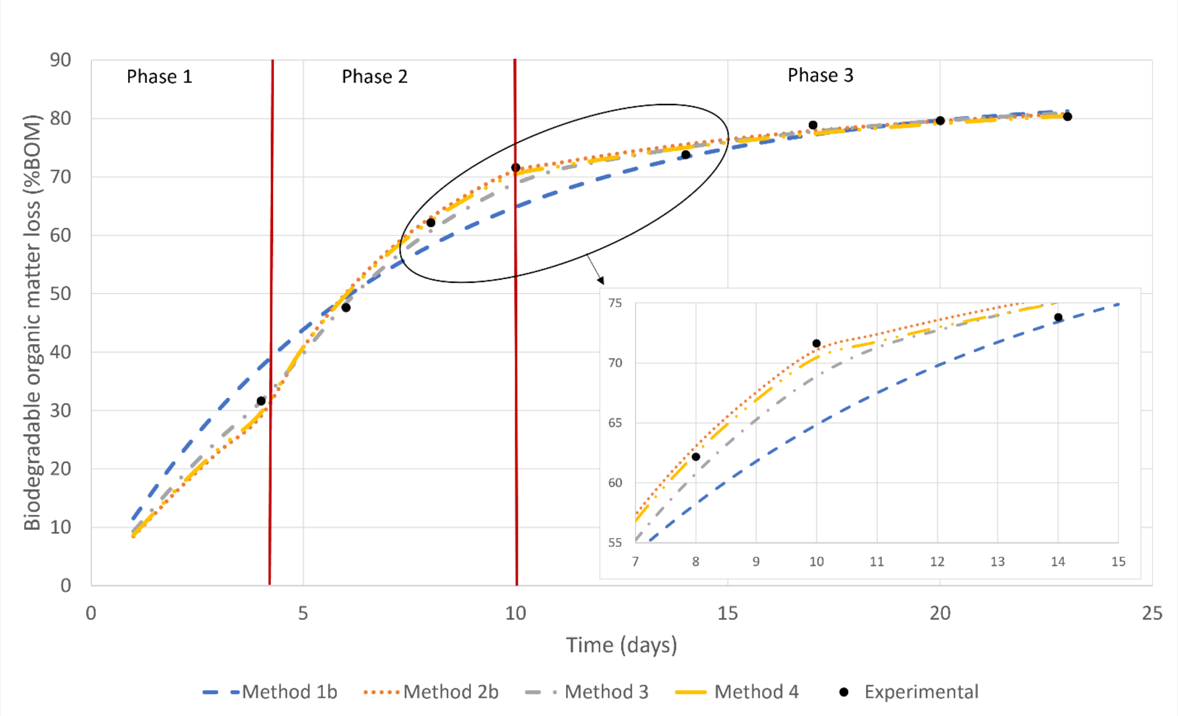


Figure 7.2 Comparison of modelling approaches with experimental data for trial 2 of Malamis et al.'s (2016) dataset. Note the ability of the proposed modelling approaches (2b through 4) to better approximate the impact of variable degradation rate when compared to method 1b.

7.5.1.4 Comparison with models implementing full correction functions

The last comparison that the authors believe is important to make is a comparison of the results of these simple models, using only degradation rates and phase duration information to those of first-order models using temperature, oxygen, and moisture correction functions (and data). The most precise version of these models, implementing eq. 1, use optimized degradation rates ($\mathrm{k_d}$) alongside the cardinal temperature or Haug (1993) models for temperature, Haug (1993) model for moisture and Monod equation for oxygen (combination found through data not presented in this work). In the aim of seeing how the novel simple models compare to these models implementing correction functions, a first-order model (eq. 7.1) with the cardinal temperature, Haug (1993) (moisture) and Monod corrections was applied, using a finite difference numerical approach. This assessment was undertaken with Petric et al.'s (2012) and Malamis et al.'s (2016) datasets, totalling in seven different trials. The results of this assessment are provided in the rows denoted as "CF model" in Table 7.3.

Of the seven trials compared, four models using the full correction functions managed to slightly outperform the simple modelling approaches with the lowest NRMSEs (one from Malamis et al. (2016) and three from Petric et al. (2012)), while three performed significantly worse (three from Malamis et al. (2016)). Of these models that outperformed the simple modelling approaches, the difference in NRMSE was small, once again pointing to the potential benefits of these new approaches. Indeed, the largest difference between a model using full correction functions with a lower NRMSE than a simple modelling approach was 0.57% (Petric et al. (2012), trial 2), with the "full" model providing an NRMSE of 0.99% vs method 2's 1.56%. On the other hand, when looking at the cases where the simple approaches outperformed the more complex ones, a much more significant difference is observed. The largest of these differences was observed in the case of trial 4 from Malamis et al. (2016), with a difference of 5.83% (1.97% method 4 vs 7.80% with full correction functions). Therefore, the modelling approaches proposed in this paper might also benefit from being less sensitive to different combinations of correction functions, which can lead to significant differences in results. For example, using the case of Malamis et al.'s (2016) trial 4, as mentioned above, the combination of correction functions led to an NRMSE of 7.80%, while the most optimal combination of correction functions led to an error of 6.71% (in this case, a combination of Haug (1993) for temperature, Stombaugh and Nokes (1996) for moisture, and Higgins and

Walker (2001) for oxygen), though this is still significantly outperformed by method 4 in this particular case.

Another possible reason for the apparent benefit of the simpler models is that the use of correction functions on such small timescales (daily variations) might further contribute to the sensitivity of the models, producing overly reactive responses. This impact can be compounded when using the traditional finite differences resolution approach, given that the degradation of each time step is dependent on that of prior steps, something that is not the case in the models of methods 3 and 4. Indeed, when implementing correction functions, a sharp increase or decrease in one of the controlling variables can relate to an equally important stimulation or inhibition of microbial activity through these methods, not taking into consideration a potential lag in the response of the system to the environmental conditions. This will be further discussed in section 7.5.4.

7.5.2 Values of the correction coefficients and time relationships

Given the central role of correction coefficients in the proposed modelling approaches, the authors thought it pertinent to investigate the values of the correction coefficients for the first and last phases, given that the second phase had a coefficient set to 1 in all trials. The mean value of the temperature correction coefficient for phase 1, $c_{T,1}$, was 0.45, with a standard deviation of 0.06. The lowest and highest observed values were 0.32 and 0.55. It is important to note, however, that not all experimental trials exhibited a first phase, with all of the experiments from Kulcu (2016) and one experiment from Petric et al. (2012) starting directly in the highly active thermophilic phase ($t_1 = 0$). For the third phase, the mean temperature correction coefficient, $c_{T,3}$, was 0.64, with a standard deviation of 0.09, and a low and high of 0.47 and 0.87. Of the processes exhibiting three phases, the mean duration of the second phase was 1.93 times longer than the first phase, with a standard deviation of 0.75. However, the authors stress that this information on timing is based on a very limited set of experimental data and is in no way intended to be a generalizable guideline; it is purely for informational purposes.

7.5.3 Sensitivity and scenario analysis

The newly proposed modelling approaches are built around the notion of splitting the degradation rate into distinct phases with different degradation rates and lengths. Therefore, uncertainty on these parameters could potentially have a significant impact on the output of the models. This is especially important given how the duration of the phases were based on experimental temperature data in this paper, something that may not be available when applying such a model. To assess this, a sensitivity analysis and scenario analyses were applied.

Regarding the sensitivity analysis, model parameters ($\mathrm{k_d}, \mathrm{c_T}, \mathrm{c_{MC}}, \mathrm{c_{O_2}}$) were varied between -75% and 400% of their initial (optimized) value, examining the impact on the NRMSE; the results of which are shown in Figure 7.3. Note that, given the mathematical form of the modelling approaches, $\mathrm{k_d}$ is always multiplied by the correction coefficients, and so the response of varying one of these parameters is the same as varying the others. Looking at Figure 7.3, we note that, despite differences in approaches, all models, including the traditional first-order model (methods 1), responded in nearly the same manner. NRMSE increased to 43% at -75% of the parameter value and decreased nearly linearly approaching 0%. The increase in error associated with increasing parameter values was quasi-logarithmic, increasing to around 6% at a 25% increase, near 16% at 100% increase and 27% at 400% increase. Of note is that methods 3 and 4 were slightly less sensitive than the first-order model (method 1), though overall, the differences were minor. Method 2 appeared to be slightly more sensitive than methods 3 and 4, likely due to the compounding of errors stemming from the finite differences resolution approach, as mentioned in section 7.5.1.4. Therefore, given the similarity in the results of the sensitivity analysis for all methods, a scenario analysis was devised to glean more information on the models.

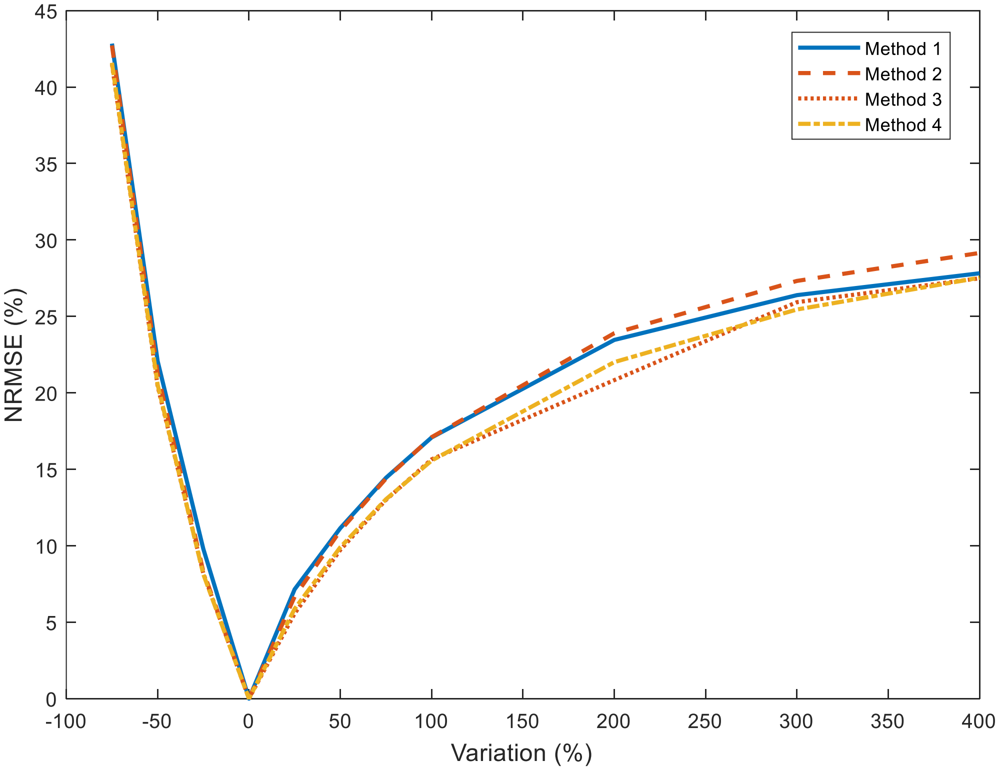


Figure 7.3 Sensitivity analysis on variations in modelling parameters $(\mathbf{k_d}, \mathbf{c_T}, \mathbf{c_{MC}}, \mathbf{c_{O_2}})$.

For the scenario analysis, to make the assessment manageable, given the large number of potential scenarios and datasets, only three of the trials were assessed: the one with the lowest NRMSE (Kulcu (2016) trial 2), the highest NRMSE (Malamis et al. (2016) trial 1), and a middle ground (Petric et al. (2012) trial 1). For these cases, the following modifications were applied: complete removal of phase 3, replacement of phase 1 with phase 2, replacement of phase 2 with phase 1, change in the timing of the phases to see whether the NRMSE could be lowered, and an increase in the duration of phase 1 or 2 of around 30%, with an equivalent decrease in the other phase. These tests were undertaken for methods 2b, 3 and 4, in every case.

In all cases, only minor differences were observed between the three methods, so the following results apply to all three, an overview of which is presented in Table 7.5. Overall, the results demonstrate the resilience of the proposed approaches, showing consistently low errors, even when faced with significant changes in timing. For example, some of the highest errors were obtained when removing phase 3, which usually accounted for more than half of the process duration. In these cases, the NRMSEs increased to between 2.94% to 7.32%, though errors on later readings were more significant, increasing to 5% to 16%. The other main source of error was the complete omission of one of the other two phases by replacing it with another (replacing phase 1/2 with the other), with errors increasing to between 2.13% to 7.52%. However, whenever the three phases were maintained, even with significant changes in timing, the errors remained relatively low and even decreased in some cases. Indeed, the highest NRMSE for this kind of scenario being 4.13% in the case of Malamis et al.'s (2016) trial 1, which is only 0.83% higher than the average of the optimal scenarios presented previously. This all points to two main conclusions: (1) the three-phased approach is beneficial to these methods, given the much more important increase in error when removing a phase; and (2) potential uncertainty in the duration of the phases may not circumvent the benefits of splitting the degradation into multiple phases, even if these phases do not completely coincide with reality. Indeed, in the latter case, when comparing the results in Tables 7.3 and 7.5, it can be noted that increasing/decreasing the first two phases still leads to a lower NRMSE than model 1b for two of the three scenarios, the exception being trial 2 of Kulcu (2016), though this also happens to be the trial with the lowest NRMSE overall.

Table 7.5 Results of the various modelling scenarios applied. Given the similarity in the values of the results, an average of the NRMSE for methods 2b, 3 and 4 is provided. In the table, P1 refers to phase 1, P2 phase 2, and P3 phase 3.

Scenario	**Average NRMSE (%)**		
	Malamis et al. (2016), trial 1	**Kulcu (2016), trial 2**	**Petric et al. (2016), trial 1**
No scenario	3.30	1.26	2.04
Remove P3	7.38	2.95	5.21
Replace P2 with P1	6.23	3.23	2.66
Replace P1 with P2	7.52	-	2.13
Modify duration	3.09	1.20	2.04
Increase P1/decrease P2	4.13	2.26	2.10
Increase P2/decrease P1	3.13	-	1.98

In the aim of further validating the resiliency of these methods and the benefits of a three-phase structure, "general" models were applied using the parameter values and timing relationships identified in section 7.5.2, the results of which are shown in Table 7.6. In this case, phase 1 was assumed to last 3 days, while phase 2 was set as being twice as long (rounding up of 1.93). The temperature correction coefficients were 0.45 for the first phase, 1 for the second, and 0.64 for the third. The results of this application using general parameters yielded good results, with the NRMSE varying between 2.13%

to 5.29%, with method 4 providing the lowest NRMSE in all three cases, though the difference in errors between the methods is very close.

Table 7.6 Results from the application of the modelling methods with the "general" parameters and time relationships identified in section 7.5.2.

Modelling approach	**NRMSE (%)**		
	Malamis et al. (2016), trial 1	**Kulcu (2016), trial 2**	**Petric et al. (2016), trial 1**
Method 2b	4.21	2.16	3.51
Method 3	5.29	2.13	2.96
Method 4	3.48	2.13	2.59

7.5.4 Model usability and limitations

All of the approaches explored and developed in this study aimed at being simple, both conceptually and regarding their numerical application. However, there are some differences between a few of the methods that could influence which one a modeller might want to implement. One of these particularities is notably regarding methods 3 and 4 when compared to methods 2/2b. Unlike methods using finite differences, these methods provide an estimation of degradation with respect to time that is in a way independent of prior degradation. In the case of methods 2/2b, the use of finite differences means that the degradation over a time interval is dependent on the amount of substrate at the beginning of the time-step and is therefore affected by prior degradation. As highlighted earlier when comparing to models implementing correction functions, this might contribute to a propagation in errors by causing an overreactive model, an issue which may be less present in methods 3 and 4 and that might offer an advantage when it comes to simple modelling.

It is also important to address the potential for under and overfitting when it comes to such simple models. Given the simplicity of the models and how they are based on first-order kinetic expressions, over-fitting was not an issue. There were fears though that the low NRMSEs obtained throughout this study could be a product of underfitting. However, this was found to not be the case through a visual comparison of data with the model outputs, as highlighted in Figure 7.2, as well as through comparison of the results of the simple models with traditional models.

Regarding limitations, it is important to once again note that these simple approaches are aimed at providing models that can give a very general idea of degradation during composting and are not intended as a fundamental representation of the biodegradation process. Indeed, following the work of chapter 6, these models are intended at being simple, approachable, and understandable. As such, these assessments have been undertaken using the aforementioned assumption that the process is well operated. It is possible that some of these assumptions might not hold true for all systems. Indeed, despite having a variable and representative range of substrates, temperature, moisture, and oxygen profiles in the experimental datasets used for this study, the models were not evaluated for extreme conditions during the process. Such conditions could be present even in well-operated systems, such as semi-batch composting, where the addition of substrate can lead to a sharp temperature decrease, or naturally aerated or windrow systems which can see more significant oxygen and moisture depletion.

7.5.5 Further research

The present work demonstrates the ability of a variety of simple mathematical approaches to model organic matter degradation during composting, without requiring temperature, oxygen or moisture content data, and their associated correction functions. However, despite the strong results provided by the simple models, further research on degradation patterns during composting would be necessary. Given the limitations highlighted in section 3.4, the main challenge for simple composting modelling is the development of generalizable models.

Being able to predict the transition between the composting phases would be of the greatest benefit, both to the models developed here and to the field of composting modelling as a whole. Given the near-inverse exponential nature of degradation, determining the duration of the earlier phases is more important when focusing on organic matter. An important part of the length of composting processes is due to curing and maturation, which are poorly understood phenomena, from a modelling perspective, and far outweigh the scope of these simple models. The advantages in applications of simple models for decision-making is that the variability of these phases can be considered in scenario analyses, which are highly recommended when modelling for decision support (Walling and Vaneeckhaute, 2020a). However, it would be interesting to establish the duration of the separate phases or if the timing of their transition can be related to other process conditions. Avenues that could potentially be explored include whether a relative rate of degradation can be associated to a change in phase (transition from more active to less active phases), or whether a relationship can be established between the duration of phases relative to one-another. Furthermore, as highlighted in section 7.5.4, separating the process into three phases appears to provide better results than a single or two-phased approach. However, further validation would be beneficial with different operating conditions. If improved performances are necessary, then it could be interesting to investigate separating the process into a few more phases, such as four or five. A separation into more phases was not investigated given that, the more phases considered, the further a model is from being "simple" and the closer it is to being a traditional model with correction functions.

In terms of application of this work, the proposed modelling approaches can provide a basis for future composting models, notably for application in decision-making scenarios where information may be lacking, or the needs for quick results and optimization may make it unfeasible to use more detailed methods. These kinetic models can also be used as a basis for simple models with a greater scope than simply predicting degradation. For example, conversion/yield factors, which are commonly used in composting modelling to relate many different phenomena to degradation, such as moisture production, oxygen consumption, gas emissions (Walling and Vaneeckhaute, 2020b), heat generation, etc. (Mason, 2006; Walling et al., 2020), could still be used to provide a wider assessment of the composting process.

7.6 Conclusion

As highlighted in the results and discussion, the novel methods provided very good estimations of the biodegradation, with the NRMSEs of these methods varying between 1.13% and 6.32% over the entirety of the datasets. These methods, notably methods 2b, 3 and 4, managed to not only provide low errors, but also ensured a better visual quality of fit with experimental data, showcasing their ability to better represent the realities of composting. These methods also managed to outperform the simplest existing kinetic models (method 1b), while also performing very closely to or significantly better than more complex models implementing correction functions for moisture content, oxygen, and temperature. Furthermore, the scenario analysis also supports the benefits of separating the degradation into three phases, instead of one or two, while demonstrating the relative resilience of the models to potential uncertainty in the timing of the phases. However, separation into more phases (four or five) was not assessed and may present potential for improvements, though it is important to balance potential benefits with the goal of simplicity in this case. Furthermore, the models also provided adequate results when using completely generalized data (i.e., non-optimized degradation rates or temperature coefficients).

Chapter 8: PCM, a parsimonious composting model for decision-making and optimization

8.1 Résumé

Dans le but de faciliter la prise de décision par l'évaluation et l'optimisation de l'opération du compostage, un modèle de compostage parcimonieux (PCM) a été développé, calibré et validé. Le modèle aborde de nombreux domaines qui ont été omis ou qui sont absents des travaux antérieurs, notamment d'une manière accessible et compréhensible. Grâce au modèle, il est possible d'obtenir des prévisions pour le ratio C/N, le carbone total (TC), l'azote total (TN), les émissions de NH_3, de N_2O, de CH_4 et de CO_2, ainsi que les propriétés physiques telles que la teneur en humidité, le volume, poids, etc. Le modèle permet également d'évaluer facilement les mélanges de compostage, le dimensionnement du procédé, ainsi que des évaluations économiques de base. Le modèle a démontré une grande précision, avec une erreur quadratique moyenne normalisée (NRMSE) variant entre 2,35 et 7,92% pour la composition solide, tandis que les estimations des émissions variaient généralement entre 1,47 et 9,48%, bien que l'estimation de la perte totale d'azote reste la facette la plus incertaine, avec un NRMSE de 25,35% sur l'ensemble de validation.

Mots clés: biodégradation aérobique; économie circulaire; modélisation; simulation; prédiction; gestion des déchets

8.2 Abstract

In the aim of facilitating decision-making through evaluation and optimization of composting operations, a parsimonious composting model (PCM) has been developed, calibrated, and validated. The model addresses many areas that have been omitted or lacking from prior works, notably in an approachable and understandable manner. Through the model, it is possible to obtain predictions for final C/N, total carbon (TC), total nitrogen (TN), NH_3, N_2O, CH_4, and CO_2 emissions, as well as physical properties such as moisture content, volume, weight, etc. The model also allows for easy evaluation of composting mixtures, process sizing, as well as the basis for economic assessments. The model has demonstrated strong accuracy, with a normalized root mean squared error (NRMSE) varying between 2.35-7.92% for solid composition, while estimates for emissions generally varied between 1.47-9.48%, though estimation of total nitrogen loss remains the most uncertain facet, with an NRMSE of 25.35% over the validation set.

Keywords: aerobic biodegradation; circular economy; modelling; simulation; prediction; waste management

8.3 Introduction

As society has shifted away from a paradigm of disposal and elimination of waste towards a model of recovery and reuse, composting has been one of the alternatives that has placed itself at the forefront of this shift. By allowing for a relatively simple and inexpensive conversion of organic waste into valuable soil amendment (compost), composting has seen itself become one of the drivers of this transition towards more sustainable and circular economies, being practiced both at industrial and individual scales (Walling et al., 2019). Currently, composting is used to treat approximately 14% of global municipal organic waste (Chen et al., 2020a), a number that will only increase as a growing number of countries and regions implement laws and directives aiming to ban landfilling, which currently represents approximately 70% of world municipal organic waste disposal (Chen et al., 2020a). Examples of such initiatives include the Landfill Directive of the European Union (EU) (EU, 1999), which has nearly eliminated landfilling in countries such as Austria, Belgium, Germany, the Netherlands and Sweden, and the recent adoption of the Circular Economy Action plan, which seeks to revise prior legislation to limit landfilling to a maximum of 10% of municipal waste by 2030. Locally, in Quebec, Canada, there is the Quebec Residual Materials Management Policy which aims to ban the landfilling and incineration of organic materials by 2022 (Hébert, 2012). Similar legislation in other countries, alongside growing social consciousness towards sustainable development and economies, has therefore placed composting as a key component of this transition.

However, organic wastes are various in sources and characteristics, each one requiring specific considerations to ensure optimal operation of composting. This variability is further compounded by the dynamic and highly variable nature of the composting process, which is defined by continually changing process variables, such as oxygen, temperature, moisture, pH, carbon to nitrogen (C/N) ratio, and chemical and biological characteristics of the waste. Given the time and effort required to evaluate composting at the laboratory and pilot scale, with results only being viable for the tested conditions, mathematical modelling has cemented itself as a powerful and necessary tool for composting process evaluation, implementation, and optimization (Walling et al., 2020). Indeed, models, when accurately developed and calibrated, can produce generalizable assessments, allowing for the rapid simulation and evaluation of various scenarios, without requiring long, costly, and tedious experimental work.

To date, a majority of composting models have focused on the fundamentals of the process, centering on biodegradation kinetics, and heat and mass balances (Mason, 2006; Walling et al., 2020). Through numerically complex models, it is possible to obtain dynamic profiles for a variety of variables, such as odor and gas emissions, temperature distribution, degradation of specific substrates, microbial populations, among many others (Walling et al., 2020). However, though such models are very useful for research or case by case process optimization, they can be problematic for decision-making. Indeed, in decision-making contexts, their complexity can detract from efficient decision-making, by rendering them hard to understand and use (Walling and Vaneeckhaute, 2020a). To favor user understanding and transparency, model flexibility and simplicity are paramount to provide high quality decision support (Hajkowicz, 2008; McIntosh et al., 2011; Walling and Vaneeckhaute, 2020a). On the other hand, most current parsimonious composting models, i.e. models that aim to provide a desired level of explanation by utilizing as few predictors as possible, lack the necessary depth to be useful for evaluation and decision-making, providing basic determination of biodegradation and process time (e.g. Nakasaki and Ohtaki, 2002; Ro et al., 2018; Walling and Vaneeckhaute, 2021b). Indeed, further consideration of factors that are primordial for decision-making, such as economic evaluations, environmental impact, and process logistics, are nearly non-existent in the literature, with only a handful of models addressing some of these issues (e.g. Proietti et al., 2016; Soto-Paz et al., 2019). Therefore, there currently exists no composting model designed around the needs of decision-makers, needs that were thoroughly identified in chapter 6, and which can provide a simple, understandable, and holistic simulation and assessment of the composting process.

Given this context and in the aim of providing approachable and usable tools for decision-makers to aid in the transition towards more circular economies, this article presents the development and application of a novel parsimonious composting model. This model seeks to provide a general and holistic evaluation of industrial composting processes at minimal computational effort. Beyond the basic considerations of most composting models, such as biodegradation and mass balances, the proposed model also includes options for evaluating composting recipes, estimates of greenhouse gas emissions and nutrient loss and transformation, process sizing, and basic economic evaluations; all of this in the aim of providing the necessary information for decision-makers.

This paper is divided as follows: materials and methods are presented in section 8.4, going in detail on the structure of the composting model, its boundaries and limitations, the assumptions and equations used throughout, the development of novel relationships, and the calibration and validation of the model using a wide set of data from the literature. Section 8.5 presents the results of the model validation through an NRMSE and global sensitivity analysis, as well as discussing model limitations and providing perspectives for future work and research, followed by a brief conclusion in section 8.6.

8.4 Materials and methods

8.4.1 Composting model

The model, named PCM (Parsimonious Composting Model), aims to a provide quick, easy to understand, accessible, and accurate evaluation of the composting process, the outputs of which can then be coupled with decision-making methods or optimization tools for use by decision-makers. The model is intended for project scoping and early assessment, as well as a certain degree of optimization, allowing for comparison between various alternatives that can be supplemented through sensitivity or scenario analyses. However, given its structure and flexibility, the model can easily be amended to fit a variety of situations. Given that environmental decision-making requires more than technical information, often necessitating economic, environmental and social considerations (Walling and Vaneeckhaute, 2020a), the model implements certain functionalities to provide general predictions for some of these areas most used by decision-makers, such as basic process sizing, general economic estimations, and greenhouse gas (GHG) emissions assessments.

The model covers the following major areas: (1) determination and optimization of composting recipes (mixture between co-substrates and/or bulking agents), (2) estimation of biodegradation and end product quality and quantity, (3) estimation of nutrient (nitrogen (N) and phosphorus (P)) loss through emissions and leaching, (4) prediction of GHG emissions, considering methane (CH_4), carbon dioxide (CO_2), and nitrogen dioxide (N_2O), and ammonia (NH_3) emissions, (5) process sizing, and (6) economic evaluation, though the latter two will not be discussed in this paper.

8.4.1.1 Model boundaries and structure

From a process perspective, the boundaries of the model extend from the mixing of the organic waste and co-substrates or bulking agents to the storage of final compost. For the time being, pre-processing steps are not included directly, such as grinding and moistening, though they are taken into account through the model inputs (section 8.4.1.2), while collection of organic matter and distribution of compost will be added in future work through coupling with a database and geographic information system (Vaneeckhaute et al., 2021). Figure 8.1 presents a conceptual overview of the model structure.

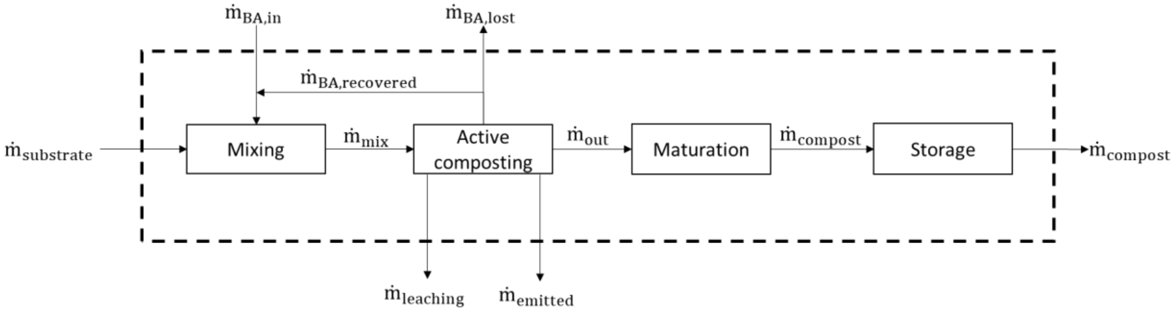


Figure 8.1 Conceptual overview of the model and its boundaries. General flow rates are presented in the figure, while the model tracts total mass (dry and wet), carbon, nitrogen, and phosphorus throughout the entire process chain.

The primary and most impactful decision on the model design has been to model the process as a steady state system, allowing for the greatest simplification by circumventing the dynamic modelling used by most composting models. Indeed, despite composting being dynamic in nature, when assessing a process, in this case a composting facility, on a long enough timescale, a steady state can be envisioned. From this perspective, and as shown in Figure 1, the composting plant can be seen as a process with substrates and bulking agents as inputs, and leachate, gaseous emissions, compost and recycled bulking agents as outputs, respective to mass. The aim of the model is not to track and predict the state of organic matter and related emissions throughout the process and at specific time intervals, but simply to determine the state of the organic matter following composting and global estimates of emissions. This, of course, does not take into consideration any variations of organic matter production over time (seasonal, peaks and lows), but such factors can be considered on their own, as will be discussed later.

8.4.1.2 Model inputs

In the aim of favoring accessibility and understanding, the composting model has been designed to use commonly known and easily obtainable inputs and parameters, given the limited information that is often available when setting up new processes or at composting facilities. As such, the different substrates of the models are defined with the following information: volumetric flow rate ($\dot{v}$), moisture content (MC), % carbon (%C) in dry matter, % nitrogen (%N) in dry matter, bulk density (ρ), degradation rate (k), and a degradable fraction of organic matter (f_d). From this information, the % organic matter (%OM) in dry matter is determined by assuming that approximately 50% of the organic matter is carbon, and thus is 2 times the %C (Pribyl, 2010). A mass flow rate ($\dot{m}$) can either be input or calculated using the volumetric flow rate and the bulk density, given the need for a mass basis in the following calculations.

8.4.1.3 Step 1: Composting recipe and preparation

The first step considered by the model is a preparation step (mixing in Figure 8.1), where the substrate(s) and potential bulking agents are mixed, providing the influent that will be used for the composting process.

During this step, the properties of this new mixture are determined:

Flow rates are combined and moisture content, % carbon, % nitrogen, C/N ratio and bulk density are determined, following the below equations (eqs. 8.1 to 8.5).

$$\mathrm{MC} = \frac{\sum(\dot{\mathrm{m}}_\mathrm{i} * \mathrm{MC}_\mathrm{i})}{\sum \dot{\mathrm{m}}_\mathrm{i}} \tag{8.1}$$

$$\%\mathrm{C} = \frac{\sum(\dot{\mathrm{m}}_\mathrm{i} * \%\mathrm{C}_\mathrm{i})}{\sum \dot{\mathrm{m}}_\mathrm{i}} \tag{8.2}$$

$$\%\mathrm{N} = \frac{\sum(\dot{\mathrm{m}}_\mathrm{i} * \%\mathrm{N}_\mathrm{i})}{\sum \dot{\mathrm{m}}_\mathrm{i}} \tag{8.3}$$

$$\mathrm{C/N} = \frac{\sum(\dot{\mathrm{m}}_\mathrm{i} * \%\mathrm{C}_\mathrm{i})}{\sum(\dot{\mathrm{m}}_\mathrm{i} * \%\mathrm{N}_\mathrm{i})} \tag{8.4}$$

$$\rho = \frac{\sum \dot{\mathrm{m}}}{\sum \dot{\mathrm{v}}} \tag{8.5}$$

where MC is moisture content (%), $\dot{\mathrm{m}}_\mathrm{i}$ is the total (wet) mass flow rate of substrate/bulking agent i (kg/d), $\%\mathrm{C}_\mathrm{i}$ is the % carbon content of substrate/bulking agent i (%), $\%\mathrm{N}_\mathrm{i}$ is the % nitrogen content of substrate/bulking agent i (%), C/N is the C/N ratio (-), and ρ is the bulk (apparent) density (kg/m^3).

At this step, the substrate and bulking agents are also deconstructed into degradable and non-degradable fractions. The degradable fraction, $\mathrm{X_{deg}}$, is the (dry) fraction of biodegradable organic matter, as described in eq. 8.6, while the non-degradable fraction, $\mathrm{X_{non-deg}}$, is the remaining dry fraction (eq. 8.7).

$$\mathrm{X_{deg,i}} = \dot{\mathrm{m}}_\mathrm{i} * \frac{\%\mathrm{OM_i}}{100} * (1 - \mathrm{MC_i}/100) * \mathrm{f_{deg,i}} \tag{8.6}$$

$$\mathrm{X_{non-deg}} = \dot{\mathrm{m}}_\mathrm{i} * (1 - \mathrm{MC_i}/100) - \mathrm{X_{deg,i}} \tag{8.7}$$

Where $\mathrm{f_{deg,i}}$ is the biodegradable fraction of organic matter (-) of substrate i.

The total flowrate of the influent (kg/d) can then be calculated using the degradable and non-degradable fractions, alongside the MC (eq. 8.8).

$$\dot{\mathrm{m}} = \frac{\sum\left(\mathrm{X_{deg,i}} + \mathrm{X_{non-deg,i}}\right)}{(1 - \mathrm{MC_i}/100)} \tag{8.8}$$

This recipe can then be optimized to try and ensure an optimal composting recipe, which is widely considered as consisting in a MC between 45 and 65, a C/N ratio between 25 and 35, and a bulk density between 300 and 700 kg/m^3 (Alberta Environment and Parks, 2018). Otherwise, outside of these ranges, there can be some detrimental or undesired impacts on the process, as will be discussed in section 8.4.1.4.

8.4.1.4 Step 2: Active composting

An overview of the active composting phase of the model is provided in Figure 8.2. Active composting, i.e., from the beginning of composting until the curing phase, is modeled through a first-order kinetic expression, as presented in eqs. 8.9 and 8.10:

$$\mathrm{X_{consumed}} = \mathrm{X_{deg,in}} - \mathrm{X_{deg,out}} = \mathrm{X_{deg,in}}(1 - \exp(-\mathrm{kt})) \tag{8.9}$$

$$\mathrm{X_{deg,out}} = \mathrm{X_{deg,in}} \exp(-\mathrm{kt}) \tag{8.10}$$

where $\mathrm{X_{consumed}}$ is the amount of substrate biodegraded (kg/d) during the process and k is the degradation rate constant (d^{-1}).

Given the aim of the model, it is assumed that the composting process is well operated, meaning that temperature is non-inhibitive (e.g., not composting at 25 °C), since modelling the impact of these parameters requires dynamic modelling, which is not the aim here. If ever oxygen is known to be inhibitive, as can be the case in naturally aerated piles, users can simply modify the degradation rate according to a Monod correction, using a half-saturation constant of 2% v/v (Haug, 1993; Richard et al., 2006; Walling and Vaneeckhaute, 2021b). Therefore, the degradation rate (k) should be measured for the "optimal" conditions described above, with the exception of temperature (Walling and Vaneeckhaute, 2021b). However, C/N ratio and moisture can have a significant impact on biodegradation. Indeed, C/N ratios above 40 are known to decrease degradation rate (Guo et al., 2012; Yan et al., 2015), given the lack of accessible nitrogen, inhibiting bacterial proliferation. As such, a switching function is implemented into the model to cut the degradation rate when outside of the optimal ranges (eq. 8.11).

$$\mathrm{X_{consumed}} = \begin{cases} \mathrm{X_{deg,in}}(1 - \exp(-\mathrm{kt})) & \text{if } \mathrm{C/N} < 40 \\ \mathrm{X_{deg,in}}(1 - \exp(-\mathrm{c_{C/N}kt})) & \text{if } \mathrm{C/N} \geq 40 \end{cases} \tag{8.11}$$

where $\mathrm{c_{C/N}}$ is a limitation on the degradation rate (-) dependent on the C/N ratio. Based on the work of Jhorar et al. (1991), we have implemented four ranges (eq. 8.12): between 40 and 60, $\mathrm{c_{C/N}}$ is equal to 0.8, meaning that 80% of optimal degradation is obtained; between 60 and 80, $\mathrm{c_{C/N}}$ is 0.7, it is 0.6 between 80 and 100, and it is 0.2 above 100.

$$\mathrm{c_{C/N}} = \begin{cases} 0.8 & \text{if } 40 \leq \mathrm{C/N} < 60 \\ 0.7 & \text{if } 60 \leq \mathrm{C/N} < 80 \\ 0.6 & \text{if } 80 \leq \mathrm{C/N} < 100 \\ 0.2 & \text{if } \mathrm{C/N} \geq 100 \end{cases} \tag{8.12}$$

Similarly, moisture contents below 40% are generally considered as being inhibitive. A variety of studies have aimed at assessing the impact of moisture on biodegradation, leading to the development of various mathematical equations to express this relationship. The most notable and commonly used examples include the models of Stombaugh and Nokes (1996) and Haug (1993); (Walling et al., 2020). Using the averaged output of both models, the following polynomial expression is used to represent the impact of MC (eq. 8.13).

$$\begin{aligned} \mathrm{MC_{limitation}} = {} & 8.246510422 * 10^{-7} * \mathrm{MC}^4 - 1.52753622 * 10^{-4} * \mathrm{MC}^3 + 0.009556 * \mathrm{MC}^2 \\ & -0.2101 * \mathrm{MC} + 1.494195 \text{ (between 20 and 70\%)} \end{aligned} \tag{8.13}$$

Below 20%, $\mathrm{MC_{limitation}}$ is given a value of 0 (completely inhibitive), while above 70%, it is given a value of 1 (non-inhibitive), independent of the type of composting system used or the type of substrate, as expressed in eq. 8.14.

$$\mathrm{X_{consumed}} = \begin{cases} \mathrm{X_{deg,in}}(1-\exp(-\mathrm{k}t)) & \text{if } \mathrm{MC} \geq 40 \\ \mathrm{X_{deg,in}}(1-\exp(-\mathrm{MC_{limitation}}\mathrm{k}t)) & \text{for } 20 \leq \mathrm{MC} < 40 \\ 0 \text{ if } \mathrm{MC} < 20 \end{cases} \tag{8.14}$$

Therefore, the equation used for degradation in the model is as follows (eq. 8.15):

$$\mathrm{X_{consumed}} = \mathrm{X_{deg,in}}\left(1-\exp\left(-\mathrm{MC_{limitation}}\mathrm{c_{C/N}}\mathrm{k}t\right)\right) \tag{8.15}$$

The same type of balances are undertaken for % carbon and nitrogen as well, but first require a consideration of the bulking agents used in the process. The main interest of bulking agents is to control moisture and density/free air space of the system, as demonstrated in eqs. 8.1 and 8.2, while adjusting the C/N ratio of the mixture. Like any organic matter, bulking agents are characterized by a wide range of biodegradability. For example, some materials have: very high biodegradability, such as cereal and cardboard (biodegradability of 70-95%), high biodegradability, such as wheat straw (biodegradability of 50% to 70%), moderate biodegradability, such as grass hay (biodegradability of 50%), and poor biodegradability, such as wood residues (biodegradability of 20% to 30%) (Loehr, 2012; Yabannavar and Bartha, 1993). Furthermore, bulking agents can be "lost" or broken down, either through mixing, compacting, or screening. Therefore, it is important to consider the balance on bulking agents throughout the process, leaving the following (eq. 8.16):

$$\dot{\mathrm{m}}_{\mathrm{BA,in}} - \dot{\mathrm{m}}_{\mathrm{BA,deg}} - \dot{\mathrm{m}}_{\mathrm{BA,lost}} = \dot{\mathrm{m}}_{\mathrm{BA,out}} \tag{8.16}$$

For the sake of simplicity and given that little research has been done on the subject, we assume that the degraded fraction of bulking agents has the same degradation rate as the substrate; the benefit from the bulking agent already being taken into account through improved composting conditions. Of the fraction that is lost ($\mathrm{X_{BA,lost}}$), it is possible that a portion could be degraded, another could remain undegraded, and another could leave the system, but the model currently assumes that it simply exits the system, with any potential degradation being simply addressed by increasing $\mathrm{X_{BA,deg}}$ and decreasing $\mathrm{X_{BA,lost}}$. The recovery of bulking agents is therefore equivalent to $\mathrm{X_{BA,out}}$, which varies for every type of bulking agent based on size and biodegradability. The range of recovery can be highly variable. Generally, considering a well operated process, highly biodegradable agents such as cardboard should not be recoverable (recovery of 0) (Itävaara et al., 1997), while poorly biodegradable substances, such as wood chips, tend to be much more recoverable, often between 60 and 90% (Wei et al., 2001), with certain agents having been designed to be as recoverable as possible (>90%).

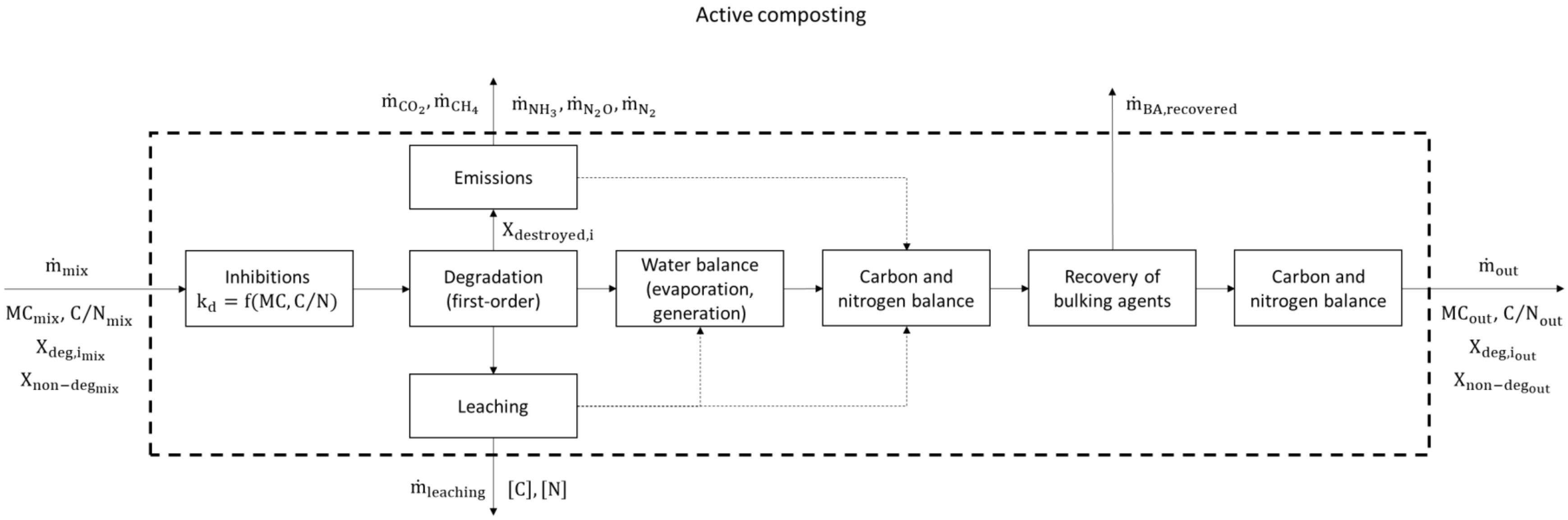


Figure 8.2 Conceptual overview of the model structure used for active composting in the model. The output of the mixing step is used as input for this section. We start with a calculation of the modified degradation rate due to potential inhibition from moisture and C/N ratio. Degradation is then determined through a first-order reaction over an input or optimized time period (t) and the amount degraded is emitted as greenhouses gases and ammonia, following the equations presented in sections 8.4.1.4.1 and 8.4.1.4.2. Leaching is a further cause of nutrient and water loss from the system. A water balance is then undertaken to determine the moisture content of the compost, using evaporation and biological water generation, alongside leaching. A carbon and nitrogen balance for the entire mixture is then calculated, followed by the removal of bulking agents, which requires the recalculation of the new nitrogen and carbon balance to determine the final C/N ratio, alongside inert and undegraded (degradable) materials.

8.4.1.4.1 Carbon emissions

Carbon loss is at the heart of the composting process, both from a technical and environmental perspective. Indeed, the main element transformed during composting is carbon, representing over 50% of the mass lost during the process (Breitenbeck and Schellinger, 2004; Hao et al., 2004). This carbon is the primary energy source for the various microorganisms in the composting environment and is mainly emitted as carbon dioxide (CO_2), with methane (CH_4) stemming from inevitable anaerobic zones in the composting environment. Therefore, carbon emissions can be directly linked to the degradation rate and we can assume that the amount of carbon emitted as both gases is equivalent to the amount of carbon degraded (Walling et al., 2020). Consequently, we can use the following equations (eqs. 8.17 and 8.18) to estimate these emissions:

$$\mathrm{CO_2} = \mathrm{X_{consumed}} * \frac{\%\mathrm{C_{degradable}}}{100} * \mathrm{CO_{2_{yield}}} * \%\text{ emitted as }\mathrm{CO_2} \tag{8.17}$$

$$\mathrm{CH_4} = \mathrm{X_{consumed}} * \frac{\%\mathrm{C_{degradable}}}{100} * \mathrm{CH_{4_{yield}}} * \%\text{ emitted as }\mathrm{CH_4} \tag{8.18}$$

where $\%\mathrm{C_{degradable}}$ is the % carbon in the substrate mixture, which is assumed to be 50%. The values of $\mathrm{CO_{2_{yield}}}$ and $\mathrm{CH_{4_{yield}}}$ are determined stoichiometrically, knowing that the decomposition of 1 kg of carbon (83 moles) will yield 3.65 kg of CO_2 or 1.33 kg of CH_4.

However, the amount of carbon emitted as CO_2 and CH_4 (%C emitted as CO_2/CH_4) can be highly variable depending on process conditions. Studies directly assessing the impact of moisture content on emissions from composting are surprisingly lacking, though recent studies have pointed to the same trend: CH_4 emissions increasing exponentially as a function of moisture content (Ermolaev et al., 2019; Xu et al., 2020). Based on data extracted from the literature, eq. 19 was obtained from a regression to describe methane emissions, as shown in Figure 3. More details on the experimental datasets used for calibration and validation will be presented in section 8.4.2.1. %CO_2 emissions are then calculated by assuming that the remainder of emissions are in the form of CO_2, as presented in eq. 8.20.

$$\%\text{ emitted as }\mathrm{CH_4} = \begin{cases} \exp(-16.6771 + 0.274338 * \mathrm{MC}) & \text{if MC} \leq 70 \\ 20 & \text{if MC} \geq 70 \end{cases} \tag{8.19}$$

$$\%\text{ emitted as }\mathrm{CO_2} = 100 - \%\text{ emitted as }\mathrm{CH_4} \tag{8.20}$$

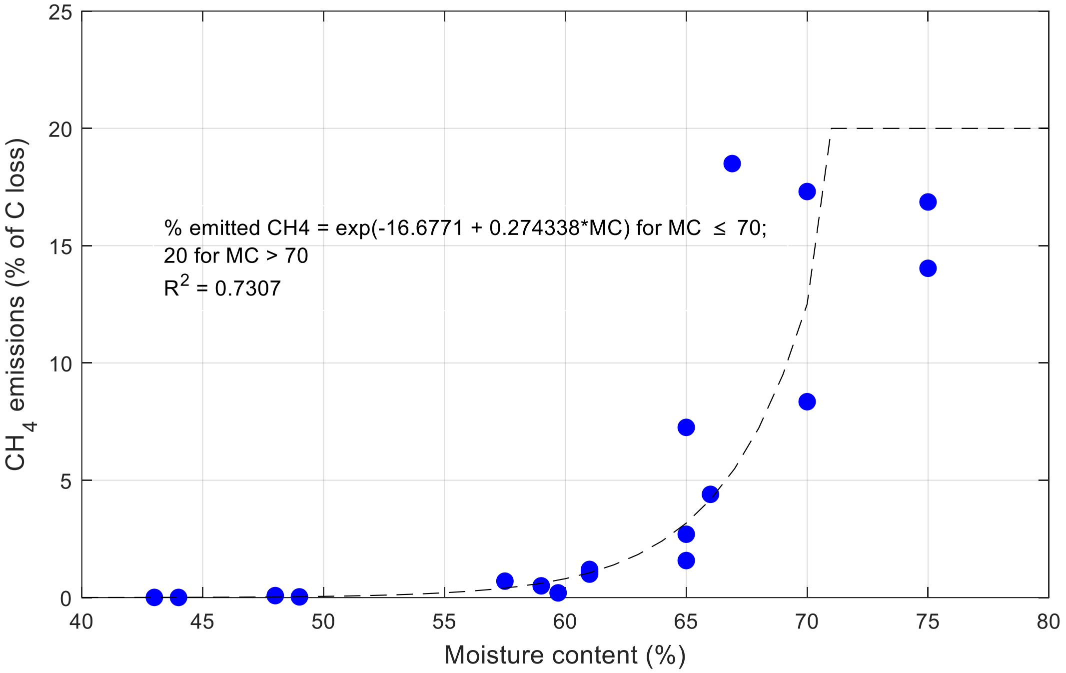


Figure 8.3 Methane emissions as a function of moisture content, based on experimental datapoints sourced from the literature.

8.4.1.4.2 Nitrogen emissions

Similarly to carbon, the main pathway for nitrogen loss during composting is through gaseous emissions, notably as ammonia (NH_3), nitrous oxide (N_2O), and nitrogen gas (N_2). Many operating variables influence the form of nitrogen emissions, such as temperature, pH, aeration rate, moisture content, and C/N ratio. The literature has once again shown a wide range of emissions, with limited guidance on the subject. Therefore, using experimental data drawn from the literature, we sought to identify potential predictors for nitrogen loss. Based on 55 datapoints (each representing a unique composting trial), discussed in section 8.4.2.1, the relationship between total nitrogen loss and other parameters, such as initial moisture, C/N ratio, NH_3, N_2O, total organic carbon (TOC) loss, and maximum temperature, were evaluated. Of the various predictors, initial moisture, initial C/N ratio, maximum temperature, and proportion of NH_3 and N_2O emissions were found to provide no predictive capabilities (R^2 varying between 0.003 to 0.11 for linear relationships). However, when applying a multivariate linear regression using TOC loss and maximum temperature as variables, an R^2 of 0.6614 was achieved based on 13 datapoints (the only points with the necessary data), as shown in Figure 4 and expressed in eq. 8.21. The fit of the relationship is far from perfect, but it is the best we could achieve without delving into more complex modelling and with the data on hand.

$$\mathrm{TN_{loss}(\%)} = 0.841126 * \mathrm{TOC_{loss}} + 0.459095 * \mathrm{T_{max}} - 49.5819 \tag{8.21}$$

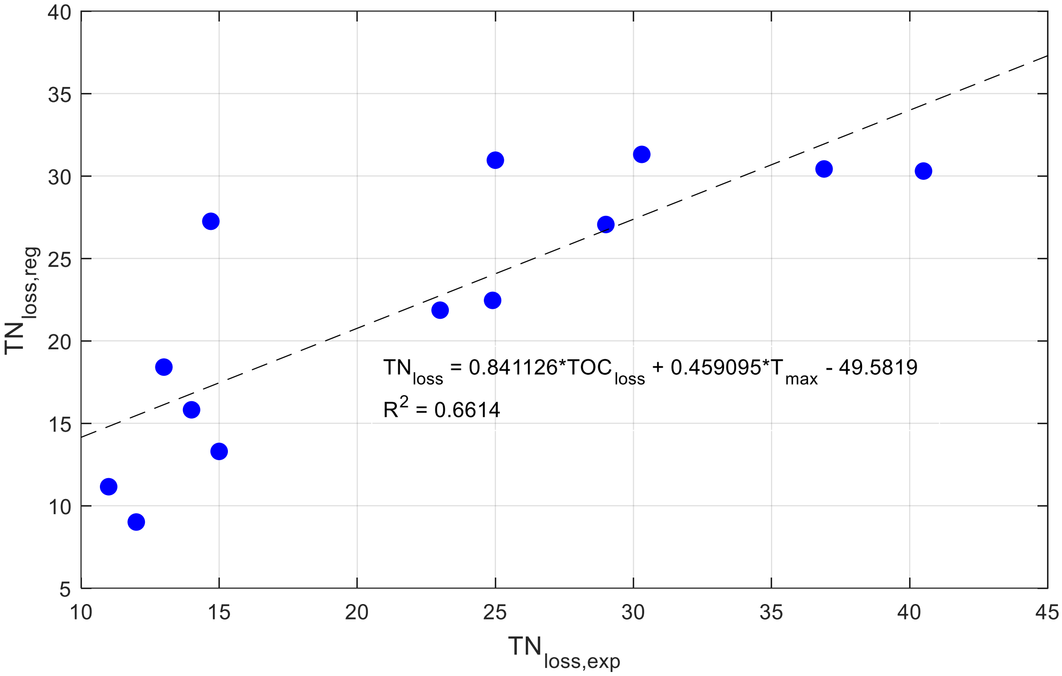


Figure 8.4 Predicted vs experimental total nitrogen loss using the multivariate linear expression obtained by regressing total nitrogen loss as a function of total organic carbon loss and maximum temperature.

This percentage can then be converted to a mass base, using the %N in the substrate mixture (eq. 8.22):

$$\mathrm{TN_{loss}(kg/d)} = \dot{\mathrm{v}} * \frac{(100 - \mathrm{MC})}{100} * \%\mathrm{N} * \frac{\mathrm{TN_{loss}(\%)}}{100} \tag{8.22}$$

From the total nitrogen loss, we then compute NH_3 and N_2O emissions. Stoichiometrically, we know that 1 kg of N (71.4 moles) yields 1.21 kg of NH_3 and 1.57 kg of N_2O, leading to the following expressions (eqs. 8.23 and 8.24):

$$\mathrm{NH_3} = \mathrm{TN_{loss}} * \%\text{ emitted as }\mathrm{NH_3} * 1.21 \tag{8.23}$$

$$\mathrm{N_2O} = \mathrm{TN_{loss}} * \%\text{ emitted as }\mathrm{N_2O} * 1.57 \tag{8.24}$$

Nitrogen emissions are also significantly affected by moisture content. Many studies have found that N_2O emissions are linearly linked (negative correlation) to moisture content (Ermolaev et al., 2019; Xu et al., 2020; Yang et al., 2019), while Wang et al. (2013a) found moisture to have the highest correlation with N_2O emissions. Building on this knowledge, we investigated the influence of moisture on N_2O emissions, based on 30 experimental trials from the calibration dataset. We chose to represent this relationship with two separate linear equations, expressed in eq. 8.25, one decreasing as moisture increases, up to a MC of 63%, where the trend reverses and emissions increase rapidly as a function of moisture, as shown in Figure 8.5.

$$\%\text{ emitted as } \mathrm{N_2O} = \begin{cases} -0.9342 * \mathrm{MC} + 59.929 & \text{if MC} < 63 \\ 3.0677 * \mathrm{MC} - 192.02 & \text{if MC} \geq 63 \end{cases} \tag{8.25}$$

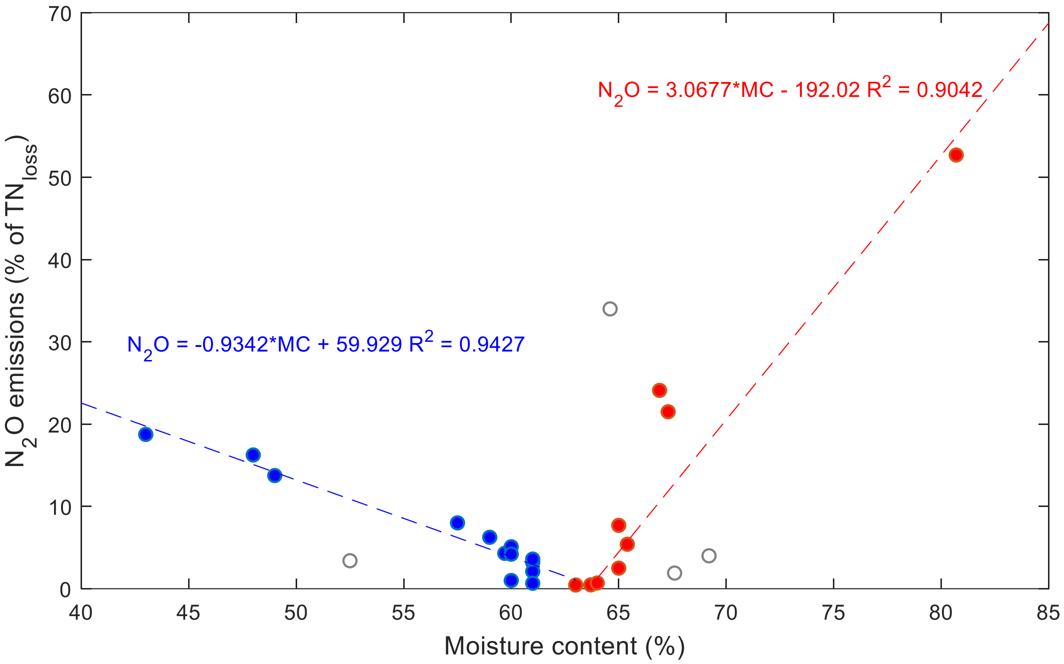


Figure 8.5 Experimental N_2O emissions as a function of initial moisture content. Between 40 and 63%, we see a negative trend, whereas this reverses and becomes positive above 63%. Grey unfilled circles were disregarded when undertaking the linear regression.

Regarding NH_3, the best predictor included in the model was found to be the maximum temperature. Based on the calibration dataset, eq. 8.26 was obtained and found to be a very good predictor of the proportion of NH_3 emissions (R^2 = 0.899). This relation is presented in Figure 8.6.

$$\%\ \text{emitted as NH}_3 = 1.7839 * \text{T}_{\text{max}} - 48.794 \tag{8.26}$$

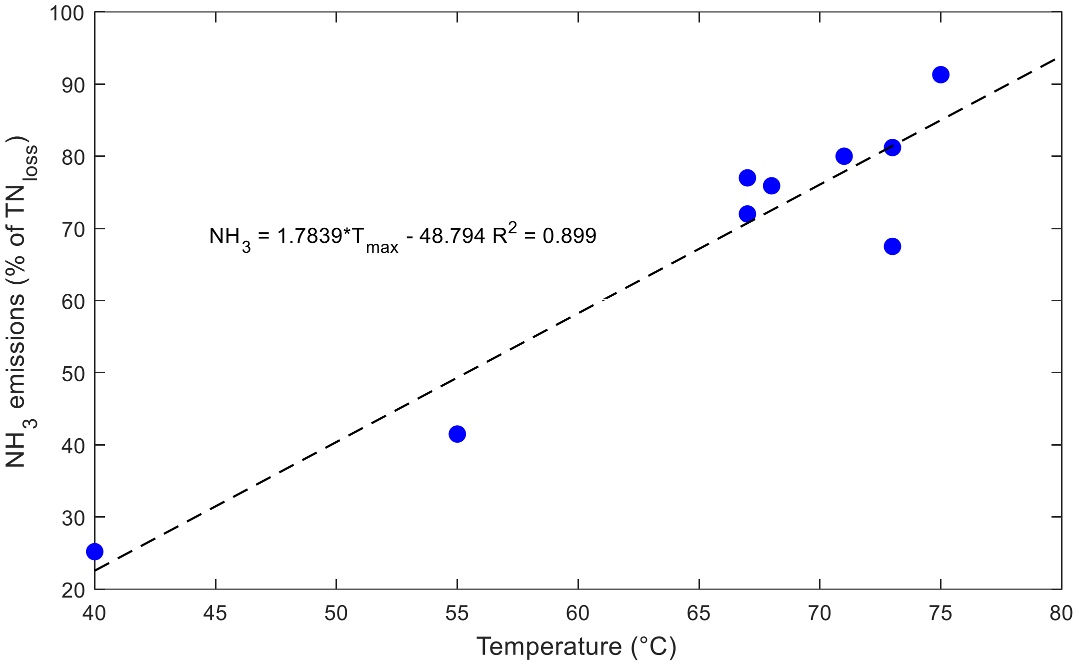


Figure 8.6 Proportion of ammonia (NH_3) emissions as a percentage of total nitrogen loss as a function of temperature.

If N_2O and NH_3 emissions do not amount to 100%, which is likely in good operating conditions, the remainder of gaseous N losses is assumed to be emitted as N_2.

8.4.1.4.5 Leaching

Leaching can be an important source of nutrient loss during composting, notably for nitrogen and phosphorus. However, the production and characterization of composting leachate is much too variable to be modeled in this situation. For example, based on Roy et al.'s (2018) review, ranges for leachate production at industrial sites treating between 1000 to 1500 tons of waste per day were between 4 and 400 m^3; while nitrogen contents of the leachates can vary by more than three orders of magnitude (Krogmann and Woyczechowski, 2000). As such, in the current model, leaching is left as a user input, where the user can either state the amount of leachate produced and its nitrogen and phosphorus content or can simply set a % N and P loss through leaching, this information then being used for water and nutrient balances. Eqs. 8.27 to 8.29 are used to determine nitrogen, phosphorus, and carbon loss through leaching:

$$N_{loss,leaching} = Leachate_{production} * N_{leachate} \tag{8.27}$$

$$P_{loss,leaching} = Leachate_{production} * P_{leachate} \tag{8.28}$$

$$C_{loss,leaching} = Leachate_{production} * C_{leachate} \tag{8.29}$$

8.4.1.4.6 Water balance

In the aim of predicting final moisture content of the compost, a global mass balance on water is applied (eq. 8.30) (Walling et al., 2020):

$$MC_{out} = \frac{\dot{m}_{in}MC_{in} + G\left(H_{A,in} - H_{A,out}\right) + Y_{H_2O}X_{destroyed} - \dot{m}_{leaching}}{\dot{m}_{out}} \tag{8.30}$$

$$H_A = 0.622\frac{H_R P_s}{P - H_R P_s} \tag{8.31}$$

$$P_s = \exp\left(A - \frac{B}{T + D}\right)P \tag{8.32}$$

Where G is the mass flowrate of air (kg air/d), $H_{A,in/out}$ are the absolute humidity at the inlet and outlet of the airflow (kg H_2O/kg air), Y_{H_2O} is the biological yield (generation) of water and is given a value of 0.4312 kg H_2O/kg of organic matter, based on (Woodford, 2009). H_R is the relative humidity of the air (-), while P_s is the pressure of saturated vapor (Pa), and P is the ambient pressure (Pa). The value of 0.622 in eq. 8.31 is the ratio of the ideal gas constant of dry air (287 J/kg.K) and vapor (461.5 J/kg.K) (Wang et al., 2015). The constants in the expression for the pressure of saturated vapor (eq. 32) in the range of composting temperatures are: A = 11.961, B = 3993.7, and D = 233.9 (Xi et al., 2005). For the relative humidity of the outlet, we assume the air is saturated, given the residence time of air in the composting environment, though this can be easily modified.

8.4.1.4.7 Output

From the information presented throughout section 8.4.1.4, the general characteristics and properties of the effluent from the active composting phase can be determined. These include the flow rates (mass and volumetric), the weight and volume reduction, the amount of carbon and nitrogen in the effluent, as well as the C/N ratio and moisture content.

For carbon and nitrogen, these are determined through a mass balance over the process, using the following equations (eqs. 8.33 and 8.34):

$$\%C_{out} = \frac{\dot{m}_{in} * (1 - MC_{in}/100) * C_{in} - X_{destroyed} * C_{degradable}}{\dot{m}_{out}(1 - MC_{out}/100)} * 100 \tag{8.33}$$

$$\%N_{out} = \frac{\dot{m}_{in} * (1 - MC_{in}/100) * N_{in} - TN_{loss,gas+leaching}}{\dot{m}_{out}(1 - MC_{out}/100)} * 100 \tag{8.34}$$

From this, we then calculate the final C and N content of the compost (eqs. 8.35 and 8.36):

$$\%C_{compost} = \frac{\dot{m}_{out} * (1 - MC_{out}/100) * C_{out} - \dot{m}_{BA,out} * C_{BA}}{\dot{m}_{compost}(1 - MC_{out}/100)} \tag{8.35}$$

$$\%N_{compost} = \frac{\dot{m}_{out} * (100 - MC_{out}) * N_{out} - \dot{m}_{BA,out} * N_{BA}}{\dot{m}_{compost}(1 - MC_{out}/100)} \tag{8.36}$$

8.4.1.5 Step 3: Maturation

The output of the active composting step is then used as the input for the final step of the process: curing. During curing, humic substances are formed by secondary reactions (condensation and polymerization of organic chains) and compost is made more suitable for agricultural application by the improvements in pH, further decrease in C/N ratio, and increased stabilization, reducing phytotoxicity (Gao et al., 2019; Wu et al., 2017; Xie et al., 2019).

Sadly, modelling of curing and maturation during composting currently presents a significant knowledge gap, so there is no available mechanistic method to predict the duration or the changes that will happen during this phase (Walling et al., 2020). The model proposes three alternatives to users: (1) the users can simply set a default duration for the curing step or, (2) a more mathematical approach can be used where a degradation rate is assumed for certain of the components over time. For example, a user could state that during this step 1% of the total carbon is expected to be emitted as CO_2 per week. However, to the best of our knowledge, no such information exists. The final option (3) would be to use a degradation rate that includes the whole process, from start to end of curing, and treat the results of the active composting model as being representative of the entire process. The output of this step can then be considered as an input for storage, during which no major change in composition should occur. Therefore, storage needs are simply calculated by considering a mass balance of compost in and compost out, over time.

8.4.2 Model calibration and validation

8.4.2.1 Calibration dataset

An extensive calibration and validation was undertaken on the model. As described throughout section 8.4.1, a large dataset of composting research was created from the literature, linking various starting properties to output properties, along with certain operating conditions, such as maximal temperature. In all, 55 experimental datapoints from 42 studies were used to calibrate the equations developed throughout the model, notably for nitrogen and CH_4 emission. Most of the studies used in the calibration dataset had been previously inventoried in the meta-analysis from Cao et al. (2019), alongside the works of Ermolaev et al. (2019) and Jiang et al. (2011).

8.4.2.1 Validation dataset

For the validation dataset, it was primordial to have a representative and diverse dataset with all the necessary data. For that reason, the literature was scoured for articles that could provide such information. Of the 13 paper initially identified, we were only capable of validating the mass balances of a small portion of these, resulting in 5 separate studies and 13 experimental trials who’s results and data were usable. The works chosen for the validation set are those of Luo et al. (2013), Shen et al. (2011), Eklind et al. (2007), Yang et al. (2013), and Mulbry and Ahn (2014). These datasets cover a range of substrates and bulking agents, including: chicken manure, corn stalks, dairy manure, dry grass, household waste, kitchen waste, pig manure, sawdust, spent mushroom substrate, and straw. Composting volumes included experiments at 60 L, 200 L, and 1900 L, with durations varying from 7 to 59 days, and total carbon losses between 32.0% and 65.1%. Aeration strategies were variable throughout the studies, including intermittent aeration, continuous aeration, and passive aeration (through weekly mixing), while moisture control was also very variable, with about half the studies maintaining constant moisture and the other half letting moisture change along with the process. Initial MCs varied from 57.5% to 66.9%, initial C/N ratios varied between 17.5 and 32.5, while maximum temperatures ranged from 40 °C to 75 °C. This variability in substrates, processes, process sizes, and operating conditions, provides a strong basis to validate the generalizability of the calibrated model.

8.4.3 Assessment of models

8.4.3.1 Quality of fit

The quality of fit of the outputs of the models were compared quantitatively to the experimental results using a Normalized Root Mean Square Error (NRMSE) using eqs. 8.37 and 38.

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(y_{\mathrm{model},i} - y_{\mathrm{exp},i}\right)^2}{n}} \tag{8.37}$$

$$\mathrm{NRMSE} = \frac{\mathrm{RSME}}{\max\left(y_{\mathrm{exp}}\right) - \min\left(y_{\mathrm{exp}}\right)} \times 100 \tag{8.38}$$

Where n is the amount of data points, $y_{\mathrm{model},i}$ is the output predicted by the model for experiment i, and $y_{\mathrm{exp},i}$ is the experimental value for output for experiment i.

8.4.3.2 Sensitivity and linear regression analyses

Global sensitivity analyses were undertaken on the model to ascertain how sensitive the various outputs are to uncertainty and to determine the impact of input variables on the model outputs. For the global analysis, the standardized regression coefficient (SRC) method was used, where the outputs of Monte Carlo simulations were fit to a linear regression. Both the Monte Carlo and linear regressions were undertaken in MATLAB, following a reprogramming of the composting model in this software. All global sensitivity analyses, which each consisted of 10000 simulations, were triplicated to assess replicability, which was found to be very high. The parameters varied during the Monte Carlo simulations were the main user inputs: moisture content, carbon and nitrogen contents, maximum temperature, degradation rate (k), and degradable fraction (f_d).

The results of the Monte Carlo simulations for the outputs of interest were then assessed as multivariate linear functions of the model factors through linear regression. These outputs include: total nitrogen loss, CH_4, NH_3, N_2O, and total emissions, final C/N ratio, moisture content, and organic matter. The aim of the multivariate linear regression was not to produce linear models, given that the composting model is purely deterministic and only a few linear relationships exist within it. The goal was instead to use the standardized regression coefficients (SRCs) of the linear models to rank the significance of their effect on the various performance indicators (i.e., the outputs mentioned above) (Vaneeckhaute et al., 2018b).

The model factors were then ranked according to the ranking thresholds presented in Table 1, taken from Vaneeckhaute et al. (2018b).

Table 8.1 Ranking thresholds based on standardized regression coefficients (SRCs) used to determine factor importance. Taken from Vaneeckhaute et al. (2018b).

Class	Cut-off threshold	Description	Importance
1	$\lvert\mathrm{SRC}\rvert > 0.1$	± 1% fraction of total variance	Very high
2	$\lvert\mathrm{tSRC}\rvert > \mathrm{t}_{\mathrm{n-p},0.95}$	Significant at the 5% confidence level	High
3	$\lvert\mathrm{tSRC}\rvert > \mathrm{t}_{\mathrm{n-p},0.90}$	Significant at the 10% confidence level	Moderate
4	$\lvert\mathrm{tSRC}\rvert > \mathrm{t}_{\mathrm{n-p},0.85}$	Significant at the 15% confidence level	Low
5	$\lvert\mathrm{tSRC}\rvert \leq \mathrm{t}_{\mathrm{n-p},0.85}$	Not significant	Very low

8.5 Results and discussion

8.5.1 Model assessment and performance

8.5.1 NRMSE analysis

The optimized models, where parameters were globally calibrated to minimize error for each specific case, were both a form of validation of the mass balances and the mathematical representation of the process, as well as a tool for initial calibration, providing insight into what relations performed adequately or needed modification. As demonstrated in Table 8.2, the calibration of the models to ensure optimization led to great results, highlighting the validity of the mass balances applied. Indeed, the NRMSE ranged from 0.98 to 3.57% for final C/N, TC, TN, and TN loss, while the absolute error over each trial varied from 0.0 to 5.7%. Discrepancies can be easily explained through data processing errors and rounding errors, especially given that the data stemmed from the literature and therefore was already somewhat manipulated beforehand. Indeed, the average absolute error for the optimized models is of 1.1%.

Following this initial step of individual calibration to achieve optimization, a global model calibration was undertaken, using the relationships developed from the literature and presented throughout section 8.4. This calibrated model was then applied to the validation set to evaluate its performance in a variety of different situations, as discussed in section 8.4.2.2. The NRMSEs of these models are also presented in Table 8.2, where we can observe a generally very strong performance. Indeed, the NRMSEs for final C/N, TC, and TN are between 2.35 and 7.92%, while, disregarding one outlier, NRMSEs for proportions of NH_3, N_2O, and CH_4 emissions varied between 1.47 and 9.48%. Given the aim of the model to provide general, quick, and easily accessible analysis, these results are extremely promising. However, estimates of total nitrogen loss remain problematic, with this relationship between the least accurate of the ones applied, as discussed in 8.4.1.4.2. Despite the NRMSE of 25.35% for TN loss being within what we consider acceptable for this type of model application, it remains high, especially when compared to the model performance on other levels. Indeed, with a more accurate prediction of total nitrogen loss, the optimization capabilities of the model would be greatly strengthened.

Table 8.2 NRMSE of the optimized and generally calibrated models.

	NRMSE (%)	
Output	**Optimized models**	**Calibrated models**
C/N	3.11	7.92
TC	3.57	3.58
TN	1.24	2.35
TN loss	0.98	25.35
NH_3-N emissions (% of nitrogen loss)	0.00	9.48
N_2O-N emissions (% of nitrogen loss)	0.00	17.87 (3.80)[a]
CH_4 emissions (% of carbon loss)	0.00	25.54 (1.47)[a]

[a] NRMSE when the results of the "CK trial" of Yang et al. (2013) are not considered, given significant N_2O (24.1%) and CH_4 (18.5%) emissions measured during this experiment.

To provide a better view of how the generally calibrated model outputs compared to experimental results, Figure 8.7 provides a comparison of both. As we can observe, the model offers very accurate predictions in most cases, while the previously mentioned outlier is clearly observable in plots e and f. One important note is that, despite the higher error in TN loss, the impact on final total nitrogen and C/N ratio appears to be minimal, given that nitrogen is present in such low quantities in composting substrates and final composts, especially in comparison to carbon. Indeed, from the validation set, initial nitrogen varied between 1.3 and 2.2%, while final nitrogen was between 1.0 and 2.9%. Therefore, a 20% error in TN loss can relate to an error of less than 5% in output composition, depending on mass loss. However, where this can have a more important impact on model results is in estimating total NH_3 and N_2O emissions, which can have a noted influence on environmental assessments following the model use. This is especially the case for N_2O emissions, given its elevated global warming potential.

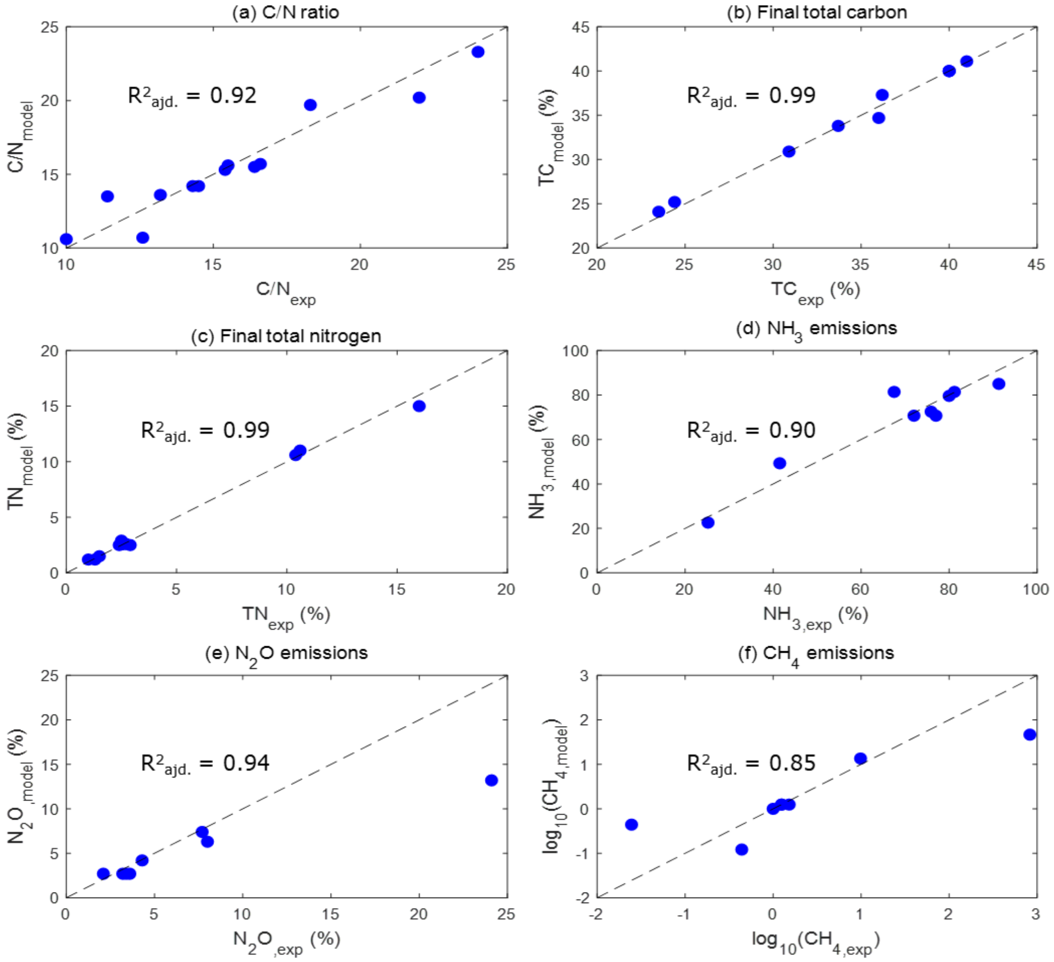


Figure 8.7 Comparison of modelling and experimental outputs. The dotted line has a slope of 1, indicating a perfect fit.

8.5.2 Global sensitivity analysis

The aim of the sensitivity analysis was to provide insight into what input variables most affected model outputs. Despite all the model relations being deterministic, as expressed through the equations of section 8.4, some output variables can be influenced by more than one factor. We hoped that the knowledge gained from the global sensitivity analysis would therefore help users identify which input properties should be targeted to modify specific outputs. However, following the assessment of the results of the sensitivity analysis, with the ranking of predictor importance being presented in Table 8.3, it appears that the six input variables assessed were important or very important in most cases. This result makes it more difficult to provide the information that was initially desired, but also points to the strength of the model design. Indeed, the fact that, in most cases, the input variables have a significant impact on outcomes is a testament to the simplicity achieved by the model. This indicates that the inputs chosen for the model are indeed the ones that best represent the composting situation, and that further simplification/model reduction is unlikely to provide benefit, the latter point having been validated through the assessment of all different model combinations during the sensitivity analysis.

Table 8.3 Ranking of predictor importance from the global sensitivity analysis. The following abbreviations are used for importance: very high (VH), high (H), moderate (M), low (L), very low (VL). Columns in the table include initial moisture content (MC_i), initial nitrogen (N_i), initial carbon (C_i), degradation rate (k_d), maximum temperature (T_{max}), and biodegradable fraction (f_d).

	Predictor importance					
Output	**MC_i**	**N_i**	**C_i**	**k_d**	**T_{max}**	**f_d**
C/N_{out}	VH	VH	VH	VH	H	VH
MC_{out}	VH	H	VH	M	H	VH
OM_{out}	H	M	H	H	H	H
TN_{loss}	H	H	H	H	VH	H
NH_3 emissions	VH	VH	H	H	VH	H
N_2O emissions	VH	VH	VL	M	VH	L
CH_4 emissions	VH	M	VH	H	H	VH
Total emissions	VH	VH	L	M	VH	M

8.5.3 Limitations and perspectives

Given the assumptions and simplifications made along the way, the model does obviously present some limitations. These limitations notably and mainly relate to certain process conditions not being considered, such as pH, dynamic temperature, and the impact of aeration on anything other than the water balance. However, as shown through this paper and discussed in Walling and Vaneeckhaute (2020a), this does not seem to have a major impact on the global mass balances when considering a well-operated system. Free airspace is another aspect that is not currently considered in the model. Its impact on process kinetics appears to be limited (Walling and Vaneeckhaute, 2021b), but it can have an important impact on emissions, given that it regulates oxygen availability throughout the environment.

Another important aspect to highlight is that this model does not take into account potential changes from traditional composting that can have an impact on the process, such as using chemical additives or undertaking mitigation strategies to reduce GHG emissions. Similarly, constant thermophilic or hyperthermophilic composting can also have an influence, both on degradation rate and emissions that are not considered in the model. This, however, can always easily be considered by changing some of the model parameters.

Regarding future work, the greatest need that became apparent through this work is for a comprehensive and exhaustive meta-analysis examining the impact of input variables and operating parameters on emissions and outputs during composting. Through this work, we have identified some relationships based on limited experimental data, but having a comprehensive dataset linking C/N ratio, aeration, temperature, carbon loss, and pH to a variety of outcomes, such as total nitrogen, NH_3, N_2O, NO_x-N, NH_4-N, and CH_4, would be of great benefit to this model, as well as any future composting models.

8.6 Conclusion

The model developed through this work has demonstrated great potential to be a valuable tool for decision-makers, allowing for quick, easy, and accurate prediction of composting outcomes, such as end quality (carbon and nitrogen content, moisture content), and greenhouse gas emissions (CH_4, CO_2, N_2O), as well as ammonia loss (NH_3). By basing itself solely on initial nitrogen and carbon, moisture content, maximum temperature, along with a degradation rate and degradable fraction, the model offers very accurate predictions. Furthermore, by having every aspect of the model clearly linked to an input parameter, it is very easy to understand how operating choices can impact the process, promoting learning among users who may be less knowledgeable about the subject.

Conclusion and perspectives

Conclusion

The aim of this PhD dissertation was to support the transition towards more sustainable and circular economies by developing tools which could aid in optimizing the composting process, one of the primary contributors to organic waste valorization. Three research phases were conducted, building on each prior phase. The first phase consisted of a consolidation and development of the fundamentals of composting modelling (Chapters 1-3), followed by an experimental and modelling investigation of nutrient loss and GHG emissions during composting in phase 2 (Chapters 4 and 5). This was then supplemented by the third and final phase of the PhD, which aimed at facilitating the use of models for successful environmental decision support (Chapters 6-8). Through these three phases, fundamental and practical knowledge on composting modelling were advanced equally, resulting in a well-rounded work that pushed our knowledge and produced creative and usable tools. In the introduction, five research questions were identified, with the answers to these questions and the main conclusions and outputs from this dissertation being presented below.

Phase 1: Consolidation and development of the fundamentals of composting modelling

Research question 1: What is the current state of knowledge in the field of composting modelling?

From the first phase of the project (Chapters 1 to 3), a consolidated basis of knowledge on composting modelling was achieved through a systematic review on composting modelling, and the first review on the subject since 2006 (Chapter 2). This review pointed towards the strong support, both experimental and theoretical, of mass and energy balances in the process, as well as the validity of first-order degradation kinetics to represent biodegradation due to hydrolysis' role as the rate-limiting step in composting. Furthermore, a variety of understudied research areas that would benefit from further research were identified, including modelling of: different processes (non-reactor systems), physical parameter variation during the process (volume, bulk density), quality and nutrient composition of composts, substrate biodegradability, as well as the great potential for emerging modelling approaches, such as machine learning.

This was then supplemented by the development of fundamental knowledge on composting, with the identification of which pairings of correction functions provided the most accurate predictions, out of the large quantity of functions proposed throughout the literature (Chapter 3), aiming at answering the second research question:

Research question 2: What correction functions (if any) are most appropriate to model composting kinetics?

The answer to this question can be found in Table 3.6 of Chapter 3, which identified the best pairings as comprising of either the Haug (1993) or cardinal temperature correction for temperature, the Stombaugh and Nokes (1996) or Haug (1980/1993) moisture correction, and the Monod oxygen correction.

Phase 2: Experimental and modelling investigation of nutrient loss and GHG emissions during composting

Research question 3: How can we mathematically model emissions of GHGs and nutrient loss during composting in a mechanistic fashion?

Building on the work of phase 1 and in the aim of answering the third research question, the second phase produced a brief but consolidated overview of experimental composting methods, aimed at bridging a gap in the accessibility of this information. This was followed by the detailing of our own experimental plan to evaluate the composting process, along with its GHG emissions and nutrient transformation and loss (Chapter 4); a plan whose implementation faced significant delays due to COVID-19. Chapter 5 then presented the development and attempted calibration and validation of a comprehensive composting model aimed at predicting traditional composting outputs (degradation, temperature, moisture) with a deepened focus on GHG emissions and nitrogen. The model proved to be capable of predicting degradation, temperature, and moisture with good accuracy, but nitrogen remains an area that requires more development. Profiles for TKN, nitrate and ammonia nitrogen can be accurately predicted, depending on calibration, but not alongside carbon and the other outputs, pointing towards a decoupling in some of the model's foundations. Due to having to base the calibration and validation on an experimental dataset from the literature, given the lack of our own experimental data because of COVID-19, it was not possible to develop the model further, having fully exhausted the options available to us. Nevertheless, the model was analyzed through multiple Monte Carlo analyses to understand its behaviour and what areas should be targeted for further development, allowing a methodology and the numerical methods to be in place to quickly calibrate and validate the model when the information becomes available. Beyond this, key takeaways from the model development process were identified, which will hopefully provide valuable insight and guidance for future modelling efforts seeking to explore composting.

Phase 3: Facilitating the use of models for successful environmental decision support

Given some of the challenges encountered in phase 2, particularly regarding the accessibility of the models identified throughout the literature, as well as the one developed in Chapter 5, this phase aimed at developing our knowledge on what makes a model approachable and usable, as well as applying this knowledge in developing more usable composting models, leading to the identification of the fourth research question:

Research question 4: What practices, notably regarding mathematical modelling, should be implemented to favor successful environmental decision-making and system design?

To answer research question 4, a comprehensive review of environmental models and decision support systems was undertaken, focusing on what factors promoted their success and the primary challenges faced by these systems. In the end, 13 major challenges were categorized into three primary categories (stakeholder, model, and system-oriented challenges), with over 60 recommendations provided (Chapter 6). Table 6.1 identifies the key challenges faced by many environmental decision-oriented models and systems, while Figures 6.1 to 6.3 provides our recommendations on model and system development to mitigate these challenges and promote a successful design process.

This knowledge was then applied in the following two chapters to answer the final research question:

Research question 5: How can we model the composting process in both a simple and generalizable fashion?

The first effort to answer this question was the development and assessment of three novel modelling approaches to composting kinetics, presented in Chapter 7. The approaches are based on a first-order kinetic expression and consist in breaking the process down into three or more phases, based on the traditional phases observed during composting (mesophilic, thermophilic, mesophilic). The three proposed modelling approaches managed to consistently outperform the traditional first-order degradation expression widely used throughout composting literature, with NRMSEs varying between 1.13% and 6.32%. Furthermore, these approaches were also found to outperform the most optimal combination of correction functions that had previously been identified in Chapter 3. Finally, all of the work undertaken in the prior seven chapters was leveraged into the development of a parsimonious composting model (PCM). The model aimed at being understandable, easy to approach, efficient, and accurate, all of which it achieved. Using only one process (a first-order biodegradation kinetic) and five parameters, the model achieved NRMSEs varying between 2.35% and 7.92% for C/N, total carbon, and total nitrogen contents, while errors on emissions estimates were generally between 1.47% and 9.48%. This was achieved through the development of empirical relationships relating a variety of process outcomes (e.g., NH_3, CH_4 and N_2O emissions) to starting or operating conditions, alongside strong mechanistic foundations for carbon and moisture dynamics, all of which was validated and calibrated with datasets comprising experimental results from nearly 50 independent studies, contributing to the generalizability of the model. However, despite these very good outcomes, estimation of nitrogen loss remains problematic, as was the case for Chapter 5. Total nitrogen loss through the PCM only achieved an NRMSE of 25.33% which, though not particularly consequential in the grand scheme, given the low concentration of nitrogen in composts compared to carbon, highlights a more fundamental issue with nitrogen prediction in composting. As mentioned previously in this section, the hypothesis of the author is that this one area lacking precision is most likely due to the absence of pH in both the models of Chapter 5 and 8.

Perspectives

Throughout this Ph.D., with the constant questioning and learning that came with it, many interesting and stimulating issues which deserve to be addressed have been raised, as well as some areas that the author had hoped to address but was unable to. These questions can be divided into three primary axes, seeking to study or optimize: (1) the composting process, (2) composting modelling, and (3) environmental decision support.

1. The composting process

The process at the heart of this dissertation has been extensively studied over the past decades, though the inherent complexity of the process, with so many factors impacting its outcomes, and its widespread and growing implementation, keep it a deeply exciting and valuable area to explore. Regarding the composting process, the author is of the opinion that the main interests for future studies are in the realm of process modification and optimization, with the following notable examples coming to mind:

- **Optimization of biodegradation:** The focus of significant research, optimization of biodegradation remains among the most important aspects of composting research. Of particular interest are the growing areas of "non-traditional" composting, such as constant temperature processes (including both mesophilic and thermophilic composting), hyperthermophilic composting, and composting with additives and inoculants to favor certain aspects of the process. Indeed, it is the long treatment period necessary for certain composting operations which presents one of the process' biggest drawbacks, leading to larger spatial and equipment requirements, and thus being one of the main factors contributing to costs.

- **Investigation of nutrient recovery and recycling approaches:** The work in this dissertation has focused primarily on recycling nutrients through traditional composting methods. However, recovery can also be promoted through control and changes to the process, many of which can benefit from further assessment. Examples of areas that could be of benefit to study include the inoculation of compost with certain microbial species that can either favor nutrient retention or render them more accessible to crops (see works of Kumar and Singh (2001), Wei et al. (2017), and Estrada-Bonilla et al. (2017)), using certain bulking agents (see works of Dias et al. (2010), Chan et al. (2016) and Lim et al. (2017)), and composting in acidic conditions alongside inoculation with acid-tolerant microbes to decrease ammonia emissions (see works of Nakasaki et al. (2013) and Kuroda et al. (2015)) and favor phosphorus solubilization. Another interesting pathway is the addition of magnesium to the composting environment to promote struvite precipitation (see works of Wang et al. (2013b) and Chan et al. (2016)).

  Furthermore, composting could also be applied alongside nutrient recovery technologies, such as nitrogen and phosphorus recovery, especially from liquid (leachate) streams. Though the production of leachate and their compositions can vary widely, these streams can be charged in nutrients, which either need to be removed or recovered. Ammonia stripping and adsorption for nitrogen removal/recovery and struvite precipitation or ion-exchange/adsorption for phosphorus could be targeted to these flows. Indeed, based on the study of Roy et al. (2018), nutrient concentrations of composting leachates from large-scale facilities have been reported as varying between 5 to 21 180 mg NH_4-N/L (36–2275 mg/L for mixed municipal solid waste; 5.1-558 mg/L for yard waste; 4-2720 mg/L for green waste; 218-21180 mg/L for wastewater treatment sludge; 443-1091 mg/L for digestate) and 0.5 to 485 mg TP/L

(0.5-288 mg/L for mixed municipal solid waste; 1.5-485 mg/L for green waste; 22-88 mg/L for wastewater treatment sludge).

- **Investigation of phosphorus, potassium, and micronutrients during composting:** In a similar vein, as was noted in a few places throughout this dissertation, as well as by Li et al. (2013), there is a particular lack of research on the state of nutrients and their transformation during composting, with nitrogen having been the primary target of research to this point. Chapter 1 presented a brief but near comprehensive review of the works on phosphorus speciation during composting, while potassium and micronutrients have seen even less study. However, these remain valuable areas of research, given the necessity of having a complete and balanced fertilization scheme, as much for agriculture as for environmental health and sustainability. This will become ever more valuable with the inevitable transition towards more restrictive fertilizer application guidelines.

- **Consolidation of knowledge on the fate of contaminants during composting:** Regarding these strictening guidelines, an understandably growing focus in the realm of organic waste management is the elimination of contaminants, including heavy metals, organic and inorganic compounds, pathogens, as well as emerging contaminants, such as brominated diphenyl ethers (PBDES), chlorinated paraffins, polydimethylsiloxanes (PDMS), per-and polyfluoroalkyl substances (PFAS), microplastics, and pharmaceuticals. Unlike some of the prior perspectives, the area of contaminants in composting has seen strong interest for a long time. Works have explored all of these highlighted areas, ranging from early works on "traditional" contaminants, such as pathogens and organic compounds, in the 1980s (e.g., Bishop and Chesbro (1982), Hurst and Gerba (1989) and Racke and Frink (1989)), while recent works have explored a wide slew of emerging contaminants (Choi et al., 2019; Dubey et al., 2021). However, as of writing this dissertation, the knowledge on the impact of composting on various contaminants is dispersed throughout the literature, with no consolidation of this knowledge into an easily accessible source. This leads to varying degrees of conflicting information being presented throughout literature on the fate of these contaminants, even with regard to pathogen elimination (Franke-Whittle and Insam, 2013). Therefore, a systematic review on the fate of contaminants during composting would be of high value to research in the field moving forward, as well as serving for the much larger fields of agriculture and environmental management.

- **Comprehensive and systematic review of emissions from composting:** As was seen in chapter 8, when trying to determine relationships between emissions and certain operating conditions/process variables empirically, as well as in some works, notably the meta-analysis of Cao et al. (2019), there appears to be a strong correlation between specific conditions and emissions. However, a stronger validation, undertaken through a meta-analysis, would be warranted. The author believes that a study of emissions through a meta-analysis would be of much greater value than an experimental study, given the inherent variability that impacts the composting process, which is highly unlikely to be observable at an individual experimental scale. Indeed, significant experimental and field work has been undertaken on composting emissions and consolidating this information to develop empirical models would be of great benefit to the field. The work of Cao et al. (2019) can present a great basis for this, but given that it was not the intention of their study, many important parameters, variables, and outcomes (N_2O, CH_4) are not included.

- **Study and review of economics of composting processes and facilities:** Similarly to the meta-analysis on emissions, when undertaking the work of chapter 8, the author wanted to include a simple but robust economic assessment module for the parsimonious model. The intention was to use traditional techno-economic assessment tools such as Lang factors for cost estimates, as well as estimating process costs on a weight, volume, or area basis. However, such information was surprisingly difficult to find and, in most cases, unavailable. Indeed, the two main works that were identified on the subject were those of Wei et al. (2001) and van Haaren (2009). The prior studied small and mid-scale composting processes for sewage sludge treatment and found a range of US$ 35 to US$ 187 per ton (dry) for aerated static piles and US$ 11 to US$ 87 for windrows. The latter focused on evaluating large-scale composting processes in the US and obtained a cost of approximately US$ 22 per ton for open-air windrow composting, including capital investments, while operating costs were estimated at around US$ 12 per ton. Such ranges made it difficult to come to any conclusions. Therefore, having an up to date and in-depth study of the costs of composting operations, with the development of economical assessment tools, such as Lang factors, could be of great benefit to the study and evaluation of composting processes and research.

  Regarding information that the author can provide that may aid in such an endeavour, the only insight that can be given is that, currently, tipping fees in Quebec, Canada, range between US$ 47 to US$ 55 per ton received, which matches with the present range of US$ 40 to US$ 72 reported by the Environment Research & Education Foundation for the United States, with a national average of US$ 55 per ton received (EREF, 2021).

- **Inventory of composting kinetic rates:** In any composting model, the most likely factor limiting the use of the model or the validity of the assessment is the rate of the reaction. As was demonstrated in chapters 3 and 7, when fitting a relatively simple kinetic expression (first-order, modified first-order) to experimental data, great accuracy could be achieved, with NRMSEs frequently below 5%. However, despite being at the heart of nearly every composting model, obtaining accurate composting kinetics remains one of the most nebulous aspects in the field. As was discussed in chapter 4, the work of Baptista et al. (2012), which found a variability of 3900% in composting kinetic rates reported at laboratory scales, vs 300% for full-scale operations, clearly highlights the need to standardize how rates are measured and to move towards more realistic and representative studies. Having an inventory of degradation rates, either at specific process conditions (temperature, moisture content, oxygen content, pH), or generalized for a process with known (variable) conditions, and for individual substrates, could be of great help to make the various tools developed throughout the field of composting modelling much more accessible and usable. Moving towards a standardization in this regard should help alleviate part of the great amount of uncertainty that surrounds composting modelling.

- **Study of the role of pH in controlling the composting process:** What the author believes to be the missing link in allowing for the PCM to accurately predict nitrogen loss, pH remains a very pertinent subject to explore. Currently, pH is mainly an observed variable in most of the composting field, serving at most as a way to track the progression of biodegradation (decreasing pH during early stages due to production of organic acids, increasing pH as these acids are consumed and the compost matures).

2. Composting modelling

Modelling of composting, seeking to either understand and emulate in detail the complex processes going on during the composting process, as was done in chapter 5, or trying to capture this complexity while distilling the process into an approachable and streamlined framework, such as in chapter 8, remains an area with great potential for development. Notable areas for future work include:

- **Study of the aspects highlighted in the perspectives of chapter 2 (see section 2.6 for full details):**
    - Composting systems other than reactors and windrows;
    - Variation in volume and the impact of compaction in composting;
    - Maturation (humic matter development);
    - pH and chemical speciation for nutrients and heavy metals;
    - Biodegradability of substrates.
- **Development of machine learning coupled with imaged-base approaches:** Another extremely interesting aspect of composting modelling that was identified during the comprehensive review of chapter 2, the (slowly) growing sector of artificial intelligence and image-based modelling in composting is an area which has significant potential to become a key actor in composting monitoring, control, and optimization. The promise of being capable of predicting and optimizing process conditions and outcomes, based solely on images, would be a major step towards producing models that would see strong interest at the industrial level. Such approaches can also be of value to other organic waste treatment processes, such as for assessing the quality of digestates from anaerobic digestion. However, acquiring the significant amount of data needed to train these models, as well as ensuring that the pathways they use are understandable and communicable (see chapter 6), remain major challenges that modellers must be aware of.
- **Continuation of the work undertaken in this dissertation:** This thesis has provided a strong validation for modelling of carbon, energy, and water dynamics in composting, while providing a valuable foot forward with modelling of nitrogen during the process. However, as detailed in chapters 5 and 8, nitrogen remains an aera that requires more development. Chapter 8 highlighted our ability to accurately estimate the proportion of nitrogen emissions (as N_2O vs NH_3 vs N_2), but quantifying nitrogen loss remains a challenge. Furthermore, the comprehensive model of chapter 5 still requires re-evaluation, modification, and appropriate calibration and validation with

the planned composting experiments. Once this process is done, new perspectives will present themselves. Of interest will be to undertake a global sensitivity analysis to ascertain both the sensitivity of the model and evaluate model simplification, following the methodology of Vaneeckhaute et al. (2018b) and the one used in chapter 8.

- **Increased importance of sensitivity assessments:** As discussed in chapter 2 (section 2.5.5), there is a surprising lack of inclusion of sensitivity assessments in the literature on composting modelling (26% of reviewed literature). Such assessments, as undertaken in chapters 5 and 8, provide invaluable insight into a model and should be commonplace for modellers. Indeed, it is sensitivity analyses which allow us to identify key sources of uncertainty, as well as highlighting the relative weight and importance of parameters within a model. Through these assessments, we can reflect on model design, identify and work to reduce uncertainty as well as potential errors, calibrate models, and perform model simplification, contributing significant added value to the design process. Moving forward, it would be important for future modelling efforts in the field to undertake a more robust model calibration, validation and evaluation by including sensitivity assessments.

3. Environmental decision support

Throughout phase 3 of this dissertation (chapters 6 to 8), we identified how, for a model or system to find practical use, a variety of design considerations focusing on the desires of users are paramount, including a focus on accessibility, transparency, and understandability. The work of phase 3 has provided what the author believes to be a deep but concise foray into the world of environmental decision support systems, followed by the application of this knowledge to produce composting modelling tools that meet these requirements. However, there remains much to be worked on in this area, particularly given its high importance in ensuring the valorization of research and development efforts. The following are some key points for work moving forward:

- **Development of a clear guideline/standard for environmental model and system development:** As stated in the conclusion of Chapter 6, "the production of high-quality EDSSs would greatly benefit from the creation of a detailed and formal framework to help developers with the challenges they face." This is indeed one of the areas that would most contribute to ensuring the success of environmental decision modelling and system design efforts. Having a clear standard or development guide to undertake modelling or system design work surrounding environmental decision support would be of great boon to ensuring the success of future endeavours. Indeed, as detailed throughout Chapter 6, there is a significant amount of resources being spent on developing many of these models and systems, when in practice very few find a level of use capable of justifying such an investment.

- **Push towards model and system evaluation:** Though not a research perspective per se, as was noted in Chapter 6, model and system evaluation (not to be confused with validation) is a massive gap that pervades the literature, at least in environmental fields. Without researchers and developers evaluating their models and systems, we find ourselves faced with an important lack of information regarding how certain design strategies or development choices impacted their products, information which is highly valuable to guide future development initiatives. Pushing for model and system evaluation to become more common place and placing value on the findings of this process will be of great benefit.

- **Increasing focus on stakeholders, users, and decision-makers in the field of composting modelling (and other, wider, waste-management and environmental fields):** Finally, following in the same vein as the prior perspective, the consideration of stakeholders and users throughout the literature assessed during this thesis, both relating to composting modelling and the wider environmental management field, remains grossly lacking. These issues were highlighted through a few examples in Chapter 6, but the same issues were observed throughout the inventoried composting literature. Of the over 200 composting models assessed in the review of Chapter 2, targeted considerations focusing on model users were nearly non-existent, with a plethora of models being developed without much clarity as to the target use-case or users. To a certain extent, the model developed in Chapter 5 of this thesis also suffers from this, due to its complex nature and non-identifiability, though phase 3 was undertaken as a way to remediate this and future work will also seek to address this. As work on modelling and system design expands, with our ever-growing dependence on computer-based planning and optimization, proper identification and documentation of target users and model/system purpose will only contribute to better design.

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Appendix A: List of correction functions used in composting literature.

This appendix presents all the correction functions used in the reviewed literature. The equations are presented in the tables in order of use (most used at the top, less used at the bottom). Given the varying nomenclature between models, we have maintained their original formats and recommend readers consult the references for more details.

Table A.1 Temperature correction functions used in the reviewed literature in order of use. In nearly all cases, T is expressed in degrees Celsius, with the exception of some of the Arrhenius equations.

Temperature correction function	References
$f_T = \frac{(T - T_{max})(T - T_{min})^2}{(T_{opt} - T_{min})[(T_{opt} - T_{min})(T - T_{opt}) - (T_{opt} - T_{max})(T_{opt} + T_{min} - 2T)]}$	(Rosso et al., 1995; Rosso et al., 1993)
$f_T = e^{\frac{-E}{R}\left(\frac{1}{273T} - \frac{1}{273+T_r}\right)}, f_T = e^{\frac{-E}{R}(T-273)}, f_T = e^{\frac{-E}{R}(T_2 - T_1)}, f_T = \frac{A_1 \exp\left(-\frac{E_1}{RT}\right)}{1 + A_2 \exp\left(-\frac{E_2}{RT}\right)},$ $f_T = Ae^{\frac{-E}{RT}}$	Various forms of the Arrhenius equation
$f_T = C_1^{T - T_{R1}} - C_2^{T - T_{R2}}$; often, $C_1 = 1.066$ and $C_2 = 1.21$. (for biomass growth)	(Haug, 1993)
$f_T = 0.0182T$ (for hydrolysis)	(Haug, 1996)
$f_T = -3.11 \times 10^{-4}T^2 + 3.48 \times 10^{-2}T + 0.0265$ (for biomass activity)	(Lin et al., 2008)
$f_T = 2.142 \times 10^{-4}T^2 - 2.356 \times 10^{-2}T + 1.348$ (for biomass decay)	(Ekinci, 2001)
$f_T = 1 - \frac{1}{1 + e^{2(T_1 - T)}} + \frac{12}{1 + e^{-0.8(T - T_2)}}$ (for biomass decay)	(Bialobrzewski et al., 2015)
$f_{T,mesophilic} = \begin{cases} 0.033T & 0 \leq T \leq 30 \\ 1.0 & 30 \leq T \leq 40 \\ -0.067T + 3.667 & 40 \leq T \leq 55 \end{cases}$ (for hydrolysis) $f_{T,thermophilic} = \begin{cases} 0.1T - 4.0 & 40 \leq T \leq 50 \\ 1.0 & 50 \leq T \leq 55 \\ -0.05T + 3.75 & 55 \leq T \leq 75 \end{cases}$	(Yu et al., 2009) (based on Ryckeboer et al. (2003))
$f_T = \alpha[\beta - \gamma^{\delta(T-20)}]$ (for hydrolysis)	(Petric et al., 2015)
$f_T f_{MC} = 0.089 \exp\left(-0.5\left[\left(\frac{MC - 44.22}{19.87}\right)^2 + \left(\frac{T - 58.31}{16.72}\right)^2\right]\right)$	(Ekinci et al., 2004b)
$f_T = -8 \times 10^{-6}T^3 + 0.008T^2 - 0.0238T - 0.2643$ (for hydrolysis)	(Mohee et al., 1998)
$f_{T,bacteria} = T(80 - T)/1600 \quad T < 80$ (for biomass growth) $f_{T,actinomycetes\ and\ fungi} = T(60 - T)/20(80 - T) \quad T < 80$	(Kaiser, 1996)
$f_T = \begin{cases} T/(T_2 - T_1) & T_1 < T \leq T_2 \\ 1.0 & T_2 < T \leq T_3 \\ 3.75 - T/(T_2 - 10) & T_3 < T \end{cases}$	(Stombaugh and Nokes, 1996)
$f_T = \exp(-(T - 57)^2/254))$ (for hydrolysis)	(Smith and Eilers, 1980)

Table A.2 Moisture correction functions used in the reviewed literature from most to least used.

Moisture content correction function	References
$f_{MC} = \frac{1}{\exp(-17.684MC + 7.0622) + 1}$	(Haug, 1993)
$f_{MC} = \begin{cases} 0 & m_1 < m \leq m_2 \\ m/m_2 - 1.0 & m_2 < m \leq m_3 \\ 1.0 & m_3 < m \end{cases}$	(Stombaugh and Nokes, 1996)
$f_{MC} = \begin{cases} 1 - 17.3(1 - m/100)^{6.94} & m \geq 40 \\ 20.6614(m/100)^{4.06} & m < 40 \end{cases}$	(Haug, 1980)
$f_T f_{MC} = 0.089 \exp\left(-0.5\left[\left(\frac{MC - 44.22}{19.87}\right)^2 + \left(\frac{T - 58.31}{16.72}\right)^2\right]\right)$	(Ekinci et al., 2004b)
$f_{MC} = 0.012m - 0.18$	(Mora-Naranjo et al., 2004)
$f_{MC} = \begin{cases} 0 & m < m_1 \\ (m - m_1)/(m_2 - m_1) & m_1 < m < m_2 \\ 1 & m_2 < m < m_3 \\ (m - m_4)/(m_3 - m_4) & m_3 < m < m_4 \\ 0 & m_4 < m < 1 \end{cases}$ (for biomass growth)	Shishido (1999) as referenced by Seki (2002)
$f_{MC} = -56.97 + 57.98 \exp[(-0.5(m - 0.56)/1.52)^2]$	(Mohee et al., 1998)
$f_{MC} = \begin{cases} 0 & 0 < w < w_L : 38.5\% \\ (a_w - a_{w_0})/(1 - a_{w_0}) & w_L < w < w_M : 60\% \\ \frac{(a_w - a_{w_0})}{(1 - a_{w_0})} \times \frac{(w_H - w)}{(w_H - w_M)} & w_M < w < w_H : 80\% \\ 0 & w_H < w \end{cases}$ (for biomass growth) $a_W = w/[(1 - K_a)w + K_a]$	(Kaneko and Fujita, 1986; Seng et al., 2016)
$f_{MC} = \exp(-10.973(FS - 0.3)^2)$	(Smith and Eilers, 1980)

Table A.3 Oxygen content correction functions used in the reviewed literature in order of use.

Oxygen content correction function	References
$f_{O_2} = \frac{O_2}{O_2 + k_{O_2}}$	Monod expressions (see Richard et al. (2006))
$f_{O_2} = \frac{O_2}{\left(\frac{20.95}{0.83 + 20.95}\right)(0.83 + O_2)}$	(Baptista et al., 2010)
$f_{O_2} = \frac{O_2}{0.79 - 0.041T + 0.040X_{H_2O} + O_2}$	(Higgins and Walker, 2001)
$f_{O_2} = \frac{O_2/\rho_a}{O_2\rho_a + 0.07}$	(Petric and Selimbašić, 2008)
$f_{O_2} = x_1 \text{ atan } (x_2 O_2)$	(Keener, 1973)

Table A.4 Free air space correction functions used in the reviewed literature in order of use.

Free air space content correction function	References
$\mathrm{f_{FAS}} = \dfrac{1}{\exp(-23.675\mathrm{FAS} + 3.4945) + 1}$	(Haug, 1993)
$\mathrm{f_{FAS,mesophile}} = 0.01 + 0.90\exp\left(-\exp\left(-15.0(\mathrm{FAS} - 0.53)\right)\right)$ $\mathrm{f_{FAS,thermophile}} = 0.01 + 0.70\exp\left(-\exp\left(-12.3(\mathrm{FAS} - 0.55)\right)\right)$	(Yu et al., 2009)
$\mathrm{f_{FAS}} = -0.0051\mathrm{MC} + 0.7567$	(Ekinci, 2001)

Table A.5 pH correction function used in the reviewed literature in order of use.

pH correction function	References
$\mathrm{f_{pH}} = \begin{cases} 0 & \mathrm{pH} \leq 5 \\ 0.5 \times \mathrm{pH} - 2.5 & 5 < \mathrm{pH} \leq 7 \\ 1.0 & 7 < \mathrm{pH} \leq 9 \\ 3.97 - 0.33 \times \mathrm{pH} & 9 < \mathrm{pH} \leq 12 \\ 0 & 12 < \mathrm{pH} \end{cases}$	(Liang et al., 2004)
$\mathrm{f_{pH}} = 0.526 \times \mathrm{pH} - 2.636$	Petric et al. (2015) based on Liang et al. (2004)

Appendix B: Results of the modelling assessment of chapter 3.

The following tables provide more detailed results on the results of the assessments undertaken in this work, notably regarding the average normalized root mean squared errors (NRMSEs) and the optimal sets for every trial.

Fixed $\mathbf{k_{max}}$:

Table B.1 Average NRMSE for trials with a fixed $\mathbf{k_{max}}$.

		average NRMSE (% error)			
	Correction function	**Trial 1**	**Trial 2**	**Trial 3**	**Trial 4**
Temperature functions	Cardinal temperature	5.90	14.15	16.07	21.03
	Arrhenius	5.96	19.00	16.66	18.04
	Haug (1993)	6.03	17.16	14.35	19.44
	Haug (1996)	8.42	17.93	20.80	25.08
	Lin et al. (2008)	11.78	23.95	24.75	27.00
	Stombaugh and Nokes (1996)	13.66	26.81	25.76	25.74
	Kaiser (1996)	12.88	25.50	24.29	21.63
Moisture functions	Haug (1993)	7.78	14.46	14.02	18.19
	Stombaugh and Nokes (1996)	8.18	15.29	15.84	19.18
	Haug (1980)	7.77	14.42	13.92	18.16
	Mora-Naranjo et al. (2004)	13.44	43.29	41.46	35.10
Oxygen functions	Monod	8.90	20.89	19.34	20.99
	Baptista et al. (2010)	9.86	20.88	21.69	24.46
	Higgins and Walker (2001)	8.94	20.15	20.11	22.25

Table B.2 NRMSE for individual application of select temperature corrections for trials with a fixed $\mathbf{k_{max}}$.

	NRSME (% error)			
Correction function	**Trial 1**	**Trial 2**	**Trial 3**	**Trial 4**
Cardinal temperature	5.32	8.92	14.18	23.16
Arrhenius	3.46	5.55	10.91	14.53
Haug (1993)	4.26	5.19	10.21	20.31

Table B.3 Optimal set for trial 1 with a fixed $\mathbf{k_{max}}$.

Combination (Temperature + Moisture + Oxygen)	**NRSME (% error)**
Rosso + Haug (1980) + Monod	2.16
Arrhenius + Haug (1980) + Baptista et al.	2.53
Arrhenius + Haug (1993) + Higgins and Walker	2.56
Arrhenius + Stombaugh and Nokes + Higgins and Walker	2.57
Rosso + Stombaugh and Nokes + Monod	2.58
Arrhenius + Stombaugh and Nokes + Monod	2.76
Haug (1993) + Stombaugh and Nokes + Monod	2.89
Haug (1993) + Haug (1980) + Higgins and Walker	2.97
Haug (1993) + Haug (1993) + Monod	3.01
Haug (1993) + Haug (1980) + Baptista	3.18

Table B.4 Optimal set for trial 2 with a fixed $\mathbf{k_{max}}$.

Combination (Temperature + Moisture + Oxygen)	**NRSME (% error)**
Rosso + Haug (1980/1993) + Monod	4.40
Rosso + Stombaugh and Nokes + Monod	4.69
Haug (1993) + Stombaugh and Nokes + Baptista et al.	4.97
Rosso + Stombaugh and Nokes + Higgins and Walker	5.34
Rosso + Haug (1980) + Baptista et al.	5.36
Haug (1993) + Haug (1993) + Baptista et al.	5.47
Arrhenius + Stombaugh and Nokes + Baptista et al.	5.57
Rosso + Haug (1993) + Monod	6.21
Haug (1993) + Stombaugh and Nokes + Higgins and Walker	6.53
Rosso + Stombaugh and Nokes + Baptista	7.63

Table B.5 Optimal set for trial 3 with a fixed $\mathbf{k_{max}}$.

Combination (Temperature + Moisture + Oxygen)	**NRSME (% error)**
Haug (1993) + Stombaugh and Nokes + Monod	3.77
Haug (1993) + Haug (1993) + Monod	4.21
Haug (1993) + Haug (1980) + Higgins and Walker	4.44
Rosso + Haug (1980) + Monod	4.97
Arrhenius + Stombaugh and Nokes + Monod	6.60
Haug (1993) + Haug (1980) + Baptista et al.	6.62
Haug (1993) + Stombaugh and Nokes + Higgins and Walker	6.69
Arrhenius + Haug (1980) + Higgins and Walker	7.19
Rosso + Haug (1980) + Higgins and Walker	7.72
Arrhenius + Haug (1980) + Monod	7.80

Table B.6 Optimal set for trial 4 with a fixed $\mathbf{k_{max}}$.

Combination (Temperature + Moisture + Oxygen)	**NRSME (% error)**
Arrhenius + Stombaugh and Nokes + Monod	8.28
Arrhenius + Haug (1993) + Monod	8.96
Arrhenius + Haug (1980) + Higgins and Walker	9.45
Haug (1993) + Haug (1980) + Monod	9.75
Arrhenius + Stombaugh and Nokes+ Higgins and Walker	9.93
Haug (1993) + Stombaugh and Nokes + Monod	10.85
Arrhenius + Haug (1980) + Baptista et al.	12.12
Rosso + Haug (1980) + Monod	12.24
Arrhenius + Stombaugh and Nokes + Baptista	13.19
Rosso + Stombaugh and Nokes + Monod	13.56

Optimized $\mathbf{k_{max}}$:

Table B.7 Average NRMSE for trials with an optimized $\mathbf{k_{max}}$.

		average NRMSE (% error)			
	Correction function	**Trial 1**	**Trial 2**	**Trial 3**	**Trial 4**
Temperature functions	Cardinal temperature	2.20	4.17	4.76	8.32
	Arrhenius	5.96	19.00	16.66	18.04
	Haug (1993)	2.68	4.80	3.83	7.86
	Haug (1996)	2.88	3.47	6.81	9.71
	Lin et al. (2008)	5.03	7.11	9.48	10.98
	Stombaugh and Nokes (1996)	6.91	11.70	12.25	12.35
	Kaiser (1996)	10.23	17.12	16.80	14.87
Moisture functions	Haug (1993)	4.43	7.96	8.73	10.21
	Stombaugh and Nokes (1996)	4.63	7.76	8.63	9.94
	Haug (1980)	4.64	7.98	8.75	10.25
	Mora-Naranjo et al. (2004)	7.17	14.81	15.45	17.21
Oxygen functions	Monod	5.11	9.89	10.17	11.67
	Baptista et al. (2010)	4.95	8.85	10.2	12.12
	Higgins and Walker (2001)	5.33	8.98	9.83	11.40

Table B.8 NRMSE for individual application of select temperature corrections for trials with an optimized $\mathbf{k_{max}}$.

	NRSME (% error)			
Correction function	**Trial 1**	**Trial 2**	**Trial 3**	**Trial 4**
Cardinal temperature	2.35	4.27	4.70	7.90
Arrhenius	3.46	4.49	10.73	14.50
Haug (1993)	2.88	5.00	3.78	7.42

Table B.9 Optimal set for trial 1 with an optimized $\mathbf{k_{max}}$.

Combination (Temperature + Moisture + Oxygen)	**NRSME (% error)**
Rosso + Mora-Naranjo et al. + Monod	1.84
Rosso + Mora-Naranjo et al. + Baptista et al.	1.85
Rosso + Mora-Naranjo et al. + Higgins and Walker	1.96
Rosso + Haug (1980) + Monod	2.15
Rosso + Haug (1980) + Baptista et al.	2.16
Rosso + Stombaugh and Nokes + Monod	2.34
Rosso + Stombaugh and Nokes + Baptista et al.	2.34
Rosso + Haug (1980) + Higgins and Walker	2.39
Haug (1996) + Mora-Naranjo et al. + Higgins and Walker	2.41
Haug (1996) + Stombaugh and Nokes + Higgins and Walker	2.48

Table B.10 Optimal set for trial 2 with an optimized $\mathbf{k_{max}}$.

Combination (Temperature + Moisture + Oxygen)	**NRSME (% error)**
Haug (1996) + Haug (1980) + Higgins and Walker	3.20
Haug (1996) + Stombaugh and Nokes + Higgins and Walker	3.24
Haug (1996) + Mora-Naranjo et al. + Higgins and Walker	3.36
Haug (1996) + Haug (1980) + Baptista et al.	3.44
Haug (1996) + Stombaugh and Nokes + Baptista et al.	3.45
Haug (1996) + Haug (1980) + Monod	3.62
Haug (1996) + Stombaugh and Nokes + Monod	3.64
Haug (1996) + Mora-Naranjo et al. + Baptista et al.	3.66
Rosso + Mora-Naranjo et al. + Monod	3.67
Arrhenius + Stombaugh and Nokes + Baptista et al.	3.71

Table B.11 Optimal set for trial 3 with an optimized $\mathbf{k_{max}}$.

Combination (Temperature + Moisture + Oxygen)	**NRSME (% error)**
Haug (1993) + Stombaugh and Nokes + Monod	3.57
Haug (1993) + Haug (1993) + Monod	3.67
Haug (1993) + Stombaugh and Nokes + Baptista et al.	3.69
Haug (1993) + Stombaugh and Nokes+ Higgins and Walker	3.80
Haug (1993) + Haug (1993) + Baptista et al.	3.80
Haug (1993) + Haug (1993) + Higgins and Walker	3.88
Haug (1993) + Mora-Naranjo et al. + Monod	4.11
Rosso + Stombaugh and Nokes + Monod	4.50
Rosso + Stombaugh and Nokes + Higgins and Walker	4.61
Rosso + Stombaugh and Nokes + Baptista et al.	4.61

Table B.12 Optimal set for trial 4 with an optimized $\mathbf{k_{max}}$.

Combination (Temperature +Moisture + Oxygen)	**NRSME (% error)**
Haug (1993) + Stombaugh and Nokes + Higgins and Walker	6.71
Haug (1993) + Stombaugh and Nokes + Monod	6.81
Haug (1993) + Stombaugh and Nokes + Baptista et al.	7.14
Rosso + Stombaugh and Nokes + Higgins and Walker	7.19
Haug (1993) + Haug (1993) + Higgins and Walker	7.25
Haug (1993) + Haug (1993) + Monod	7.33
Rosso + Stombaugh and Nokes + Baptista et al.	7.33
Haug (1993) + Haug (1993) + Baptista et al.	7.68
Rosso + Haug (1993) + Higgins and Walker	7.68
Rosso + Haug (1993) + Monod	7.81

Experimental data use for the model evaluation, adapted from Malamis et al. (2016)

Table B.13 Experimental data for trial 1

Time (day)	Temperature (°C)	Moisture content (%)	Oxygen content (%)	BOMloss (%)
0	25.7	65.8	16.3	
1	27.3	65.5	16.8	
2	33.0	66.2	17.4	9.5
3	40.7	64.2	15.7	
4	47.3	63.3	14.2	27.6
5	56.7	61.7	12.5	
6	58.7	60.4	9.8	
7	59.7	60.9	9.1	
8	59.0	58.9	11.2	52.1
9	55.0	60.0	13.7	
10	57.0	59.5	13.0	
11	56.0	58.4	14.3	
12	51.3	57.1	16.0	66.6
13	48.7	55.9	16.4	
14	49.3	54.4	17.8	
15	46.3	53.9	18.6	
16	46.0	53.3	18.6	70.2
17	43.7	55.5	18.4	
18	43.7	53.7	19.3	
19	42.7	52.2	19.8	
20	41.0	51.7	19.9	76.8
21	39.0	51.2	19.9	
22	37.0	51.2	19.6	
23	36.3	50.8	20.0	
24	34.3	49.9	19.8	80.8
25	34.3	50.5	20.1	

Table B.14 Experimental data for trial 2

Time (day)	Temperature (°C)	Moisture content (%)	Oxygen content (%)	BOMloss (%)
0	28.0	59.3	17.0	
1	31.0	57.0	17.5	
2	40.8	60.7	15.9	
3	49.7	58.1	14.4	31.6
4	57.5	57.9	12.1	
5	61.1	61.3	10.4	47.6
6	59.2	58.6	11.5	
7	59.8	59.2	11.0	62.3
8	55.2	57.2	13.7	
9	53.9	55.8	14.3	
10	50.0	53.5	14.7	
11	48.4	56.6	15.6	
12	46.1	55.0	15.4	
13	47.0	56.0	16.4	73.8
14	44.8	53.2	17.0	
15	43.4	52.9	18.4	
16	42.1	52.0	18.5	78.9
17	37.2	51.6	18.9	
18	37.9	50.0	18.5	79.6
19	34.9	49.0	18.9	
20	34.9	48.3	19.4	
21	31.6	47.7	19.0	
22	28.4	47.4	19.3	80.4

Table B.15 Experimental data for trial 3

Time (day)	Temperature (°C)	Moisture content (%)	Oxygen content (%)	BOMloss (%)
0	28	60.4	19.1	
1	37.2	57.9	16.8	
2	50	60.7	15.7	15.0
3	58.9	58.9	14.4	
4	60.5	55.6	13.8	
5	57.5	57.6	15.6	32.1
6	58.5	58.5	16.2	
7	54.9	59.4	16.9	
8	52.6	57.6	16.3	
9	51.6	56.5	17.8	50.7
10	52.0	54.2	17.2	
11	49.3	55.8	18.6	
12	47.7	54.4	18.1	
13	48.7	55.9	18.5	
14	48.4	54.3	19.0	59.3
15	45.4	52.7	18.8	
16	44.4	52.3	17.9	
17	42.5	53.8	18.6	60.7
18	40.5	52.9	19.1	
19	40.8	51.8	19.8	
20	38.5	51.7	19.3	62.1
21	39.5	51.3	19.8	
22	37.5	51.0	19.6	
23	34.6	51.0	19.8	
24	32.3	50.1	19.6	62.9

Table B.16 Experimental data for trial 4

Time (day)	Temperature (°C)	Moisture content (%)	Oxygen content (%)	BOMloss (%)
0	32.0	68.2	14.9	
1	51.0	66.4	12.2	
2	58.9	63.1	12.5	21.4
3	58.9	60.0	13.6	
4	57.9	62.2	14.2	43.2
5	58.5	58.5	15.7	
6	54.6	61.0	15.6	
7	52.0	58.8	16.2	62.1
8	52.3	57.2	17.5	
9	49.7	60.8	17.3	
10	48.4	57.6	18.3	72.6
11	45.4	55.8	17.9	
12	43.4	54.2	18.1	
13	42.8	54.8	18.1	76.8
14	40.2	53.6	18.3	
15	39.5	51.8	18.9	
16	39.5	51.3	18.6	
17	38.5	50.6	18.9	79.7
18	36.6	50.0	19.3	
19	33.3	49.7	19.0	79.7

Appendix C: Petersen matrix for the comprehensive composting model (chapter 5)

Table C.1 Petersen matrix for the comprehensive composting model developed in chapter 5.

		1	2	3	4	5	6	7	8	9
	Process	S_I	S_S	X_I	X_S	X_{HB}	X_{FH}	X_{AOB}	X_{NOB}	X_{DP}
Bacteria	1. Aerobic growth of HB		$-\frac{1}{Y_{HB}}$			1				
	2. Anoxic growth of HB on nitrate		$-\frac{1}{\eta Y_{HB}}$			1				
	3. Anoxic growth of HB on nitrite		$-\frac{1}{\eta Y_{HB}}$			1				
	4. Anoxic growth of HB on nitric oxide		$-\frac{1}{\eta Y_{HB}}$			1				
	5. Anoxic growth of HB on nitrous oxide		$-\frac{1}{\eta Y_{HB}}$			1				
Fungi	6. Aerobic growth of HF		$-\frac{1}{Y_{HF}}$				1			
	7. Anoxic growth of HF on nitrate		$-\frac{1}{\eta Y_{HF}}$				1			
	8. Anoxic growth of HF on nitrite		$-\frac{1}{\eta Y_{HF}}$				1			
	9. Anoxic growth of HF on nitric oxide		$-\frac{1}{\eta Y_{HF}}$				1			
	10. Anoxic growth of HF on nitrous oxide		$-\frac{1}{\eta Y_{HF}}$				1			
Ammonia oxidizing bacteria	11. Aerobic growth of AOBs							1		
	12. AOB denitrification of NO_2									
	13. AOB denitrification of N_2O									

		10	11	12	13	14	15	16	17	18
	Process	S_O	S_{NO3}	S_{NO2}	S_{NO}	S_{N2O}	S_{N2}	S_{NH}	S_{ND}	X_{ND}
Bacteria	1. Aerobic growth of HB	$-\frac{1-Y_{HB}}{Y_{HB}}$						$-i_{XB}$		
	2. Anoxic growth of HB on nitrate		$-\frac{1-\eta Y_{HB}}{1.143\eta Y_{H}}$	$\frac{1-\eta Y_{HB}}{1.143\eta Y_{HB}}$				$-i_{XB}$		
	3. Anoxic growth of HB on nitrite			$-\frac{1-\eta Y_{H}}{0.571\eta Y}$	$\frac{1-\eta Y_{HB}}{0.571\eta Y_{HB}}$			$-i_{XB}$		
	4. Anoxic growth of HB on nitric oxide				$-\frac{1-\eta Y_{HB}}{0.571\eta Y_{HB}}$	$\frac{1-\eta Y_{HB}}{0.571\eta Y_{HB}}$		$-i_{XB}$		
	5. Anoxic growth of HB on nitrous oxide					$-\frac{1-\eta Y_{H}}{0.571\eta Y}$	$\frac{1-\eta Y_{HB}}{0.571\eta Y_{HB}}$	$-i_{XB}$		
Fungi	6. Aerobic growth of HF	$-\frac{1-Y_{HF}}{Y_{HF}}$						$-i_{XB}$		
	7. Anoxic growth of HF on nitrate		$-\frac{1-Y_{HF}}{1.143\eta Y_{H}}$	$\frac{1-Y_{HF}}{1.143\eta Y_{HF}}$				$-i_{XB}$		
	8. Anoxic growth of HF on nitrite			$-\frac{1-Y_{H}}{0.571\eta Y}$	$\frac{1-Y_{HF}}{0.571\eta Y_{HF}}$			$-i_{XB}$		
	9. Anoxic growth of HF on nitric oxide				$-\frac{1-Y_{HF}}{0.571\eta Y_{HF}}$	$\frac{1-Y_{HF}}{0.571\eta Y_{HF}}$		$-i_{XB}$		
	10. Anoxic growth of HF on nitrous oxide					$-\frac{1-Y_{H}}{0.571\eta Y}$	$\frac{1-Y_{HF}}{0.571\eta Y_{HF}}$	$-i_{XB}$		
Ammonia oxidizing bacteria	11. Aerobic growth of AOBs	$1-\frac{3.43}{Y_{AOB}}$		$\frac{1}{Y_{AOB}}$				$-i_{XB}-\frac{1}{Y_{AOB}}$		
	12. AOB denitrification of NO_2			-1	1.33					
	13. AOB denitrification of N_2O				-1	1.5				

		19	
	Process	S_{alk}	**Process rate (M L^{-3} T^{-1})**
Bacteria	1. Aerobic growth of HB	$-i_{XB}/14$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_O+S_O}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)X_{HB}f$
	2. Anoxic growth of HB on nitrate	$-i_{XB}/14$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_O}{K_O+S_O}\right)\left(\frac{S_{NO3}}{K_{NO3}+S_{NO3}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)\eta_{NO3}X_{BH}f$
	3. Anoxic growth of HB on nitrite	$-\frac{1-\eta Y_{HB}}{14*0.571\eta Y_{HB}}-\frac{i_{XB}}{14}$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_O}{K_O+S_O}\right)\left(\frac{S_{NO2}}{K_{NO2}+S_{NO2}}\right)\left(\frac{K_{I3NO}}{K_{I3NO}+S_{NO}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)\eta_{NO2}X_{BH}f$
	4. Anoxic growth of HB on nitric oxide	$-i_{XB}/14$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_O}{K_O+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}+S_{NO}^2/K_{I4NO}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)\eta_{NO}X_{HB}f$
	5. Anoxic growth of HB on nitrous oxide	$-i_{XB}/14$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{OH}}{K_{OH}+S_O}\right)\left(\frac{S_{N2O}}{K_{N2O}+S_{N2O}}\right)\left(\frac{K_{I5NO}}{K_{I5NO}+S_{NO}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)\eta_{N2O}X_{HB}f$
Fungi	6. Aerobic growth of HF	$-i_{XB}/14$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_O+S_O}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)X_{HB}f$
	7. Anoxic growth of HF on nitrate	$-i_{XB}/14$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_O}{K_O+S_O}\right)\left(\frac{S_{NO3}}{K_{NO3}+S_{NO3}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)\eta_{NO3}X_{BH}f$
	8. Anoxic growth of HF on nitrite	$-\frac{1-\eta Y_{HF}}{14*0.571\eta Y_{HF}}-\frac{i_{XB}}{14}$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_O}{K_O+S_O}\right)\left(\frac{S_{NO2}}{K_{NO2}+S_{NO2}}\right)\left(\frac{K_{I3NO}}{K_{I3NO}+S_{NO}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)\eta_{NO2}X_{BH}f$
	9. Anoxic growth of HF on nitric oxide	$-i_{XB}/14$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_O}{K_O+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}+S_{NO}^2/K_{I4NO}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)\eta_{NO}X_{HB}f$
	10. Anoxic growth of HF on nitrous oxide	$-i_{XB}/14$	$\mu_{HB}\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{OH}}{K_{OH}+S_O}\right)\left(\frac{S_{N2O}}{K_{N2O}+S_{N2O}}\right)\left(\frac{K_{I5NO}}{K_{I5NO}+S_{NO}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)\eta_{N2O}X_{HB}f$
Ammonia oxidizing bacteria	11. Aerobic growth of AOBs	$-i_{XB}-\frac{1}{7Y_{AOB}}$	$\mu_{AOB}\left(\frac{S_{FA}}{K_{FA}+S_{FA}+S_{FA}^2/K_{I8FA}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)\left(\frac{K_{IFNA}}{K_{IFNA}+S_{FNA}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)X_{AOB}f$
	12. AOB denitrification of NO_2		$\mu_{AOB}\eta_{AOB}\left(\frac{S_{NO2}}{K_{NO2}+S_{NO2}}\right)\left(\frac{K_{OH}}{K_{OH}+S_O}\right)X_{AOB}f$
	13. AOB denitrification of N_2O	$\frac{1}{14}$	$\mu_{AOB}\eta_{AOB}\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\left(\frac{K_{OH}}{K_{OH}+S_O}\right)X_{AOB}f$

		1	2	3	4	5	6	7	8	9
	Process	S_I	S_S	X_I	X_S	X_{HB}	X_{FH}	X_{AOB}	X_{NOB}	X_{DP}
Nitric oxidizing bacteria	14. Aerobic growth of nitric oxidizing bacteria								1	
Reduction of nitrate to ammonia	15. Assimilative nitrate reduction to nitrite		-1.14							
	16. Assimilate nitrate reduction to ammonia		-3.43							
Decay	17. Decay of heterotrophic bacteria				$1 - f_p$	-1				f_p
	18. Decay of heterotrophic fungi				$1 - f_p$		-1			f_p
	19. Decay of AOBs				$1 - f_p$			-1		f_p
	20. Decay of NOBs				$1 - f_p$				-1	f_p
Ammonification/hydrolysis	21. Ammonification of soluble organic nitrogen by bacteria									
	22. Ammonification of soluble organic nitrogen by fungi									
	23. Hydrolysis of entrapped organics by bacteria		1		-1					
	24. Hydrolysis of entrapped organics by fungi		1		-1					
	25. Hydrolysis of entrapped organic nitrogen									

		10	11	12	13	14	15	16	17	18
	Process	S_O	S_{NO3}	S_{NO2}	S_{NO}	S_{N2O}	S_{N2}	S_{NH}	S_{ND}	X_{ND}
Nitric oxidizing bacteria	14. Aerobic growth of nitric oxidizing bacteria	$1 - \frac{1.14}{Y_{NOB}}$	$\frac{1}{Y_{NOB}}$	$-\frac{1}{Y_{NOB}}$				$-i_{XB}$		
Reduction of nitrate to ammonia	15. Assimilative nitrate reduction to nitrite		-1	1						
	16. Assimilate nitrate reduction to ammonia			-1				1		
Decay	17. Decay of heterotrophic bacteria								$i_{XB} - f_p i_{XP}$	
	18. Decay of heterotrophic fungi								$i_{XB} - f_p i_{XP}$	
	19. Decay of AOBs								$i_{XB} - f_p i_{XP}$	
	20. Decay of NOBs								$i_{XB} - f_p i_{XP}$	
Ammonification/hydrolysis	21. Ammonification of soluble organic nitrogen by bacteria							1	-1	
	22. Ammonification of soluble organic nitrogen by fungi							1	-1	
	23. Hydrolysis of entrapped organics by bacteria									
	24. Hydrolysis of entrapped organics by fungi									
	25. Hydrolysis of entrapped organic nitrogen								1	-1

		19	
	Process	S_{alk}	**Process rate (M L^{-3} T^{-1})**
Nitric oxidizing bacteria	14. Aerobic growth of nitric oxidizing bacteria	$\frac{-i_{XB}}{14}$	$\mu_{NOB}\left(\frac{S_{FNA}}{K_{FNA}+S_{FNA}+S_{FNA}^2/K_{I9FNA}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)\left(\frac{K_{IFNA}}{K_{IFNA}+S_{FNA}}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_{alk}}{K_{alk}+S_{alk}}\right)X_{NOB}f$
Reduction of nitrate to ammonia	15. Assimilative nitrate reduction to nitrite		$1.2\cdot i_{XB}\left(\frac{S_{NO_3}}{K_{6NO_3}+S_{NO_3}}\right)\left(\frac{K_{INH}}{K_{INH}+S_{NH}}\right)\left(\frac{K_{I6NO_2}}{K_{I6NO_2}+S_{NO_2}}\right)\left(\sum_{i=1}^{13}R_i-R_{21}-R_{22}\right)$
	16. Assimilate nitrate reduction to ammonia	$\frac{1}{14}$	$1.2\cdot i_{XB}\left(\frac{S_{NO_2}}{K_{7NO_2}+S_{NO_2}}\right)\left(\frac{K_{INH}}{K_{INH}+S_{NH}}\right)\left(\sum_{i=1}^{13}R_i-R_{21}-R_{22}\right)$
Decay	17. Decay of heterotrophic bacteria		$b_{HB}X_{HB}$
	18. Decay of heterotrophic fungi		$b_{HF}X_{HF}$
	19. Decay of AOBs		$b_{AOB}X_{AOB}$
	20. Decay of NOBs		$b_{NOB}X_{NOB}$
Ammonification/hydrolysis	21. Ammonification of soluble organic nitrogen by bacteria	$\frac{1}{14}$	$k_{A,HB}S_{ND}X_{HB}$
	22. Ammonification of soluble organic nitrogen by fungi	$\frac{1}{14}$	$k_{A,HB}S_{ND}X_{HF}$
	23. Hydrolysis of entrapped organics by bacteria		$k_h(T)\frac{X_S/X_{HB}}{K_{X,HB}+(X_S/X_{HB})}\left[\left(\frac{S_O}{K_O+S_O}\right)+\eta_h\left(\frac{K_O}{K_O+S_O}\right)\left(\frac{\sum S_{NO_X}}{K_{NO_3}+\sum S_{NO_X}}\right)\right]X_{HB}$
	24. Hydrolysis of entrapped organics by fungi		$k_h(T)\frac{X_S/X_{HF}}{K_{X,HF}+(X_S/X_{HF})}\left[\left(\frac{S_O}{K_O+S_O}\right)+\eta_h\left(\frac{K_O}{K_O+S_O}\right)\left(\frac{\sum S_{NO_X}}{K_{NO_3}+\sum S_{NO_X}}\right)\right]X_{HF}$
	25. Hydrolysis of entrapped organic nitrogen		$(R23+R24)\left(\frac{X_{ND}}{X_S}\right)$

Appendix D: Initial range of parameters for the Monte Carlo simulation (step 1) (chapter 5).

Table D.1 Parameter range for the Monte Carlo in step 1.

	Parameter	**Min**	**Max**
Growth rates	$\mathbf{\mu_{HB}}$	0	50
	$\mathbf{\mu_{AOB}}$	0	50
	$\mathbf{\mu_{NOB}}$	0	50
Half-saturation coefficients	$\mathbf{K_s}$	0	200
	$\mathbf{K_{NH}}$	0	5
	$\mathbf{K_{S5}}$	0	200
	$\mathbf{K_{OH}}$	0	0.1
	$\mathbf{K_{NO_3}}$	0	0.1
	$\mathbf{K_{15NO_3}}$	0	0.1
	$\mathbf{K_{NO_2}}$	0	0.1
	$\mathbf{K_{16NO_2}}$	0	0.1
	$\mathbf{K_{NO}}$	0	0.1
	$\mathbf{K_{N_2O}}$	0	0.1
	$\mathbf{K_{FA}}$	0	0.1
	$\mathbf{K_{FNA}}$	0	0.1
	$\mathbf{K_{OA}}$	0	0.1
	$\mathbf{K_{ON}}$	0	0.1
	$\mathbf{K_X}$	0	1
Inhibition coefficients	$\mathbf{K_{I3NO}}$	0	0.1
	$\mathbf{K_{I4NO}}$	0	0.1
	$\mathbf{K_{I5NO}}$	0	0.1
	$\mathbf{K_{I15NO_2}}$	0	0.1
	$\mathbf{K_{INH}}$	0	0.1
	$\mathbf{K_{I11FA}}$	0	0.1
	$\mathbf{K_{I14FA}}$	0	0.1
	$\mathbf{K_{I11FNA}}$	0	0.1
	$\mathbf{K_{I14FNA}}$	0	0.1
Anoxic adjustment factors	$\mathbf{\eta_y}$	0	1
	$\mathbf{\eta_{NO_3}}$	0	1
	$\mathbf{\eta_{NO_2}}$	0	1
	$\mathbf{\eta_{NO}}$	0	1
	$\mathbf{\eta_{N_2O}}$	0	1
	$\mathbf{\eta_H}$	0	1
	$\mathbf{\eta_{AOB}}$	0	1
Decay coefficients	$\mathbf{b_{HB}}$	0	5
	$\mathbf{b_{AOB}}$	0	5
	$\mathbf{b_{NOB}}$	0	5
Hydrolysis and ammonification	$\mathbf{k_{H,HB}}$, $\mathbf{k_{a,HB}}$	0	5
Heat generation	$\mathbf{\Delta H_S}$	0	20000

Appendix E: Parameters of the comprehensive composting model used during validation (chapter 5).

Table E.1 Parameters used during validation of the comprehensive model of chapter 5.

Type	Variable	Description	Units	Value	Reference
Biomass yields	Y_{HB}	Yield coefficient heterotrophic bacteria	g cell TOC formed/g TOC oxidized	0.667	adapted from ASM/Hiatt and Grady (2008)
	Y_{HF}	Yield coefficient heterotrophic fungi	g cell TOC formed/g TOC oxidized	0.667	adapted from ASM/Hiatt and Grady (2008)
	Y_{AOB}	Yield coefficient AOB	g cell TOC formed/g N oxidized	0.48	adapted from ASM/Hiatt and Grady (2008)
	Y_{NOB}	Yield coefficient NOB	g cell TOC formed/g N oxidized	0.06	adapted from ASM/Hiatt and Grady (2008)
	f_p	Fraction of biomass going to inert products	-	0.08	ASM/Hiatt and Grady (2008)
	i_{XB}	Nitrogen content of active biomass	g N/g cell TOC	0.032	adapted from ASM/Hiatt and Grady (2008)
	i_{XP}	Nitrogen content of biomass debris	g N/g debris TOC	0.022	adapted from ASM/Hiatt and Grady (2008)
CO_2, CH_4 and NH_3	Y_{CO_2}	CO_2 yield coefficient	kg CO_2/kg O_2	1.375	Stoichiometry
	K_{PC}^{H}	Henry constant	atm L mol^{-1}	0.04	Sommer et al. (2006)
	R	Gas constant	L Pa mol^{-1} K^{-1}	8.31E3	Known property
Energy balance	ΔH_S	Biological heat generation coefficient	kJ/kg O_2 consumed	14000	Finstein (1986) (see chapter 2)
	H_i	Inlet enthalpy	kJ/kg of air	-	Calculated
	H_o	Outlet enthalpy	kJ/kg of air	-	Calculated
	U	Global heat transfer coefficient	kW (m^2 °C)$^{-1}$	0.05	Known/measured /assumed
	c	Heat capacity of the substrate	kJ (kg °C)$^{-1}$	1.9	Known/measured /assumed

Mass transfer	Y_{H_2O}	Metabolic yield of water	kg H_2O produced/kg O_2 consumed	0.84	Hénon (2008)
	ρ_{DM}	Dry bulk density of the substrate	kg/m^3	600	Measured/Assumed
	ρ_a	Density of air	kg/m^3	1.225	Known property
	ε	Porosity of the bed	-	0.4	Measured/Assumed

Appendix F: Continuity check on the comprehensive composting model (chapter 5)

Table F.1 For a model using chemical oxygen demand (COD) inputs: equivalences of the various model fractions for COD, nitrogen, and charge (alkalinity).

	COD	**Nitrogen (N)**	**Charge (HCO_3^-)**
S_I	1	0	0
S_S	1	0	0
X_I	1	0	0
X_I	1	0	0
X_{HB}	1	0.086	0
X_{HF}	1	0.086	0
X_{AOB}	1	0.086	0
X_{NOB}	1	0.086	0
X_{DP}	1	0.06	0
S_O	-1	0	0
S_{NO3}	-4.57	1	-0.071
S_{NO2}	-3.43	1	-0.071
S_{NO}	-2.86	1	-0.071
S_{N2O}	-2.29	1	-0.071
S_{N2}	-1.72	1	-0.071
S_{NH}	0	1	0.071
S_{ND}	0	1	0
X_{ND}	0	1	0
S_{alk}	0	0	-1

Table F.2 For a model using total organic carbon (TOC) inputs: equivalences of the various model fractions for TOC, nitrogen, and charge (alkalinity).

	TOC	Nitrogen (N)	Charge (HCO_3^-)
S_I	0.373	0	0
S_S	0.373	0	0
X_I	0.373	0	0
X_I	0.373	0	0
X_{HB}	0.373	0.032	0
X_{HF}	0.373	0.032	0
X_{AOB}	0.373	0.032	0
X_{NOB}	0.373	0.032	0
X_{DP}	0.373	0.023	0
S_O	-0.373	0	0
S_{NO3}	-1.705	0.373	-0.027
S_{NO2}	-1.279	0.373	-0.027
S_{NO}	-1.067	0.373	-0.027
S_{N2O}	-0.854	0.373	-0.027
S_{N2}	-0.642	0.373	-0.027
S_{NH}	0	0.373	0.027
S_{ND}	0	0.373	0
X_{ND}	0	0.373	0
S_{alk}	0	0	-0.373

Table F.3 Continuity check on the comprehensive model.

		1	2	3	4	5	6	7	8	9	10	11	12
	Process	S_I	S_S	X_I	X_S	X_{HB}	X_{FH}	X_{AOB}	X_{NOB}	X_{DP}	S_O	S_{NO3}	S_{NO2}
Bacteria	1. Aerobic growth of HB		-1.4993			1					-0.49925		
	2. Anoxic growth of HB on nitrate		-1.6658			1						-0.58253	0.58253
	3. Anoxic growth of HB on nitrite		-1.6658			1							-1.16608
	4. Anoxic growth of HB on nitric oxide		-1.6658			1							
	5. Anoxic growth of HB on nitrous oxide		-1.6658			1							
Fungi	6. Aerobic growth of HF		-1.4993				1				-0.49925		
	7. Anoxic growth of HF on nitrate		-1.6658				1					-0.58253	0.58253
	8. Anoxic growth of HF on nitrite		-1.6658				1						-1.16608
	9. Anoxic growth of HF on nitric oxide		-1.6658				1						
	10. Anoxic growth of HF on nitrous oxide		-1.6658				1						
Ammonia oxidizing bacteria	11. Aerobic growth of AOBs							1			-18.05556		5.55555
	12. AOB denitrification of NO_2		-0.57										-1
	13. AOB denitrification of N_2O		-0.57										

		13	14	15	16	17	18	19	**Continuity on**		
	Process	S_{NO}	S_{N2O}	S_{N2}	S_{NH}	S_{ND}	X_{ND}	S_{alk}	C	N	Charge
Bacteria	1. Aerobic growth of HB				-0.086			-0.00614	-5.55E-17	-7.8E-5	1.35E-5
	2. Anoxic growth of HB on nitrate				-0.086			-0.00614	-6.52E-4	7.8E-5	1.35E-5
	3. Anoxic growth of HB on nitrite	1.16608			-0.086			-0.00614	-4.35E-4	7.8E-5	1.35E-5
	4. Anoxic growth of HB on nitric oxide	-1.16608	1.16608		-0.086			-0.00614	-4.35E-4	7.8E-5	1.35E-5
	5. Anoxic growth of HB on nitrous oxide		-1.16608	1.6608	-0.086			-0.00614	-4.35E-4	7.8E-5	1.35E-5
Fungi	6. Aerobic growth of HF				-0.086			-0.00614	-5.55E-17	7.8E-5	1.35E-5
	7. Anoxic growth of HF on nitrate				-0.086			-0.00614	-6.52E-4	7.8E-5	1.35E-5
	8. Anoxic growth of HF on nitrite				-0.086			-0.00614	-4.35E-4	7.8E-5	1.35E-5
	9. Anoxic growth of HF on nitric oxide				-0.086			-0.00614	-4.35E-4	7.8E-5	1.35E-5
	10. Anoxic growth of HF on nitrous oxide				-0.086			-0.00614	-4.35E-4	7.8E-5	1.35E-5
Ammonia oxidizing bacteria	11. Aerobic growth of AOBs				-5.6416			-0.79979	8.88E-16	7.8E-5	9.29E-5
	12. AOB denitrification of NO_2	1							2.22E-16	0	0
	13. AOB denitrification of N_2O	-1	1						-1.11E-16	0	0

		1	2	3	4	5	6	7	8	9	10	11
	Process	S_I	S_S	X_I	X_S	X_{HB}	X_{FH}	X_{AOB}	X_{NOB}	X_{DP}	S_O	S_{NO3}
Nitric oxidizing bacteria	14. Aerobic growth of nitric oxidizing bacteria								1		-18	16.66667
Reduction of nitrate to ammonia	15. Assimilative nitrate reduction to nitrite		-1.14									-1
	16. Assimilate nitrate reduction to ammonia		-3.43									
Decay	17. Decay of heterotrophic bacteria				0.92	-1				0.08		
	18. Decay of heterotrophic fungi				0.92		-1			0.08		
	19. Decay of AOBs				0.92			-1		0.08		
	20. Decay of NOBs				0.92				-1	0.08		
Ammonification/hydrolysis	21. Ammonification of soluble organic nitrogen by bacteria											
	22. Ammonification of soluble organic nitrogen by fungi											
	23. Hydrolysis of entrapped organics by bacteria		1		-1							
	24. Hydrolysis of entrapped organics by fungi		1		-1							
	25. Hydrolysis of entrapped organic nitrogen											

		12	13	14	15	16	17	18	19	**Continuity on**		
	Process	S_{NO2}	S_{NO}	S_{N2O}	S_{N2}	S_{NH}	S_{ND}	X_{ND}	S_{alk}	C	N	Charge
Nitric oxidizing bacteria	14. Aerobic growth of nitric oxidizing bacteria	16.66667				-0.086			-0.00614	0	-7.8E-5	1.35E-5
Reduction of nitrate to ammonia	15. Assimilative nitrate reduction to nitrite	-1	1							0	0	0
	16. Assimilate nitrate reduction to ammonia		-1			1			0.14286	2.20E-16	0	-1.43E-5
Decay	17. Decay of heterotrophic bacteria							0.0812		2.43E-17	8.76E-5	0
	18. Decay of heterotrophic fungi							0.0812		2.43E-17	8.76E-5	0
	19. Decay of AOBs							0.0812		2.43E-17	8.76E-5	0
	20. Decay of NOBs							0.0812		2.43E-17	8.76E-5	0
Ammonification/hydrolysis	21. Ammonification of soluble organic nitrogen by bacteria					1	-1		0.07143	0	0	-1.57E-4
	22. Ammonification of soluble organic nitrogen by fungi					1	-1		0.07143	0	0	-1.57E-4
	23. Hydrolysis of entrapped organics by bacteria									0	0	0
	24. Hydrolysis of entrapped organics by fungi									0	0	0
	25. Hydrolysis of entrapped organic nitrogen						1	-1		0	0	0

Appendix G: Publications and communications undertaken during the course of this PhD.

Journal articles:

- Walling E, Vaneeckhaute C. PCM, a parsimonious composting model for optimization and decision-making. Bioresource Technology (Under Review)

- Walling E, Vaneeckhaute C. Modelling composting kinetics: An evaluation of temperature, moisture and oxygen correction functions. Compost Science & Utilization. (Under Review)

- Vaneeckhaute C, Walling E, Rivest S, Belia E, Chartrand I, Fortin F, Mostafavi M. (2021). Towards an integrated decision-support system for sustainable organic waste management. npj Urban Sustainability, 1(1), 1-6.

- Walling E, Vaneeckhaute C. (2021). Novel simple approaches to modelling composting kinetics. Journal of Environmental Chemical Engineering, 9:3, 105243.

- Walling E. Vaneeckhaute C. (2020) Greenhouse gas emissions from inorganic and organic fertilizer production and use: A review of emission factors and their sources of variability. Journal of Environmental Management, 276, 111211.

- Walling E, Trémier A, Vaneeckhaute C. (2020). A review of mathematical models for composting. Waste Management, 113, 379-394.

- Walling E, Vaneeckhaute C. (2020). Developing successful environmental decision support systems: Challenges and best practices. Journal of Environmental Management, 264, 110513.

Book chapters:

- Walling E, Moerman W, Verstraete W, Vaneeckhaute C. (2021) Resource recovery from industrial wastewater: What and how much is there? In Resource Recovery from Water: Principles and Application. IWA publishing.

- Walling E, Vaneeckhaute C. (2021). Nitrogen fertilizers and the environment. Ed. Tsadilas C - In Nitrate Handbook: Environmental, Agricultural and Health Effects. CRC Press Taylor and Francis.

- Walling E, Babin A, Vaneeckhaute, C. (2019). Nutrient and Carbon Recovery from Organic Wastes. In Biorefinery (pp. 351-373). Springer, Cham.

International conferences:

- Walling E, Vaneeckhaute C. (2021). A comprehensive mathematical model to optimize nutrient recovery and recycling during composting. 4th IWA Resource Recovery Conference, 2021. Virtual. (Oral)

- Walling E, Vaneeckhaute C. (2021). The importance of considering emissions variability in environmental and sustainability analyses. 17th International Conference on Renewable Resources and Biorefineries. Aveiro, Portugal. (Oral)

- Walling E, Vaneeckhaute C. (2021). Optimizing nutrient recycling from composting through modelling. 17th International Conference on Renewable Resources and Biorefineries. Aveiro, Portugal. (Poster)

- Walling E, Belia E, Vaneeckhaute C. (2021). Enhancing nutrient recovery and reducing GHG emissions from composting through modeling. WEF Innovations in Process Engineering 2021. Virtual. (Oral)

- Walling E, Vaneeckhaute C. (2021). The role of decision support systems in promoting sustainable development and knowledge use. 5th CIGR International Conference, virtual. (Oral)

- Walling E, Vaneeckhaute C. (2021). Greenhouse gas emissions from fertilizers: The necessity for case-specific emissions data for environmental assessments of agricultural systems. 5th CIGR International Conference, virtual. (Oral)

- Walling E, Rivest S, Mostafavi M, Vaneeckhaute C. (2019). The challenges and opportunities of getting digestate to market in sparsely populated areas: a case study of Quebec. ManuREsource, Hasselt, Belgium. (Oral)

- Walling E, Vaneeckhaute C. (2019). How important are GHG emissions from organic fertilizers? A comparison with inorganic fertilizers and best practices. ManuREsource, Hasselt, Belgium. (Oral)

- Cormier N, Walling E, Vaneeckhaute C. (2019). Developing a novel treatment train for nutrient recovery from digestate combining ammonia recovery and membrane bioreactors. ManuREsource, Hasselt, Belgium. (Oral)

- Walling E, Belia E, Vaneeckhaute C. (2019). The current state of composting modelling and the need for a better understanding of these microbial ecosystems. The International Society for Ecological Modelling Global Conference 2019, Salzbourg, Autriche. (Oral) (Accepted)

- Walling E, Rivest S, Belia E, Mostafavi M, Vaneeckhaute C. (2019). Towards integrated spatio-temporal and socio-ecological modelling of organic waste valorization chains. The International Society for Ecological Modelling Global Conference 2019, Salzbourg, Autriche. (Affiche) (Accepted)

- Vaneeckhaute C, Walling E, Belia E, (2019). Nutrient and energy recovery from pig manure and sludge: Economic optimization using a new process model library. Agro2019, Rhodes, Grèce. (Oral)

- Vaneeckhaute C, Walling E, Styles D, Prade T, Adams P, Thelin G, Rodhe L, D'Hertefeldt T, (2019). Decentralized recycling of digestated wastes in agricultural regions: A multi-dimensional sustainability assessment. Agro2019, Rhodes, Grèce. (Oral)

- Walling E, Vaneeckhaute C. (2019). Critical comparison of conversion technologies for organic waste valorization. Value of Biogas East, Toronto Eaton Center, ON, Canada (Invited poster)

- Vaneeckhaute C, Walling E, Rivest S, Belia E, Fortin F, Mostafavi M. (2019). Optim-O : Decision-support system for organics valorization. Value of Biogas East, Toronto Eaton Center, ON, Canada (Invited poster)

- Walling E, Rivest S., Mostafavi M., Vaneeckhaute C. (2018). Outil d'aide à la décision pour la valorisation des matières organiques résiduelles au Québec. 15^{e} conférence biogaz et bioénergie, Centre de congrès, Saint-Hyancinthe, QC, Canada (Invited poster)

<u>Other publication/presentations:</u>

- Fréchette J, Walling E, Vaneeckhaute C, Messaddeq Y. (2021) New insight on the use of cellulose-based membranes for wastewater treatment and reclamation in northern regions. Sentinelle Nord Scientific Meeting 2021, virtual. (Oral and Poster)

- Vaneeckhaute C, Walling E, Boleydei H, Fréchette J, Messaddeq Y. (2021) Development of a wastewater treatment train adapted to northern regions. Sentinelle Nord Scientific Meeting 2021, virtual. (Oral and Poster)

- Walling E, Boleydei H, Fréchette J, Messaddeq Y, Vaneeckhaute C. (2021) Development of a wastewater treatment system by membrane bioreactor designed for the northern reality. Sentinelle Nord Scientific Meeting 2021, virtual. (Poster)

- Walling E, Vaneeckhaute C. (2021) Exploring novel avenues to sewage sludge digestate conditioning. Journée Québécoise des étudiants CentrEau 2021, virtual. (Oral)

- Walling E, Rivest S, Mostafavi M, Vaneeckhaute C. (2020) Outil d'aide à la décision pour la valorisation des matières organiques résiduelles au Québec. Journée Québécoise des étudiants CentrEau 2020, Montreal, Canada. (Poster)

- Walling E. (2019). Challenges and opportunities for biomethanation and composting in Quebec. Journée de la Recherche en Sciences et Génie, Québec, Canada. (Oral)

- Veillette D, Walling E, Jamaludin Z, Vaneeckhaute C. (2019). Valorisation de biochars issus de boues municipales comme adsorbant pour la récupération de l'ammonium. Journée de la Recherche en Sciences et Génie, Québec, Canada. (Poster)

- Walling E. (2019). Towards the development of a decision support system for the valorization of organic residual matter. Chemical engineering research day, Polytechnique Montréal, QC, Canada (Oral)

- Walling E, Vaneeckhaute C. (2019). Optimiser l'efficacité de l'économie circulaire : Défis et solutions. Conseil canadien du compost : Le Compost ça compte!, Centre de recherche industriel du Québec, QC, Canada (Oral)

- Mostafavi M, Rivest S, Walling E, Vaneeckhaute C. (2018). Un outil géospatial multidimensionnel d'aide à la décision pour l'optimisation de la chaîne de valorisation des matières résiduelles. Géomatique; 45(1): 22-25.

- Walling E, Mostafavi M, Belia E, Fortin F, Vaneeckhaute C. (2018). Review of decision-support systems for bio-waste valorization. Journée de réseautage du Département de génie chimique, Université Laval, QC, Canada. (Oral)