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Are our models keeping pace with the evolving data deluge?

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Abstract: Environmental sensors collect information on a broad suite of variables at a range of spatial and temporal scales. At one extreme are remote sensing devices on satellites that provide information at regular intervals (days) over scales of tens to hundreds of metres. At the other extreme are in situ sensors that collect data from a fixed point at intervals of seconds to minutes. The integration and harmonisation of these data (see O'Grady et al. 2021) provide an unprecedented opportunity to test the predictive capability of process based models. The question arises: are we fully utilising this opportunity to improve our water models?

High frequency data can greatly increase the number of measurements available for comparison with state variable outputs from dynamic models, as well as supporting determination of kinetic parameters from rates of change of variables. For example, high frequency measurements of dissolved oxygen in water can be compared directly to modelled dissolved oxygen or used to derive indices like lake metabolism, as well being useful for quantifying key kinetic parameters like production and respiration. Variables such as temperature and dissolved oxygen, with appropriate quality control/quality assurance, are highly suitable for these types of assessments. Some variables measured with sensors (e.g., turbidity, chlorophyll fluorescence) require careful and skilled interpretation because they may only be proxies for model state variables and are often subject to a number of interferences. For this reason, sensors require user expertise through a full sequence of probe selection, deployment, calibration and quality assurance/quality control (QA/QC).

I contend that for a number of reasons, modellers have not yet exploited the potential of sensor data for model calibration and validation. First, compensation for sensor interference is often inadequate and readings can be misinterpreted; QA/QC of data is critical. Second, comparisons of measurements against model state variables remain the 'standard' for calibrating models. This option may be suitable for sparse, non-sensor data but it negates opportunities for direct calculation of kinetic parameters from, for example, using first and second time derivatives of sensor data (i.e., to identify rates of change and inflection points, respectively). Third, working with sensor data requires strong disciplinary expertise – similar to working with numerical models – and we need to break the disciplinary shackles to harmonise data and develop data assimilation techniques to drive model simulations and align measured proxies with state variables in models.

For calibration of water quality models, we often still rely on routine water sampling (e.g., collecting 'grab samples') at a measurement frequency that is orders of magnitude less than that used for sensors. This problem is relevant to many of the water quality issues that interest managers, e.g., whether an algal bloom will appear; the level of water contamination by pathogens; and whether nutrient levels are high enough to trigger water quality problems (e.g., deoxygenation of bottom waters). However, a new generation of smart field sensors that uses optical chemical and biosensors, automated eDNA methods and miniaturised laboratory instruments is beginning to address the issue of disparity of monitoring frequency for biogeochemical constituents that is relevant to models. Integration of data from these sensors into well-established sensor networks should enable the development of a new generation of biogeochemical algorithms for water models and allow us to progress beyond the lumped state variable approaches and Michaelis-Menten kinetics descriptions that characterise most current applications. With these advances, we will be in a better position to apply process based models to address the specific questions of relevance to water managers and narrow the confidence intervals of model projections.

REFERENCE

O'Grady, J., Zhang, D., O'Connor, N., Regan, F., 2021. A comprehensive review of catchment water quality monitoring using a tiered framework of integrated sensing technologies. Science of the Total Environment 765:142766.

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