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Coelho, Lineker Goulart

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Towards a framework to incorporate metagenomics in ecological modeling of lake water quality simulations: challenges and perspectives

Lineker Max Goulart Coelho

Nowadays, lake water quality modeling presents highly embedded advanced models for hydraulic simulations and physico-chemical processes but normally considers biological processes and biodiversity using a simplified kinetics species-based approach [1]. In this context, with the availability of metagenomics, bioinformatic methods can support the development of new ecological models representing biochemical processes for different biogeochemical cycles like carbon, nitrogen, phosphorus, etc. combining gene expression data and conventional water quality parameters to simulate ecosystem dynamics [2, 3]. So, further studies in this area are needed and will represent a turning point in terms of the accuracy of such models as well as from the point of view of the usefulness of metagenomics in supporting policymakers. The goal of this study is to provide an overview of challenges and perspectives concerning a framework addressed to incorporate metagenomics data to enhance biochemical processes in ecological water quality modeling. So, this study intends to use a gene function perspective based on metagenomics data to support lake ecosystem prevision modeling addressing water quality forecasting. To accomplish these goals a literature review was carried out followed by a critical analysis and a conceptual framework was developed. From previous works, it is noted a lack of available models exploring metagenomics-based models not only for lake ecosystem prediction models but also for aquatic systems as a whole. On the other hand, some pilot systems based on linear optimization and single objective models reveals promising results of bioinformatic practical use as inputs in water quality modeling, but they do not consider hydraulic simulations or chemical process [4]. In this context, the combination of Stochastic Community Models based on spatial data from metagenomics sampling can be used to calibrate a function-expression biochemical model embedded in Computational Fluid Dynamics (CFD) simulations, which will enable a much more detailed estimation of ecosystem biological dynamics and behaviour. This prospective study revealed an important scientific gap in water quality modeling altogether with some directions and perspectives for a framework addressing a more holistic approach. Such models can support decision-making in long-term depollution plans as well as in predicting emergency algae bloom events.

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