Hydrology & Water Resources Symposium
12-15 November | Sydney

ENGINEERS AUSTRALIA | National Committee on Water Engineering

ISBN number for HWRS 2023 is 978-1-925627-81-7

A New Approach to Integrated Environmental Modelling

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ABSTRACT

Linking catchment hydrology and pollutant export models with downstream hydrodynamic and water quality receiving models has underpinned environmental catchment management for decades. Despite this state of practice, there has been an equally long-standing disconnect between the conceptual, scientific and computational approaches taken by linked catchment and receiving models. This paper presents a new GPU accelerated platform for holistic catchment simulation that overcomes these disconnects and through automation eliminates error prone legacy model linking tasks. This platform executes direct rainfall (rain-on-grid) calculations in the catchment domain, and solves the shallow water and transport equations to predict surface runoff and pollutant export at gridded spatial scales of tens of metres, and at timesteps of seconds. It also simulates associated subsurface flows and pollutant transport, and automatically locates and generates inflow conditions for use in a downstream three dimensional receiving model, which it then executes. This innovative, novel platform is described, and a selection of calibration results from the application to a catchment is presented as a proof-of-concept.

INTRODUCTION

Numerical modelling has long been used to quantitatively inform environmental management via the deployment of manually coupled catchment (upstream) and receiving water quality (downstream) models. Although this coupling has been commonplace for some time, it has often been problematic for a range of scientific and practical reasons, including (but not limited to):

- A divergence in the currency of the underlying science of the coupled models, with the scientific rigour of the receiving model sometimes not being mirrored by the catchment model
- Confounding conceptual disconnects in linking models of materially different time and space discretisations and pollutant type predictions (e.g. total versus speciated nutrients, minutes vs daily timesteps), and
- The nontrivial potential for human error in executing inter-model data translation

Given this, an upgraded and properly integrated whole-of-system modelling platform has been developed with the support of the Queensland Government through the Queensland Water Modelling Network (QWMN) and Healthy Land and Water (HLW). Brisbane City Council (BCC) kindly provided some environmental data sets to support this project. The key intent has been to realign catchment and receiving water quality modelling to best practise standards, and therefore fully exploit current scientific and compute capabilities to better support management of our shared natural resources. This paper describes briefly both the platform itself and a small suite of outcomes from its pilot application to the Oxley Creek catchment, Queensland. The latter develops an initial understanding of the impact applying a robustly constructed hydrologic and pollutant export catchment model has on predicting downstream water quality dynamics. Importantly, proof-of-concept has been established through validation to hydraulic and environmental measurements.

METHODS

A New Platform

Overarching Platform

A key functional requirement of the new modelling platform (other than it be scientifically robust, field validated, and have strong predictive power) was that it present to the user a single, integrated and one-stop modelling interface that automates the synchronisation, linking and execution of underlying numerical engines. These underlying engines together simulate catchment scale hydrologic, hydraulic, pollutant export and transport, and receiving water processes. To do so, this platform draws on the power of two existing (and enhanced) TUFLOW products and – most importantly – removes the user burden of manually integrating and interrogating models deployed on typical whole of catchment scales. These existing TUFLOW products are:

- TUFLOW HPC, having been enhanced to deliver this new platform, computes:
    - Catchment surface and subsurface hydrology, and routing by using rain-on-grid (direct rainfall) methods and a full 2D solution of the fluid flow equations
    - Drainage structure hydraulics (such as 1D culvert and bridge flow) using well established methods commonly applied in flood studies
    - Catchment pollutant export (also in 1D and 2D) using a first principles export model, and subsequently solving the equations of constituent transport to route pollutants with the above surface and subsurface hydrology and hydraulics
    - Resultant highly resolved (both temporally and spatially) catchment based inflow volumes and pollutant loads for delivery to a downstream receiving waterway model (TUFLOW FV) as inflow boundary conditions
- TUFLOW FV, that computes:
    - Three dimensional in stream hydrodynamics, sediment transport and water quality dynamics, automatically using the inflow boundary conditions developed and preprocessed by TUFLOW HPC above

Key features of the new platform are as follows. It:

- Allows the user to build, from scratch, TUFLOW HPC (catchment and rivers/creeks) and TUFLOW FV (receiving water) models from a single unified control file that points directly to all underlying data sets and lower tier commands
- Draws on the scientific rigour and computational power of the TUFLOW suite of products
- Automatically determines the locations at which catchment inflows enter the receiving model, and therefore links the TUFLOW HPC and TUFLOW FV models without user intervention

- Has its outputs combined and interrogated as a single data set, which allows on-the-fly results interpretation of catchment and receiving water predictions in a single coordinated interface

Upgrades to TUFLOW HPC (Catchment Model)

TUFLOW HPC has allowed simulation of rain on grid surface and limited subsurface hydrology for some time (Ryan et al. 2022). In order to support the needs of the modelling platform described here, the following enhancements were made to TUFLOW HPC in addition to those described in the 2023-03 TUFLOW Release Notes:

- Material based (i.e. spatially variable at the discretion of the user) surface generation of constituent pollutant loads. A runoff properties file allows the user to specify the choice of pollutant generation model and required input parameters for each constituent for each surface material. This avoids the need for lumping, and allows setting pollutant models and parameters for individual sites that may be of interest, such as known gully erosion locations
- Accumulation of constituents. A new "dry store" surface layer for pollutants was introduced. A generation model can then be directed as to whether it liberates a constituent during dry weather only, wet weather only, or both, and whether the constituent is assigned to the dry store, or the wet (dissolved) surface field for subsequent transport
- Wet weather release of constituents. The generation model determines dry store field to wet field pollutant conversion, including use of a time of concentration, T_c. Once in the wet field, a constituent will advect with the surface water and may (see next point), infiltrate to groundwater. User defined minimum rainfall intensity (mm/hr) and minimum cell depth (m) can be set, and both need to be exceeded before the dry store is released to the wet field
- Selective infiltration of constituents. Constituents can be selectively prohibited from infiltrating into ground water layers (for example particulate constituents), and therefore will only be exported during rain events. Soluble constituents are allowed to infiltrate into the ground water layers and eventually be exported as base flow
- Simulation of pollutant transport through 1D drainage structures (e.g. pipe networks, culverts)

The above is intended to enable modelling of water and constituent transport as illustrated in Figure 1.

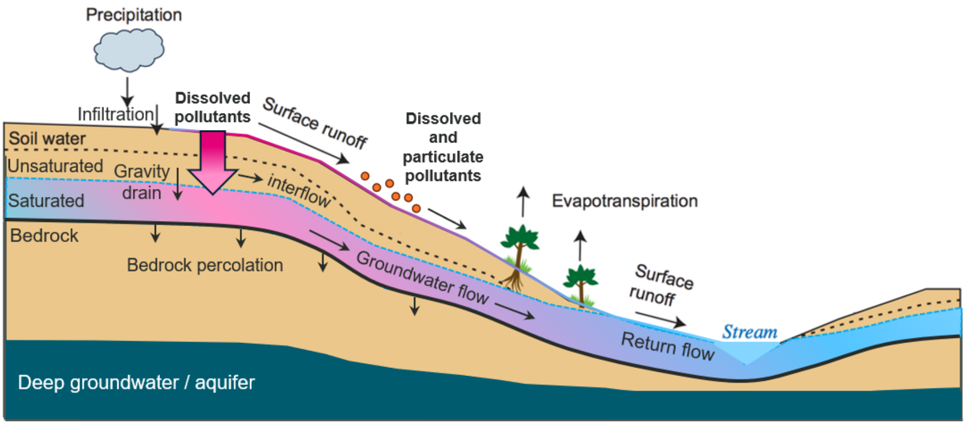

Figure 1. Hydrology and constituent production conceptual diagram.

Considering the shift in paradigm towards a grid-based approach for this new platform, a literature review was conducted to ascertain common approaches for parameterising associated pollutant export. The review covered 68 publications focusing on catchment models that simulate pollutant export. Of those, 46 were found to be relevant because they included water quality constituent models, erosion models, or erosion susceptibility models. All but two of these were published between 2000 and 2022, and most articles on distributed (i.e. grid-based, or semi-distributed) models were published from 2020 onwards.

This literature review motivated a return to first principles and therefore implementation of an accumulation/washoff basis for the pollutant export model in the new platform, rather than resorting to event mean/dry weather concentration based approaches which dominate the literature. As such, two parameters were proposed for implementation: areal accumulation rate (e.g. in kg/ha/yr); and areal wash-off/release rate (also in kg/ha/yr). This approach was adopted to allow for both constant pollutant concentrations (i.e. washoff = accumulation) and threshold based (i.e. washoff occurs after a threshold) pollutant export, in addition to the ability to parameterise each of the component elements (accumulation rate, washoff rate, thresholds etc). It also allows the initial parameterisation to be developed based on widely available values of areal accumulation or washoff rates. The literature was interrogated to ascribe values for the former, for every water quality constituent simulated in the receiving (TUFLOW FV) water quality model. These are presented in Table 1.

Table 1. Summary pollutant export parameters.
Adapted from Fletcher (2014), Bartley et al. (2012), Eyre (2002) and Alvarez-Cobelas et al. (2010)

Pollutant	Areal accumulation rate (kg/ha/yr)		Pollutant	Areal accumulation rate (kg/ha/yr)	
	Forest	Urban		Forest	Urban
Sediment	55	300	Part org C	12.154	40.514
Ammonium	0.273	2.171	Diss org N	1.021	2.194
Nitrate + Nitrite	0.662	2.364	Part org N	1.044	3.271
FRP	0.01	0.022	Diss org P	0.009	0.005
Diss org C	21.466	71.486	Part org P	0.061	0.623

For this initial population, values were ascribed based on a forested/urban land use basis, but any other appropriate categorisation (including slope, proximity to waterways, known eroding gully etc) can be used to spatially define these parameter rates: the degree of detail to which they are set is entirely up to the user and can reflect the well known variability in pollutant export behaviour within and between catchments (as noted in the references above), to the limits of the user's knowledge and supported by ongoing monitoring. This approach has been adopted specifically with model scenario execution in mind, where spatially explicit and modifiable pollutant export parameterisations are often needed to properly investigate matters such as nutrient offsetting and targeted land remediation.

The second parameter (areal washoff/release rate) was computed dynamically within TUFLOW HPC using the dry and wet store scheme described above. As such, this approach deploys physically meaningful first principles methods to predict the catchment pollutant export of speciated (as opposed to total) pollutants at a grid cell spatial resolution (usually tens of metres) and temporal resolutions of seconds, without resorting to lumping either hydrology or pollutant export.

Upgrades to TUFLOW FV (Receiving Model)

No specific updates or enhancements to TUFLOW FV were required.

Summary

The new environmental modelling platform described here uses rain on grid processes to compute 1D and 2D catchment hydrology and pollutant loads/transport by deploying first principles pollutant export methods and solving the equations of motion and transport. It automatically links these predictions to a downstream three dimensional hydrodynamic and water quality receiving model, and executes that model. This is achieved through a single point of user contact using the familiar and efficient TUFLOW script style approach. Integrated results are simultaneously viewable on platforms such as QGIS. This new platform is anticipated to greatly expedite the construction and integration of whole-of-catchment environmental modelling tools, and exploit the best available science and GPU accelerated compute techniques. To illustrate this, a description of a pilot application of the platform to the Oxley Creek catchment, Queensland, follows.

Application to Oxley Creek Catchment

The first application of this new modelling platform was to the Oxley Creek catchment, with its locality presented in Figure 2. Locations of water level and rainfall gauges used in the TUFLOW HPC model construction and validation (described subsequently) are also shown.

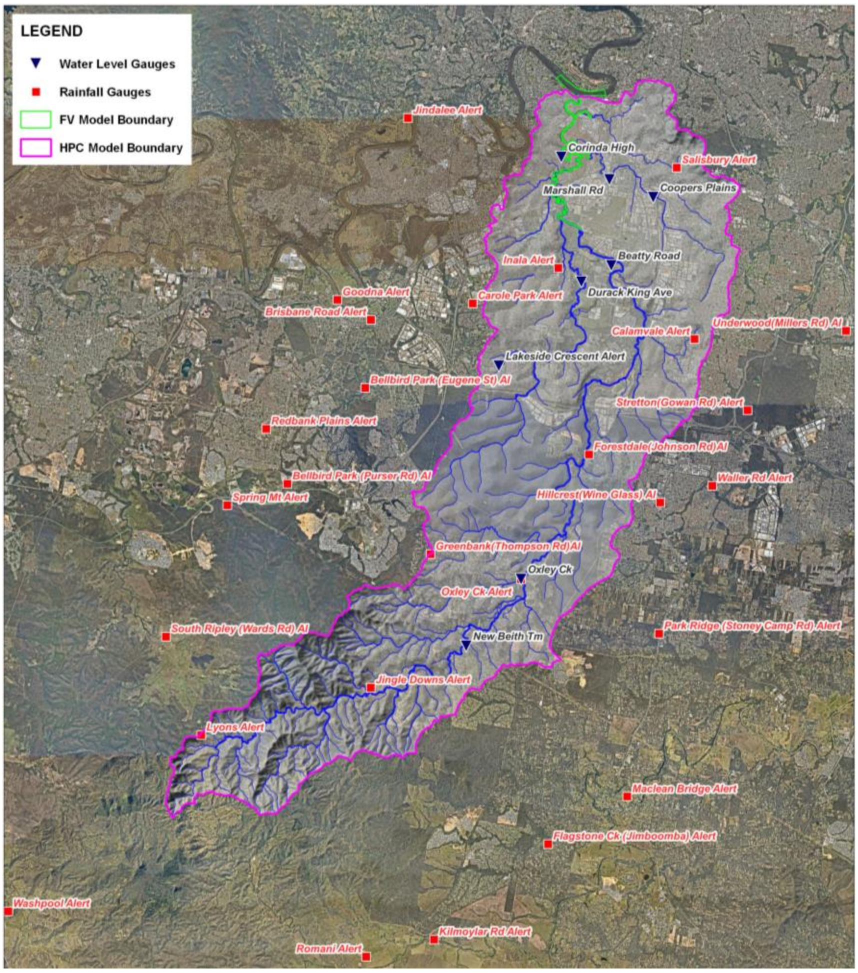

Figure 2. Oxley Creek catchment pilot model domain, with rainfall and gauge locations

TUFLOW HPC Model

A summary of data used to construct the TUFLOW HPC rain on grid hydrologic, hydraulic and pollutant export catchment model follows (and were supplemented by a targeted field trip):

- TUFLOW HPC was deployed with GPU acceleration and sub grid sampling (SGS) turned on
- Elevation data was 1m resolution topographical data sets, and instream cross sectional data
- 1D and 2D structures were included (bridges, major culverts and the Forest Lake Spillway)
- Twelve (12) land use types were used to assign Manning's *n* and impervious fractions
- Three calibration periods were selected based on data availability, recency and range of captured events, as: 2019 (dry), 2020 (typical) and 2022 (wet) calendar years

- TUFLOW's Inverse Distance Weighted (IDW) interpolation method was applied to the data from rainfall stations presented in Figure 2 to spatially and temporally vary the rainfall
- Tidal water levels at Oxley Mouth were applied as the model downstream boundary
- The Green-Ampt groundwater parameterisation is presented by (Gao et al. 2023)
- Evapotranspiration was included on a monthly timestep, using [BoM data]
- Pollutant export parameters presented in Table 1 were applied on aggregated land uses
- The model was parameterised using industry standard values of Manning's *n*, infiltration losses etc. The simulation time using off the shelf GPU hardware was 3.45 hours/year

Calibration performance of the TUFLOW HPC hydrologic model was assessed against a range of available water level gauge data, after transforming measured heights to flows. An example of the model's calibration performance at the Beatty Road gauge over the 2022 period is presented in Figure 3 as an hourly (not daily or monthly) timestep timeseries (main pane) and duration curve (inset). The data used in the duration curve is the complete set from 2019, 2020 and 2022.

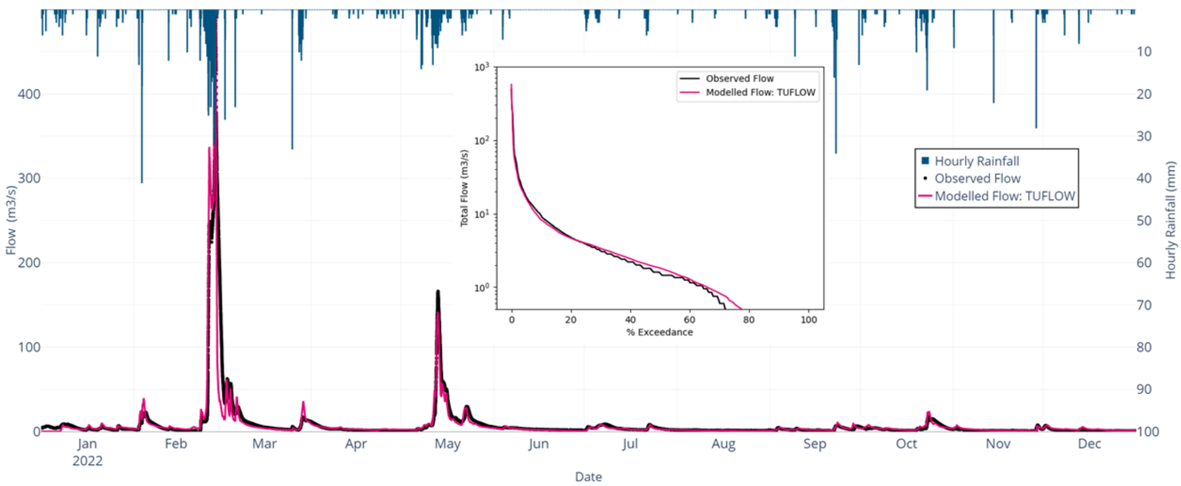

Figure 3. Example performance at Beatty Road gauge, measured (black) and modelled (red) flows (main pane). Rainfall is presented in blue. The inset presents the measured and modelled duration curves using combined hourly data across 2019, 2020 and 2020.

The Nash Sutcliffe Efficiency (NSE) and Percent bias (PBIAS) statistics for all modelled – measured comparisons at available gauges are presented in Table 2, computed from hourly data.

Table 2. NSE and PBIAS statistics for hourly gauge modelled – measured comparisons.

Gauge	Hourly statistic		Gauge	Hourly statistic	
	NSE	PBIAS		NSE	PBIAS
Beatty Road	0.81	6.34%	New Beith	0.85	11.75%
Durack King Avenue	0.83	-4.04%	Goodna Road	0.9	12.57%
Coopers Plains	0.85	9.89%	Lakeside Crescent	0.58	0.11%

Taking the D-M-A timescale benchmarks for these statistics from (Moriasi et al. 2015) (hourly benchmarks are not presented therein), all NSE statistics are classified as 'very good' other than Lakeside which was 'satisfactory'. Similarly, PBIAS metrics are generally 'good', with Durack King Avenue and Lakeside being 'very good' and Goodna Road and New Beith being 'satisfactory'.

TUFLOW HPC Pollutant Export Model

Given that this was the first application of this modelling platform, the accumulation rates presented in Table 1 were applied without change. Times of concentration (T_c) were set to 1 hour and 1 minute for forested and urban land uses, respectively. All rainfall intensity thresholds were set to 1 mm/hr and depth thresholds were set to 2 mm and 1 mm for forested and urban land uses, respectively. Water quality data for calibration of catchment loads were unavailable.

TUFLOW FV Receiving Hydrodynamic and Water Quality Model

A three dimensional hydrodynamic, sediment transport and water quality TUFLOW FV model of Oxley Creek (from the Brisbane River to its tidal limit) was built to receive the flows and pollutant loads predicted by TUFLOW HPC. The model mesh (which had 11 vertical layers), mainstream inflow nodestrings (3), lateral inflow points (454) and locations of calibration data (5) are presented in Figure 4. The nodestring locations are user defined (but optional) and the lateral inflow locations were determined automatically by TUFLOW HPC (which also automatically configured and produced all the boundary data timeseries at these locations from TUFLOW HPC predictions).

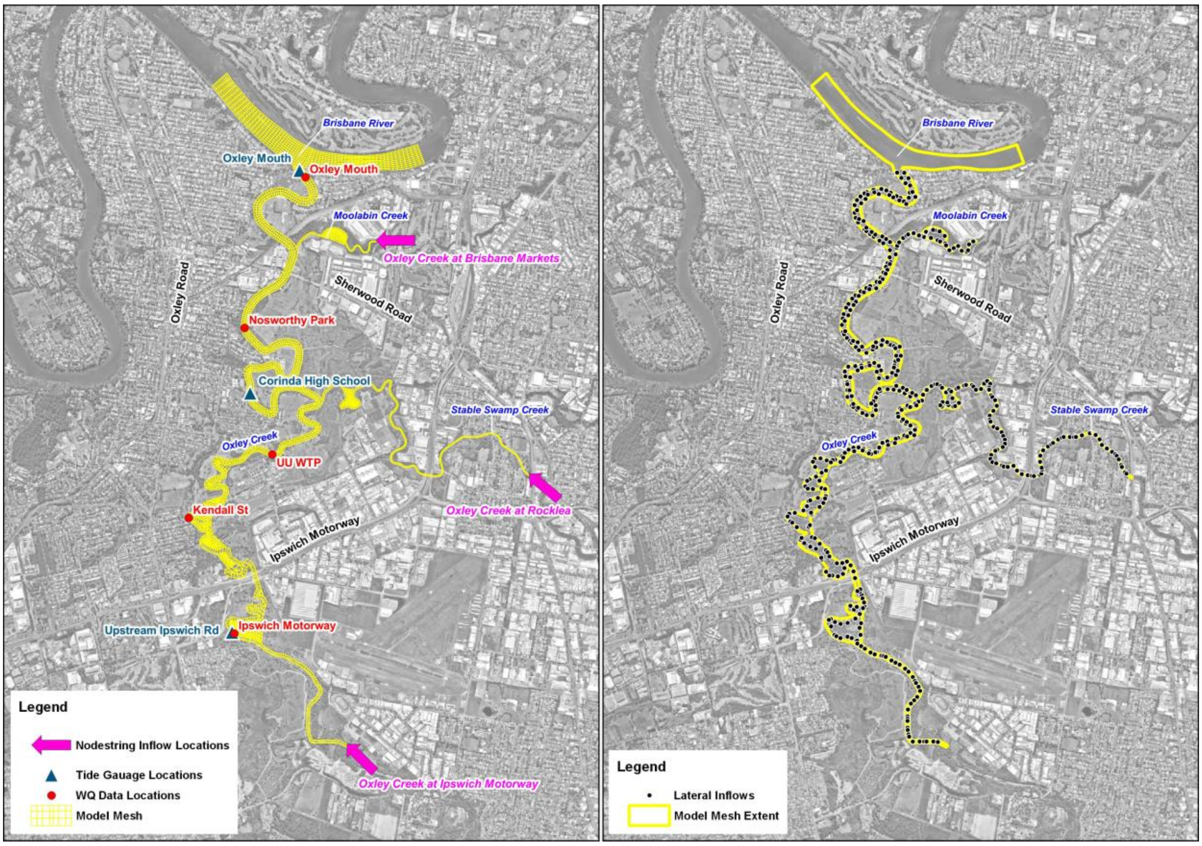

Figure 4. TUFLOW FV mesh, nodestring inflows and calibration data locations (left pane) and lateral inflow locations (right pane)

A summary of key data used to construct the TUFLOW FV receiving model is as follows:

- Bathymetric data was obtained from a combination of sources and reviewed once interpolated onto the TUFLOW FV mesh to ensure continuity of thalweg connectivity
- Meteorological data was sourced and preprocessed automatically from the ERA5 global circulation model, using the TUFLOW FV GetAtmos tool
- Tidal water levels at Oxley Mouth were applied at the two downstream boundaries in the Brisbane River. A shallow water wave calculation was used to set a lag between boundaries

- Water quality at the tidal boundaries was interpolated between measurements at Oxley Creek mouth, where available, and catchment boundaries were provided by TUFLOW HPC

Other selected model configurations were as follows:

- TUFLOW FV was configured to use the 3D Hydrodynamic (HD), Advection Dispersion (AD), Sediment Transport (ST) and Water Quality (WQ) Modules
- Simulated quantities were therefore: water level, current speed and direction, salinity, temperature, one sediment fraction, dissolved oxygen, silicate, ammonium, nitrate, filterable reactive phosphorus (FRP), adsorbed FRP, dissolved and particulate labile organic carbon, nitrogen and phosphorus, and one phytoplankton group
- For simplicity, a single suite of bottom roughness, sediment erosion and water quality benthic properties were set throughout the domain
- Two calibration periods were selected based on data availability, recency, overlap with TUFLOW HPC and range of captured events: 2019 (dry) and 2020 (typical) calendar years

The HD, ST and WQ Modules were parameterised using typical values, reflective of those applied previously to receiving models in Queensland. Water level measurements were the only hydrodynamic calibration data available, and the TUFLOW FV model was able to predict these well in amplitude and phase space (not shown). Water quality calibration data was sourced from campaign measurements at five instream sites (Figure 4) and are shown as points in the following figures.

RESULTS AND DISCUSSION

Beyond presentation of an integrated platform for the simulation of whole-of-catchment hydrologic and hydraulic runoff, and water quality dynamics, this paper's key scientific point of interest is developing an initial understanding of the potential impact that using such a robustly linked and physically based approach to simulating catchment hydrology and pollutant export may have on the prediction of receiving hydrodynamics and water quality. This is possible through interrogation of the rich data set that the Oxley Creek catchment pilot model has provided. In order to provide focus, the quantities simulated in the TUFLOW FV WQ model that are often compared to water quality objectives were considered: dissolved oxygen, total nitrogen, total phosphorus and total chlorophyll a. Salinity has also been considered given that its recovery through an estuary during low flow periods is an indicator of the robustness of (fresh) catchment inflow predictions. The total flow entering the TUFLOW FV model has also been considered.

In order to provide a point of comparison, flows and pollutant loads from an existing calibrated daily timestep lumped model of Oxley Creek catchment (which used GR4J, implemented through eWater Source, Alluvium, 2023 with a simulation time of 10 seconds/year) were extracted and applied to the TUFLOW FV receiving model described above, without any other changes.

Results are presented in Figure 5 for the Kendall Street site (refer to Figure 4) only. Other sites provided similar performance and insight. The figure has six panels that present timeseries of different constituents simulated by TUFLOW FV, in order from top to bottom: total flow delivered to the TUFLOW FV model, salinity, dissolved oxygen, total nitrogen, total phosphorus and total chlorophyll a. Predictions under the TUFLOW HPC and daily catchment model inflow boundary conditions are co-presented on all panes as dark and light blue lines, respectively. Available measurements are plotted as points, and comparison of timeseries with these points provides an indication of the predictive power of each TUFLOW FV simulation. The year 2019 is considered.

The most obvious feature of Figure 5 is that the hydrologic and pollutant export predictions of the TUFLOW HPC model – unchanged from their first principles calculations – result in hydrodynamic and water quality predictions that correspond remarkably well to measurements used to force the TUFLOW FV model of Oxley Creek. Notably, there has been no need to use the TUFLOW FV receiving water quality model as a proxy calibration tool for the upstream catchment model – rather, the TUFLOW HPC catchment model has provided robust predictions using physically meaningful first principles approaches and industry standard parameters. This is an important result that has the potential to save environmental modelling practitioners considerable rework.

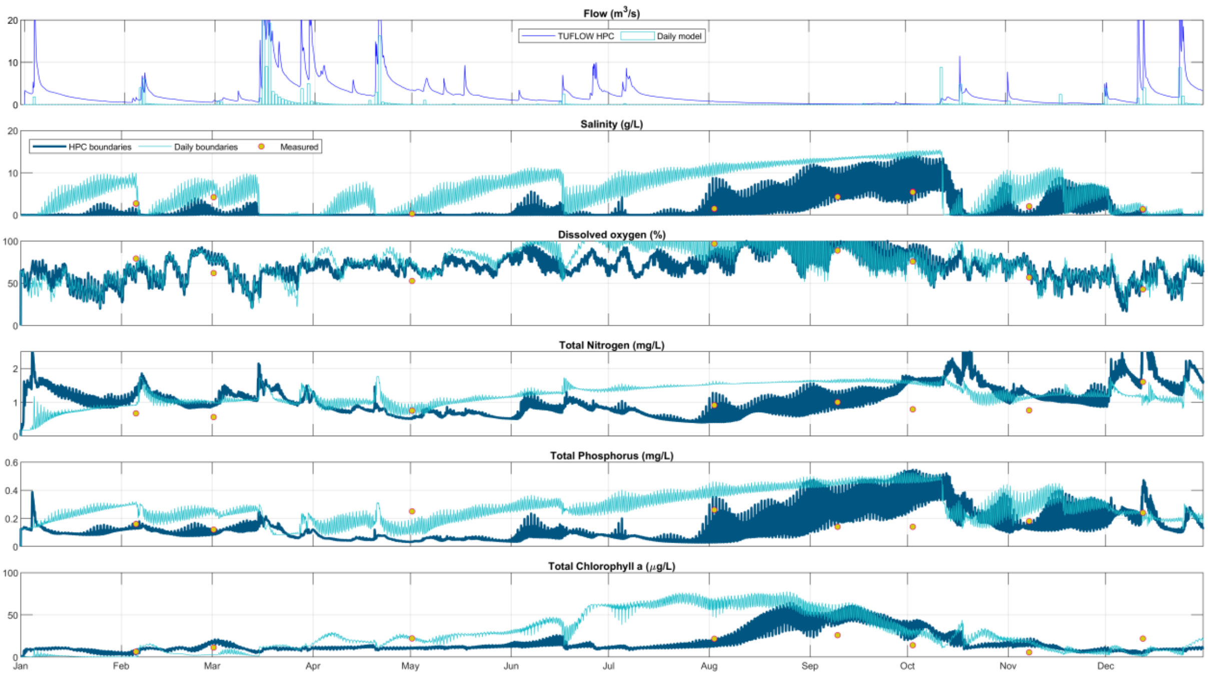

Figure 5. TUFLOW FV predictions at Kendall Street over 2019. Panes are explained in the text.

Looking more closely at Figure 5, the top pane shows a marked disparity between the TUFLOW HPC and daily lumped model total flow predictions to Oxley Creek. One notable difference is the models' representations of falling limbs post rainfall events – HPC has falling limbs that last for extended periods (up to months) whilst the daily lumped model essentially predicts zero flow for the majority of these times. The flow calibration (Figure 3) demonstrates that these falling limbs are indeed real, and that TUFLOW HPC predicts them well.

A consequence of a falling limb absence is an overprediction of salinity in the TUFLOW FV model forced by the daily lumped model (second panel): salt from the downstream Brisbane River boundary repeatedly recovers up Oxley Creek too quickly after rainfall (light blue line in the second pane), by virtue of the persistent near zero fresh inflows predicted by the daily lumped model. In contrast, the TUFLOW FV model forced by the TUFLOW HPC boundaries predicts salt recovery well under the influence of long lasting falling limb fresh inflows. The two approaches produce fundamentally different predictions of hydrodynamic estuarine responses, with the TUFLOW HPC approach producing far superior outcomes, even before water quality modelling is considered.

One follow-on consequence of the rapid salt recovery caused by the lumped daily model approach, is the increase in nitrogen and phosphorus concentrations across the middle months of 2019 in the TUFLOW FV model. It is likely that this increase is a signature of the Brisbane River tidal boundary, as was obviously the case with the rapid salt recovery. These overpredictions do not occur for the TUFLOW FV model forced by TUFLOW HPC outflows, where ongoing falling limb base flows appropriately retard the ingress of Brisbane River water to Oxley Creek. Moreover, these excess nutrients present in June, July and August in the TUFLOW FV model forced by the daily lumped catchment model trigger elevated phytoplanktonic growth well beyond that measured in the creek, as evidenced by a comparison of modelled phytoplankton concentrations (light and dark blue lines) with spot measurements in the bottom panel. This false effect is absent when forced by TUFLOW HPC.

This outcome points to a clear nexus: as practitioners modelling Oxley Creek, we can choose to either a) continue to use unphysical lumped daily catchment models that (whilst having low computational overheads) make demonstrably inadequate hydrologic predictions, or b) move our industry forward by using physically based catchment hydrology and pollutant export modelling tools that (whilst having a run time of a few hours) make accurate, and spatially and temporally resolved predictions that support meaningful downstream water quality modelling. To not consider applying modern tools to modern problems is inconsistent with our professional obligations to deploy the best tools available in order to inform evidenced-based decision making that translates to positive real world outcomes.

CONCLUSION

A new numerical platform for the integrated simulation of catchment-wide hydrologic, hydraulic and water quality processes has been presented. This platform uses first principles to predict high resolution, spatially and temporally resolved surface and subsurface catchment runoff and pollutant loads, and automatically links these predictions with a downstream three dimensional receiving hydrodynamic and water quality model. This is a major step forward in the whole-of-catchment simulation of environmental systems and has the potential to vastly improve the efficacy of assessments of real world management interventions (such as environmental offsets) within a single integrated platform that exploits state-of-the-art scientific rigour and compute power. A first step interrogation of the receiving water quality model predictions has shown that capturing the details of catchment hydrologic processes (such as extended periods of falling limb flows) is essential to the robust and defensible prediction of water quality dynamics in downstream waterways. In particular, the misprediction of the details of catchment hydrology (even before considering pollutant export) has the potential to deleteriously impact the predictive power of downstream receiving water quality models, up to and including higher trophic processes such as phytoplanktonic primary productivity.

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BIOGRAPHY

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