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A model framework to predict pesticide concentrations in runoff at improved temporal and spatial resolution

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Abstract: Nested catchment models are an important component of our environmental decision-making framework. They are used in a variety of contexts related to management of critical coastal ecosystems and land use planning. Water quality predictions from catchments have typically been made using models that have been primarily developed for use in water resource planning and allocation applications. These models resolve hydrology at sub-catchment scale (few kms) and function on daily to monthly timesteps. This modelling approach is not fully compatible for a range of applications. Pesticide modelling is a particularly important example of this short-coming.

Modelling tools like eWater SOURCE operate on a daily timescale and sub-catchment/functional unit (landuse) is the smallest spatial discretization. Pesticide generation happens at very localized scales within the sub-catchment and incumbent modelling tools cannot represent the heterogeneity in application and generation. Similarly daily timestep models cannot be used to model advection and transport due to small storm events (of the order of a few hours) and the subsequent transformations (e.g., mixing, hydrolysis, photolysis, sedimentation, resuspension etc.) that might happen at sub-daily timescales.

The current pesticide targets are concentration-based, and a novel model framework is required to address current gaps. A distributed hydrological model is proposed to address issues around spatial and temporal resolution. This distributed model consists of a flexible mesh of quadrilateral and triangular elements, each of which has their own rainfall and water balance calculations. The excess runoff is routed through a simplistic delay-based routing scheme. The model is designed and executed to predict hourly flows, therefore providing much refined granularity to usual water modelling information available to water managers.

The distributed hydrological model can be used to resolve spatial variability in generation alongside an empirical transport duration. As soon as the pollutant reaches an ephemeral or permanent stream with depth beyond a threshold, more complexity is required to model advection-dispersion and other transformations. A 1D Lagrangian model, DYRIM can be coupled with a water quality model AED2 to provide further improved predictions.

Keywords: *Distributed hydrological model, 1D model, pesticides*

1. INTRODUCTION

The Great Barrier Reef (GBR) is one of the world's largest and most complex coral ecosystems, an iconic national asset of great ecological significance. Unfortunately, the GBR is faced with challenges originating from anthropogenic activity within the region. One of the greatest threats is the discharge of sediments, nutrients, and toxicants (pesticides and herbicides) to the reef (State of Queensland, 2018). These pollutants originate in the catchments, aggregate through a network of small streams, and finally get transported to the GBR lagoon through estuarine outlets.

To mitigate these threats and improve the GBR's health, the Australian and Queensland Governments have implemented the Reef 2050 Water Quality Improvement Plan (Reef 2050 WQIP), which defines the required reductions in sediments, nutrients, and toxicants (State of Queensland, 2018). A cornerstone of the Reef 2050 WQIP is the Paddock to Reef (P2R) modelling and monitoring program, which aims to develop scientific methods to influence and enhance land management practices in the catchment to improve runoff quality.

Modelling the generation and transport of toxicants across the GBR catchments is a complex undertaking and involves the use of nested models, resolving processes at different spatial scales. The outputs from one model are often used as boundary conditions for the next model. The flexibility offered by the nesting approach is quite powerful and enables adequate representation of process complexity through the catchment to coast continuum. Figure 1 describes the different models currently being used as part of P2R modelling. The paddock simulations can simulate time and quantity of pesticide/herbicide application, their residual concentration until the next rainfall event and the runoff/drainage concentration. The catchment models simulate the generation of pesticides in a particular sub-catchment/functional unit and the transport through the stream network resulting in a certain load to the marine environment.

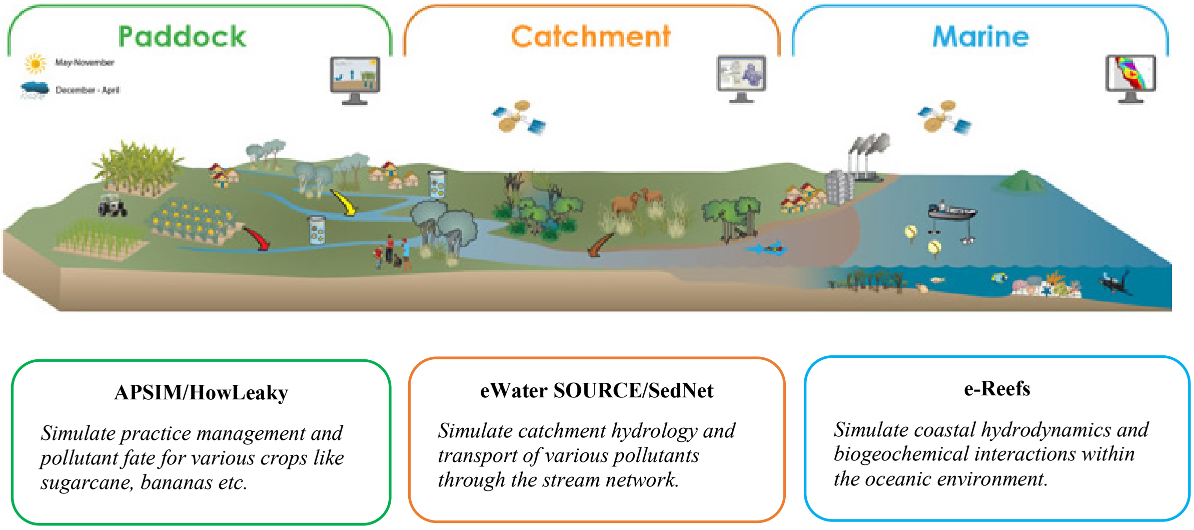


Figure 1. P2R modelling tools currently used to simulate pesticide fate and transport

The Reef 2050 WQIP specifies that the pesticides target is "*To protect at least 99% of aquatic species at the end-of-catchments*". This translates into a concentration-based target against the previous load-based target. This shift in target has major implications on model structure, particularly the catchment model. To simulate pesticide concentrations, the following additional considerations will have to be made:

- **Spatial discretisation/resolution**: Pesticide application and timing is quite localized, and the model must be able to adequately represent the spatial heterogeneity, expected to coincide with spatial scales currently represented in Paddock models.
- **Transformations in riverine systems**: River streams (both ephemeral and permanent) carry pesticides with them where they are subjected to different processes (e.g., mixing, hydrolysis, photolysis, sedimentation, resuspension etc.) that could influence concentration. The overarching advection and transport are driven by the flooding in river channels.
- **Timestep**: The model timestep must be setup to adequately match timescales at which changes occur in the system. To model concentrations and capture any transformations, timescale of the order of hours would be considered desirable. This would also enable more meaningful linkages with the downstream marine model that resolves hydrodynamics at the scale of a few minutes.

- **Model runtime**: The uncertainty in pesticide application and parameterisation of the transformations will require the use of data-assimilation based analysis techniques. Several model realisations maybe required as part of this analysis and so the model run times will have to be practical.

Based on the considerations outlined above, this paper proposes a modelling framework that utilizes a combination of existing conceptual models in catchment hydrology along with other models that simulate riverine hydraulics. The following sections provide details of the framework and its application to a case study in south-east Queensland.

2. PROPOSED MODEL FRAMEWORK

2.1. The case for a distributed hydrological model

Catchments are often viewed as a collection of largely complex (sometimes random) processes at a micro-scale that coalesce into a system whose behavior can be explained at a macro-level using basic physical relations. The main objective of a catchment water quality model is to use these physical relations to predict the generation and transport of nutrients, sediments, and other toxicants because of rainfall.

There are two major applications of hydrological models. The first involves using them to predict behavior of catchments during extreme flow events (i.e., floods). These hydrological models are used to force more refined, 2-d models that predict inundation levels and flood extent downstream. This use-case involves running the models over a few days and focuses on modelling the flood hydrograph correctly. The second use case involves the analysis of long-term behavior of the catchment and the export of nutrients, sediments, and toxicants through time scales of a year or longer. Both applications of models have a significant amount of overlap, yet different modelling tools are often used. Flood models have well developed methods to model flow routing between catchments because of the focus on getting a perfect fit on the hydrograph at sub-event time scales. Nutrient export models at the catchment scale function at a daily timestep and resolve functioning of a long-term water balance which is vaguely parameterized in flood models through initial and continuing losses. There is therefore merit in working with both classes of models to ensure they work at sub-daily (i.e., hourly) timescales and incorporate some of the complexities related to the water balance.

Most of the modelling tools available have operated on a reasonably large spatial scale of the orders of kilometers, being delineated at the sub-catchment level to comprise large extents associated with the entire catchments. These models regionalize the hydrological properties over a significantly large area and are often referred to as lumped parsimonious hydrological models (Willems et al., 2014). Each sub-catchment behaves like a bucket that drains into the next and this whole system replicates the functioning of streams constrained by a localized water balance. The main drawback with this approach is the loss of non-homogeneity within the catchment leading to an inadequate representation of underlying processes.

SOURCE uses sub-catchments as its primary hydrological unit but gives an additional option of specifying land uses (namely functional units) as a proportion of the sub-catchment area, with the provision of model outputs discretized across the different land uses (Chiew et al., 2009). This in fact makes SOURCE a semi-distributed hydrological model. The model (as used in GBR catchments) only operates at a daily time scale and has provisions for link-based storage routing, which approximates the physical functioning of the links as actual streams. Parameter regionalization happens at the sub-catchment/functional unit level, and this can often be a large area leading to potential distortion in the representation of underlying spatial variability.

To overcome the issue with parameter regionalization and loss of underlying spatial variability, a distributed hydrological model involving the use of structured mesh, with the mesh elements being the basic computational unit, can be adopted as an alternative. The size and distribution of these elements can be controlled and therefore regionalization of hydrological properties can happen at a more refined scale. Both fixed (square elements only) and flexible (quadrilateral and triangle elements) meshes can be potentially used. The water balance can be computed on each model cell and drainage from one cell to the other can be specified using an appropriate routing scheme.

Distributed hydrological models have been used extensively with several instances available in existing literature (Merritt et al., 2003). Adoption of these models within the practitioner community has been relatively slow, due to the relatively large computational requirements. This limitation has improved with greater computational power in recent times and the use of distributed models is likely to increase.

2.2. Distributed hydrological model components

The components of the distributed hydrological model developed as part of the present study are described below (refer Figure 2).

Table 1. Components of a distributed hydrology model

Component	Description
Model Mesh	Both fixed and flexible meshes can be used. Flexible meshes have the added advantage of being customizable around areas of interest within the catchment.
Rainfall Data	The rainfall used to force the model can be collected from available pluviometer sites around the catchment. An inverse distance weighted interpolation can be used to distribute the rainfall over each model cell
Water Balance	Water balance is computed for each model cell for each timestep. SIMHYD, Sacramento and AWBM are all existing water balance models within SOURCE and can be applied to each model cell.
Flow Routing	A simple delay-based, empirical routing is found to be the most effective and numerically stable. a delay separately for overland flow (Boughton & Askew, 1968) and stream channel (Boyd, 1978) based on the following empirical relationships: $$D_o = L * (A_i)^{0.57} * (Q_j)^c$$ $$D_s = 0.6 * L * (A_i)^{0.57} * (Q_j)^c$$ D_o is the overland delay, D_s is the stream channel delay, L is the lag parameter, A_i is the element i area, Q_j is the flow through the link j and c is the non-linearity constant that links flow to the lag (in hours). Usually, the non-linearity implies that larger flows pass through with less lag and smaller flows have larger lag.
Generation Models/Paddock Models	Since the model domain has been discretised into model cells, the complete heterogeneity of agricultural practices and load generation can now be accounted for and represented in the model. A complete linkage with paddock scale models can be achieved by applying the same water balance approach in the catchment model as the paddock model and running both at the same timestep. Each cell in the catchment model should map to a unique crop/pesticide management scenario in the paddock model.

2.3. DYRIM-AED2

DYRIM was developed at the University of Western Australia (UWA) and is a computationally efficient Lagrangian method for solving one-dimensional advection-diffusion transport in steady and unsteady open channel flows. The model moves parcels (or grids) with the mean flow velocity as the flood-wave propagates through the system. The numerical core is a Crank-Nicolson type scheme that can be used in explicit, semi-implicit, or fully implicit modes. Extensive validations of the model have been done against analytical solutions and numerical results from benchmark problems that included a variety of tracer distributions (Gaussian, top hat) and steep tracer fronts (step function) in both uniform flow and flow because of a traveling wave. Numerical diffusion in pure advection transport in steady, uniform flow was negligible and the Lagrangian scheme provided exact solutions. The model is computationally efficient and can function at large timesteps/courant numbers (Devkota & Imberger, 2009).

The DYRIM model setup involves specifying Lagrangian volumes along a river reach. Each Lagrangian volume is constrained by the stream and floodplain cross-sectional areas at both ends (refer Figure 3). The model setup allows for elevation and slope to be set for each section and this can be used to model disconnected pools of water or small wetlands. The model structure is quasi-2D. DYRIM can be easily linked to the distributed hydrological model described above by the following steps:

- Identify and mark cells in the distributed hydrological model that form part of the floodplain.
- Extract a timeseries for inflows from all the cells draining into the floodplain boundary.
- Apply these timeseries as external inflows to DYRIM.

A more dynamically linked setup is also possible where both the hydrological model and DYRIM function on similar timesteps.

The current DYRIM codebase has been coupled with Aquatic Eco-Dynamics (AED2), the open-source water quality model, also developed at UWA. AED2, is a flexible software library comprising standard interface that can be called directly from other hydrodynamic packages, like DYRIM. The AED2 library consists of numerous modules that are designed as individual model 'components' able to be configured in a way that facilitates custom aquatic ecosystem conceptualizations (either simple or complex). Users can define water quality and ecosystem variables to simulate and then are able to customize connections and dependencies with other modules. Support exists for easy customization at an algorithm level of how model components operate (e.g., photosynthesis functions, sorption algorithms etc.). A module with basic algorithms for modelling pesticide fate has already been developed and can be customized further.

A combination of the distributed hydrological model and DYRIM-AED2 enables a complete spatial linkage between the generation of pesticides, the transport through riverine networks and interactions within floodplains to finally a receiving model for the estuarine zone/GBR lagoon.

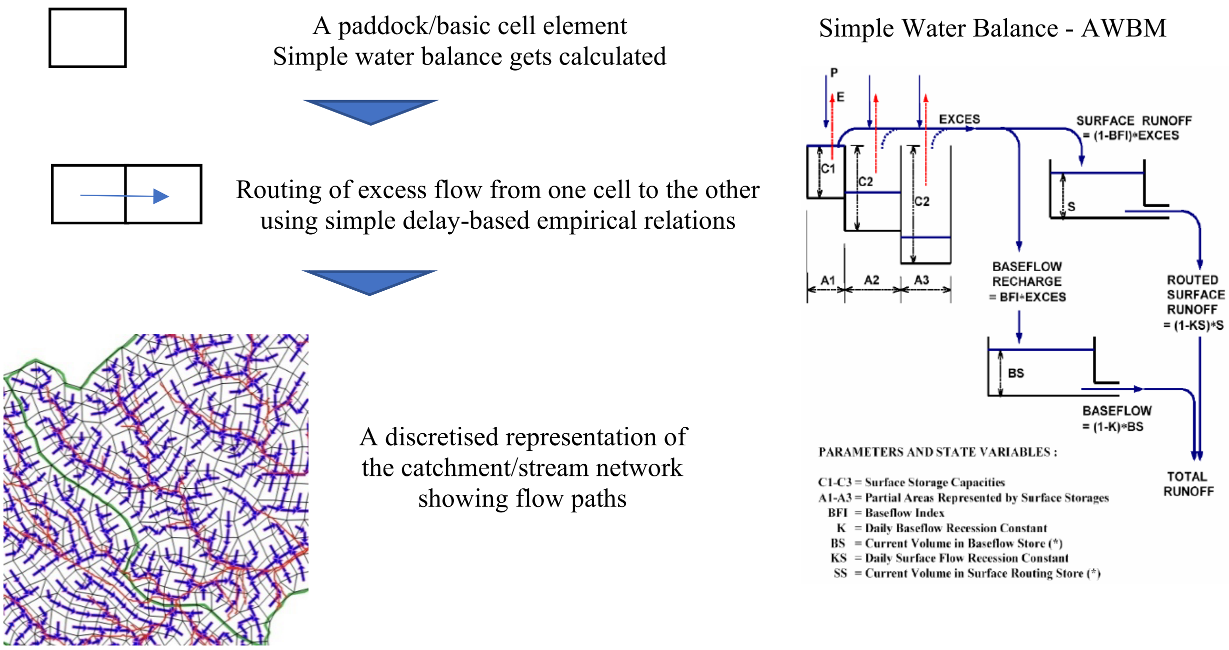
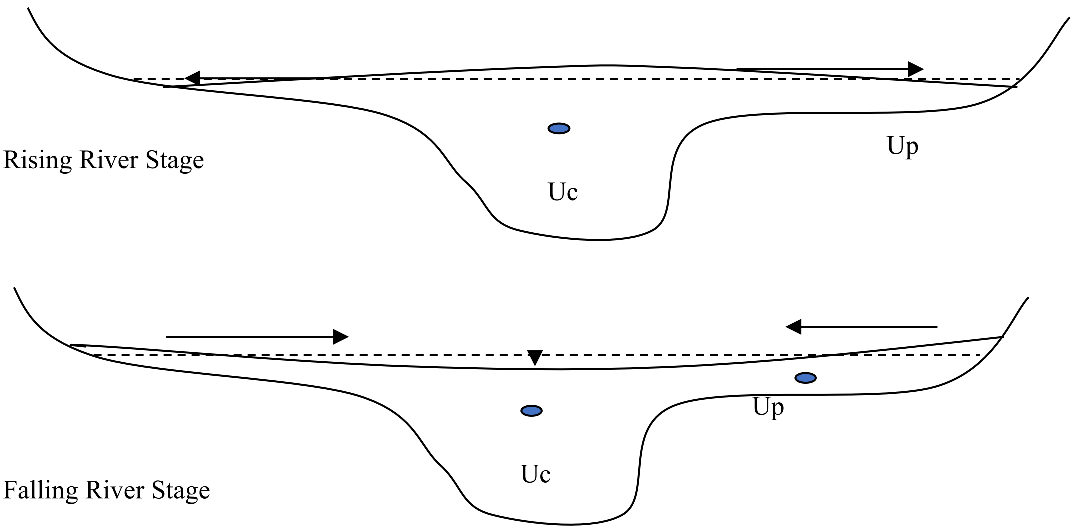


Figure 2. Structure of a distributed hydrological model with a simple water balance model (AWBM) (Yu & Zhu, 2015)



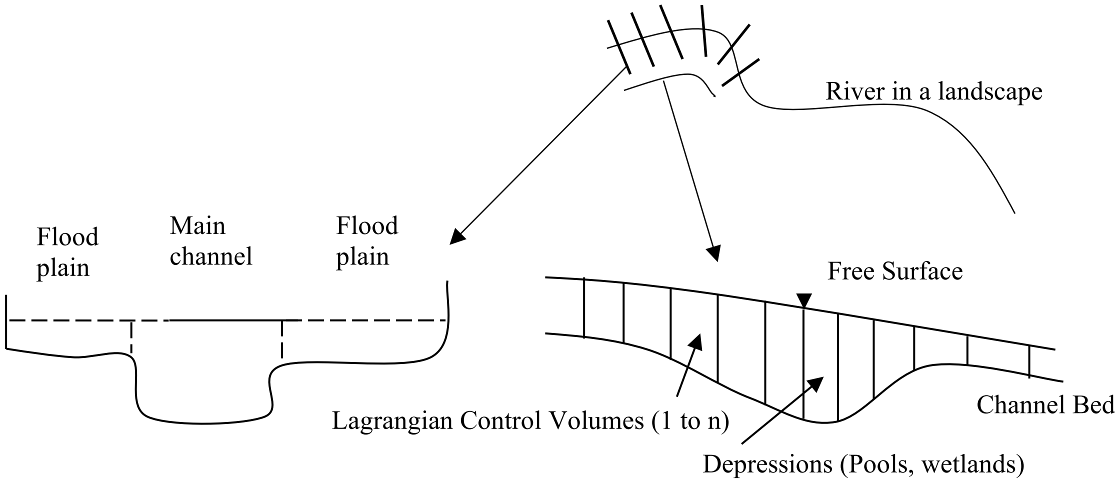


Figure 3. Structure of the 1D DYRIM model (Devkota & Imberger, 2009)

3. APPLICATION OF THE DISTRIBUTED HYDROLOGICAL MODEL – A CASE STUDY

The distributed hydrological model was applied to the Bremer River catchment in south-east Queensland. The catchment area was divided into 20,000 cells with each roughly 100m x 100 m in size. AWBM was used as a water balance model and the delay-based routing described before was also used. Rainfall data sourced from 17 pluviometer gauges around the catchment was applied to the model. A flood event in 2013 was modelled, and the results are shown below in Figure 4. Spatial distribution of rainfall and flow across the catchment indicate that the model performance matches expectations. A direct comparison of performance to SOURCE has not been carried out, but results are expected to be significantly better.

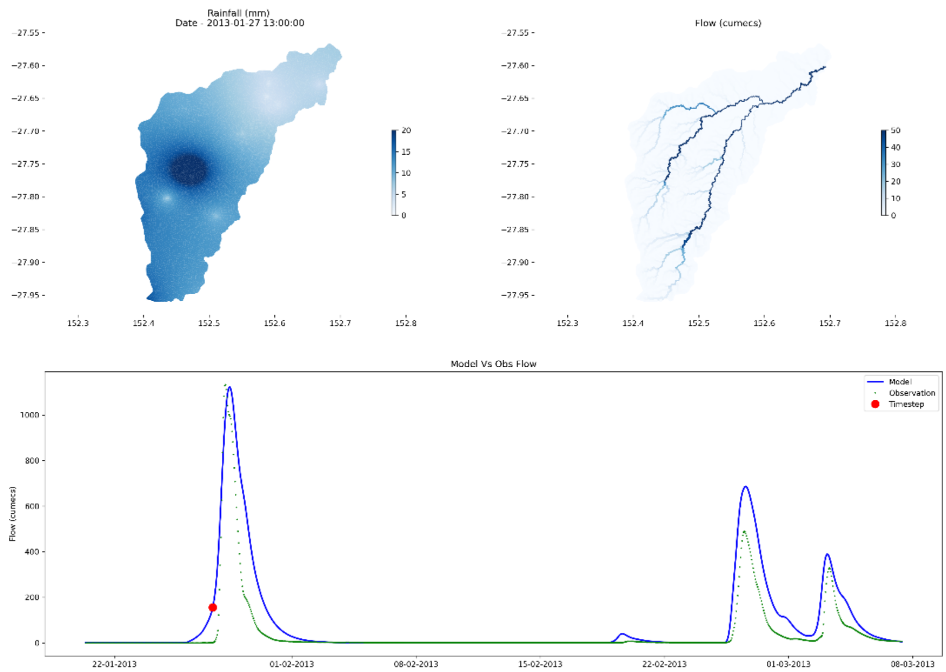


Figure 4. Results from modelling the 2013 flood event at the Bremer River catchment (animation)

Observation data for concentrations of Metalochlor was also available for this period at the catchment outlet. Metalochlor concentration was simulated as a conservative tracer generated from areas of broadscale cropping landuse based on an exponential relationship to the flow generated from individual cells.

$$E\ (conc) = \gamma * \ (Q_i)^{\delta}$$

γ and δ are constants that scale the flow generated from the i^{th} cell to predict constituent concentration. Figure 5 shows the spatial distribution and transport of Metalochlor with rainfall across the catchment.

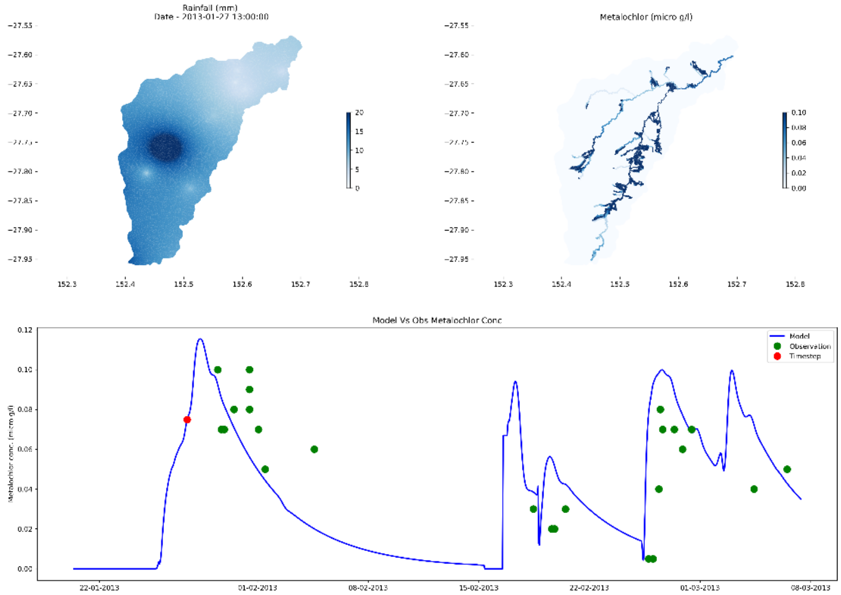


Figure 5. Results from modelling the Metalochlor concentrations during the 2013 flood event (animation)

4. CONCLUSIONS

The proposed model framework provides a novel, flexible modular approach to modelling pesticide concentrations in the catchment. The framework is built upon existing conceptual models that have been extensively applied to different catchments within the GBR. The combination of these simple models results in a much more granular (both spatially and temporally) predictive ability. Further testing of the framework and potentially combining with groundwater models will help understand the full extent of pesticide transport in GBR catchments.

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