PERSPECTIVE OPENImage: Check for updatesIntegrating resource recovery process and watershed modelling
to facilitate decision-making regarding bio-fertilizer
production and application

Céline Vaneeckhaute ^[][™]

Waste management strategies such as anaerobic digestion and composting produce bio-based fertilizer products that could be applied to agricultural soil. Although multiple modelling software tools are available to simulate the environmental effect of fertilizer application to the soil, these models do not allow specification of emerging bio-based fertilizer types. Moreover, mathematical process models exist that allow optimizing the operational settings of waste management processes in order to produce an optimal bio-fertilizer quality adjusted to the local market needs. If an integrated tool would be available that couples process modelling to watershed modelling, the valorization chain could be simulated as a whole, i.e. the bio-fertilizer type and composition could be adjusted to the local watershed and environmental impacts of bio-based fertilizer production and application could more easily be assessed and controlled. The availability of such integrated tool may as such allow for improved decision and policy making regarding bio-fertilizer production and application with environmental benefits as a result.

npj Clean Water (2021)4:15; https://doi.org/10.1038/s41545-021-00105-6

EMERGING BIO-FERTILIZER PRODUCTS

With increasingly strict environmental regulations worldwide, the implementation of waste management strategies targeting nutrient recovery and reuse has been increasing at a rapid pace^{1–4}. Particularly, anaerobic digestion and composting projects for organic waste valorization are booming across the world. These processes produce nutrient-rich products that could be valorized in the agricultural sector. Liquid digestates, the remaining product after conventional wet anaerobic digestion, can however rarely be applied to agricultural fields in their crude unprocessed form. Nutrient recovery technologies have therefore been invented over the last decades in order to produce concentrated fertilizer products, that can compete with synthetic fertilizers currently on the market⁵. Popular recovered fertilizer types include ammonium sulfates and struvite (magnesium ammonium phosphates)⁵. Ammonium sulfate can be recovered through the stripping and subsequent scrubbing of ammonia from polluted water sources⁶, whereas struvite can be recovered through the precipitation and crystallization of phosphorus at increased pH⁷. Struvite could be classified as a slow release fertilizer rich in the macronutrients phosphorus (P), nitrogen (N), and magnesium (Mg), whereas ammonium sulfates could be classified as a liquid mineral fertilizer rich in the macronutrients nitrogen (N) and sulfur (S)⁵. Although field trials provide evidence of their fertilizer value, marketing of these products remains challenging, either due to regulatory constraints, farmers' distrust, or limitations related to social acceptability⁵.

CURRENT STATE IN PROCESS MODELLING

Along with the technological developments described above, mathematical process models for waste management and nutrient recovery have seen growing development^{8–14}. One of the key tools currently available is the nutrient recovery model

(NRM) library¹⁴. It includes advanced mathematical process models for anaerobic digestion, struvite precipitation, and ammonium sulfate production through stripping and scrubbing. Since nutrient recovery processes mainly involve physicochemical reactions, the reaction chemistry should be included in these mathematical process models. One feasible approach to do so is to couple geochemical databases such as PHREEQC or MINTEQC to the dynamic process models for equilibrium calculation of chemical speciation, saturation indexes, and gas partial pressures at every time step during model simulations¹⁴. The latter then determine the driving forces for minerals precipitation/dissolution and gas transfer. As such, the models are capable of predicting mineral bio-based fertilizer properties such as the nutrient composition, particle size and purity, for variable input streams and operating conditions. The organic nutrient fraction, for example for digestate, is generally estimated as a percentage of the solids content¹⁴.

CURRENT STATE IN WATERSHED MODELLING

Over the last 50 years, multiple watershed models have been developed in an attempt to evaluate the effects of alternative management decisions on water resources and nonpoint-source pollution in large river basins¹⁵. Watershed models describe complex interactions of various terrestrial components such as precipitation, wet and dry atmospheric deposition, impact of diffuse pollution, chemicals in fertilizers and pesticides, and emissions and impact of traffic¹⁵. One of the most popular available tools is SWAT (Soil & Water Assessment Tool), which is a river basin scale model actively supported by the USDA Agricultural Research Service and developed to quantify the impact of land management practices in large, complex watersheds. SWAT operates on a daily time step and is designed to predict the impact of land use and management on water,

¹BioEngine, Research Team on Green Process Engineering and Biorefineries, Chemical Engineering Department, Université Laval, Québec, QC, Canada. ^{Ele}email: celine. vaneeckhaute@gch.ulaval.ca



C. Vaneeckhaute

sediment, and agricultural chemical yields in ungauged watersheds¹⁶. As such, potential nutrient pollution through fertilizer application can be predicted by providing estimations of plant uptake, runoff and leaching.

THE NEED FOR INTEGRATED MODELS

The interest for coupling process models to watershed models has risen from discussions and brainstorms within a stakeholder group of the Sustainable Phosphorus Alliance, i.e., the phosphorus transport modelling group (https://phosphorusalliance.org/ modeling-group/). Due to the fact that nutrient recovery processes are often physicochemical in nature, there exists a certain flexibility in operating and combining them, thereby adjusting the bio-based fertilizer type and composition to the local market needs. Moreover, at waste and wastewater treatment plants, multiple nutrient recovery processes can be installed in series. These processes are typically interdependent¹⁷. Hence, the process chain should be optimized as a whole in order to produce various interesting products, that may in some cases also be combined into one single formulated product all while minimizing costs and environmental impact. Decisions regarding technologies to be implemented or bio-based fertilizer(s) to be produced have to date often been made based on technical-economic process considerations, thereby often underestimating the importance of the fertilizer market value and applications in the initial stages of waste management projects. Hence, combined with the regulatory and societal limitations identified above, waste and wastewater treatment facilities often struggle to find a market for the produced end products, meaning that the products either have to be transported far away or have to be disposed of, both situations resulting in additional and seemingly unnecessary costs.

On the other hand, fertilizer application limits and restrictions are based on the watershed's water quality. As such, fertilizer demand is location-dependent and case specific. Hence, the interest of integrating process and watershed models relies in the fact that bio-based fertilizer production could be better adjusted to the watershed needs. Indeed, the resource recovery process chain and its operational settings (e.g., substrate ratios in anaerobic digestion, duration of composting, and pH for phosphorus precipitation) could be adjusted to simulate various bio-fertilizer production scenarios along with an assessment of their impact on watershed quality. This would allow more rapid and improved decision-making regarding bio-based fertilizer types to be produced in the region of the watershed under study and their production process.

CHALLENGES AHEAD

The overall concept of the proposed integrated modelling strategy is presented in Fig. 1. With regard to the process models, we propose the use of simplified or parsimonious mathematical models appropriately reflective of reality, with key parameters and equations in a software that allows easy integration with SWAT, for example Excel or Matlab. Indeed, an optimal balance is aimed between model accuracy and simulation times. Sensitivity analyses should be performed in order to select the most important parameters to be included in these models. Output parameters should be matched with input parameters needed for SWAT. SWAT itself should on the other hand be extended so that it allows to specify the key characteristics of alternative bio-based fertilizers, and to estimate the rate of integration of surfaceapplied nutrients (nitrogen and phosphorus) from these fertilizers into soil nutrient pools. Field data available from the various stakeholders within the Sustainable Phosphorus Alliance can be used for this purpose. Ideally, the integrated model would allow to provide quantitative outputs regarding crop uptake, nutrient runoff and leaching through the application of bio-based fertilizer



Fig. 1 Concept of integrated process and watershed modelling. Blue arrows represent nutrient flows. Interactions between process models and watershed models are marked. Image reuse permission: 1) wastewater treatment, Unsplash, Ivan Bandura, https://unsplash.com/; 2) anaerobic digestion, personal picture, Céline Vaneeckhaute; 3) composting, personal picture, Tania Santiago; 4) struvite fertilizer, Microsoft Bing Creative Commons, Ostara Nutrient Recovery, www.ostara.com, 5) liquid fertilizer, personal picture, Céline Vaneeckhaute; 6) compost, Unsplash, Gabriel Jimenez, https://unsplash.com/; 7) field application, Unsplash, Naseem Buras, https://unsplash.com/; 8) watershed, Wikimedia Commons, Unknown Author Public Domain, File:Mississippi River Watershed.gif - Wikimedia Commons.

 $\frac{np}{2}$

products. This would allow to select the optimal bio-based fertilizer to be produced and applied nearby the watershed under study. Although such problem could likely also be assessed without integrating process and watershed modelling (by using the models separately), the integration makes it possible to estimate and minimize the impact of upstream process-related choices on the watershed quality, e.g., which organic waste sources to be treated by anaerobic digestion and what is the optimal ratio of these substrates in order to reduce the impact of the resulting digestates on the local watershed's water quality. Hence, overall decision-making and holistic optimization regarding bio-fertilizer production and application can be facilitated and improved.

OUTLOOK

The availability of the integrated tool will help to reduce the environmental impact of waste management and bio-fertilizer use on local watersheds. Indeed, by providing a better link between upstream resource recovery processes and downstream markets for bio-based fertilizer products, decision-making regarding bio-fertilizer types and compositions to be produced in a certain region may be facilitated and improved. The tool can also help in assessing the efficiency of environmental best management practices and alternative waste/fertilizer management policies.

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Received: 4 November 2020; Accepted: 21 January 2021; Published online: 26 February 2021

REFERENCES

- Buckwell, A. & Nadau, E. Nutrient Recovery and Reuse (NRR) in Europe agriculture: A Review of the Issues, Opportunities, and Actions (The Rise Foundation, 2016). https://www.nutrientplatform.org/wp-content/uploads/2016/09/Nutrient-Recovery-and-Reuse-in-European-Agriculture.pdf
- IISD. Nutrient Recovery and Reuse in Canada: Foundations for a National Framework (International Institute for Sustainable Development, 2018).
- Murray, H. G. R. Bill 151, Waste-Free Ontario Act (Ministry of the Environment and Climate Change, 2016).
- USEPA. NutrientSmart (NSmart) (United States Environmental Protection Agency, 2019). https://www.epa.gov/nutrient-policy-data/nutrientsmart-nsmart
- 5. Vaneeckhaute, C. et al. Nutrient recovery from digestate: systematic technology review and product classification. *Waste Biomass.* **8**, 21–40 (2017).
- Jamaludin, Z., Rollings-Scattergood, S., Lutes, K. & Vaneeckhaute, C. Evaluation of sustainable scrubbing agents for ammonia recovery from anaerobic digestate. *Bioresour. Technol.* 270, 569–602 (2018).
- 7. Rahman, M. M. et al. Production of slow release crystal fertilizer from wastewaters through struvite crystallization: a review. *Arab. J. Chem.* **7**, 139–155 (2014).
- Yu, L., Zhao, Q., Jiang, A. & Chen, S. Analysis and optimization of ammonia stripping using multi-fluid model. *Water Sci. Technol.* 63, 1143–1152 (2011).
- 9. Batstone, D. J. et al. Towards a generalized physicochemical framework. *Water Sci. Technol.* **66**, 1147–1161 (2012).
- Flores-Alsina, X. et al. Modelling phosphorus (P), sulfur (S) and iron (Fe) interactions for dynamic simulations of anaerobic digestion processes. *Water Res.* 95, 370–382 (2016).

- Lizarralde, I. et al. A new general methodology for incorporating physicochemical transformations into multi-phase wastewater treatment process models. *Water Res.* 74, 239–256 (2015).
- Mbamba, C. K., Flores-Alsina, X., Batstone, D. J. & Tait, S. Validation of a plant-wide phosphorus modelling approach with minerals precipitation in a full-scale WWTP. *Water Res.* 100, 169–183 (2016).
- Solon, K. et al. Plant-wide modelling of phosphorus transformations in wastewater treatment systems: impacts of control and operational strategies. *Water Res.* 113, 77–110 (2017).
- Vaneeckhaute, C. et al. Development, implementation, and validation of a generic nutrient recovery model (NRM) library. *Environ. Model. Softw.* **99**, 170–209 (2018a).
 Novotny, V. Watershed Models, Encyclopedia of Ecology (Elsevier, 2009)
- Arnold, J. G. et al. SWAT: model use, calibration and validation. *Trans. ASABE* 55, 1491–1508 (2012).
- Vaneeckhaute, C. et al. Optimizing the configuration of integrated nutrient and energy recovery treatment trains: a new application of global sensitivity analysis to the generic nutrient recovery model (NRM) library. *Bioresour. Technol.* 269, 375–383 (2018b).

ACKNOWLEDGEMENTS

Céline Vaneeckhaute is financially supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) through the award of an NSERC Discovery Grant (RGPIN-2017-04838). She also holds the Canada Research Chair in Resource Recovery and Bioproducts Engineering. The author would like to thank the Sustainable Phosphorus Alliance for their initiative to set up a phosphorus transport modelling group (https://phosphorusalliance.org/modeling-group/).

AUTHOR CONTRIBUTIONS

Céline Vaneeckhaute conceptualised the work, drafted and revised the paper, and approved to the final version of the paper. She is accountable for all aspects of the work in ensuring that questions related to the accuracy or integrity of any part of the work are appropriately investigated and resolved.

COMPETING INTERESTS

The author declares no competing interests.

ADDITIONAL INFORMATION

Correspondence and requests for materials should be addressed to C.V.

Reprints and permission information is available at http://www.nature.com/ reprints

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons license, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons license and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this license, visit http://creativecommons. org/licenses/by/4.0/.

© The Author(s) 2021