

# **The Future of Water Quality Modelling**

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### Outline

What is water quality modelling?

What is particle tracking?

What is the status quo?

The Future - Advanced water quality modelling case studies









# Different environmental water modelling disciplines use different tools, but most are some form of numerical model, or a combination thereof

- Hydrologic (e.g. rainfall runoff prediction)
- Hydraulic (e.g. flood modelling)
- Hydrodynamic (e.g. estuarine tidal flows)
- Sediment transport (e.g. coastal environments)
- Waves (as additional stress to hydrodynamics)
- Groundwater (independent or linked to hydrodynamic/hydrologic models)
- Plumes (e.g. ocean outfalls)
- · Combinations of one-, two- and three-dimensional models
- Not an exhaustive list...

### **Physics**









#### When ecological process questions arise, an additional suite of models is required

- Simulate water chemistry and ecology, informed in part by physicals
- Used to examine the non-conservative fate and transport of ecologically significant constituents
  - Dissolved oxygen (core of many water quality and ecological models)
  - Nutrients (nitrogen and phosphorus)
  - Organic matter (nitrogen, phosphorus and carbon)
  - Phytoplankton (algae)
  - Zooplankton
  - Pathogens
  - Geochemistry
  - Many more
- Wide range of water quality constituents simulated to address different issues
- Basic premise: to simulate ecologically relevant processes and pathways that can be characterised by dissolved quantities to support environmental management









#### Typical questions that water quality models might be used to address (not exhaustive)

- What nutrient loading can an estuary accept from a wastewater treatment plant, before estuarine water quality fails to meet its objectives?
- What impact will catchment-based stormwater treatment have on the ecological function of a downstream creek?
- How might we best design a wetland to treat urban stormwater runoff?
- How might the frequency and severity of algae blooms change in a water supply reservoir if sediment nutrient release is suppressed?
- What risks are posed to the public by pathogens delivered to aquatic recreational areas?
- What is the likely geochemistry of a coal mine's final void if it fills with water to form a lake?



The historical approach to addressing these types of questions has typically been





#### Summary

- These assessments simulate concentration based quantities, also known as "Eulerian" or "cell" based quantities
- Relate primarily to dissolved quantities
- If not, they attempt to simulate non-dissolved quantities as water concentrations
  - Phytoplankton "concentration", but phytoplankton are discrete entities
  - Shrimp or fish "concentration", but these are also discrete entities
- Leads to particle modelling







#### When discrete entity process questions arise, they can be simulated as particles

- Particle (or particle tracking) models simulate individual entities rather then dissolved quantities
- Individual entities might include
  - Fish or crustaceans
  - Shrimp (prawns)
  - Surface scum algal blooms
  - Fish larvae
  - Turtle hatchlings
  - · Aquaculture feed pellets or waste
  - Over-boarded shipping containers
  - Solid oceanic waste / wreckage
  - Lost uncontrolled vessels
  - Many others









#### Particles can be

- · Transported by the flow field and/or wave and wind drift
- Modified by settling/buoyancy, decay, sedimentation and resuspension
- Dispersed horizontally and vertically
- Given motility behaviours over and above simple advection
- Set to crawl if on dry land
- Basic premise: to simulate processes and pathways that cannot be properly characterised by dissolved quantities to support environmental and other management efforts







The historical approach to addressing these questions has typically been





#### Summary

- These assessments rely on particle based dynamics, also known as "Lagrangian" quantities
- Not dissolved quantities
- Moved by currents, waves, wind and potential organism-based motility







### The past

- Both Eulerian and Lagrangian modelling tools have been used for decades, in increasing complexity
- Both have primarily (but not always) been driven only by hydrodynamics, and have themselves not been linked
- Restrictive in the issues that can be addressed

#### Most traditional analyses are one-way

- Water quality responds to hydrodynamics
- Particles respond to hydrodynamics
- Particles do not modify water quality
- Water quality does not modify particle behaviour
- Water quality does not alter hydrodynamics
- Some exceptions (WQ → HD, niche, often non-commercial)
  - Oil spill modelling (2D)
- Phytoplankton shading
- Fish kills







#### The past

- Hydrodynamics
  - 1D hydrodynamic models were once the norm
- Understanding of our natural environment
  - Basic processes (e.g. total nutrients and generic phytoplankton)
- Compute power
  - CPU was once the norm
  - · Desktop computers were once the norm

#### The present

- Hydrodynamics
  - 3D models are now expected
- Understanding of our natural environment
  - Multitrophics are increasingly well understood
- Compute power
  - GPU is now expected (or at least asked after)
  - Blade arrays and cloud compute options are the norm







The questions being asked of environmental models are increasing in scale and complexity







#### A glimpse of what is to come in TUFLOW

- Two way linking of HD / PT / WQ models
  - Management of dissolved oxygen in "shrimp" ponds •
  - Migration of salmon

#### Already being applied in industry

- UK Seafood Innovation Fund project
- BMT, Scottish Sea Farms, Marine Scotland Science, Aquatera and Scottish Environment **Protection Agency**
- https://www.bmt.org/news/2020/bmt-to-support-scottishseafood-industry/



STATUS: ONGOING









# **Question 1: DO (dissolved oxygen) in shrimp ponds**

### The setting

- Land based aquaculture uses grow out ponds to develop shrimp to saleable size
- Ponds are typically
  - · Up to hundreds of metres in horizontal dimension, and
  - · Several metres deep at their deepest
- Maintenance of oxygen in the ponds is critical
  - Shrimp consume oxygen via respiration
  - Shrimp waste and over-feed also consume oxygen when broken down
- For the purposes of this simple example case, "shrimp" migrate vertically on a diurnal cycle, seeking safety at depth during daylight hours

#### **Key questions**

- Does vertical shrimp migration lead to ongoing low dissolved oxygen at depth?
- If so, how might shrimp respond?









#### **Historical assessments**



Make inferences around PTM-WQ linkage

#### **Current needs**



Specifically simulate PTM-WQ linkage





#### The requirement

- · Particles are to respond to hydrodynamics, but also dynamically to
  - Temperature
  - Light (PAR)
- Particles are to consume oxygen at a user defined rate
- This will allow
  - Diurnal vertical migration
  - Interaction between PT and WQ models around oxygen







#### The implementation

- Particle tracking
  - · Migrate downwards when a user defined ambient PAR threshold is exceeded
  - Stop migrating once the PAR threshold is no longer exceeded
  - Crawl downwards if they hit a pond's sloping sides
  - Freely migrate laterally at the pond base
- Oxygen consumption
  - · Within a user defined temperature range
  - Scales with maximum mg O<sub>2</sub> per gram of shrimp biomass
  - User defined temperature dependence

#### The example model

• 3D constructed shrimp farm pond







#### The 3D pond model



Dots: shrimp Colour contours: bottom PAR











Do not respond to PAR

Do respond to PAR







Do not respond to PAR

#### Do respond to PAR







#### **Current needs**



Specifically simulate PTM-WQ linkage

#### **Future needs**



- Have WQ feed back to PTM
- Shrimp avoid low DO waters to survive







Do not respond to DO









#### Where to next

- Customisation of algorithms to reflect different behaviours (real shrimp!)
- Management of ponds, shrimp, feed and waste

#### **Example questions**

- How can paddles be arranged to promote accumulation of waste in locations that are easy to access to clean, and to minimise a low DO footprint size?
- How do different types of feed/waste travel through the pond and influence dissolved oxygen?
- What thickness of waste is likely to collect at the bottom of a pond, and how often should it be cleaned, to optimise cleaning costs and avoid low DO?
- · Is waste or overfeed resuspended and if so, what are its water quality dynamics?
- What are the carbon, nitrogen and phosphorus dynamics associated with pellet overfeed and waste and how can these be better managed to save money?









# **Question 2: Migrating salmon**

#### The setting

- Salmon migrate upstream
- They have various depth and temperature seeking behaviours
- They can become stressed due to higher water temperatures and so seek cold water refuges
- Creation of artificial refuges is being considered to assist migrating salmon

### **Key question**

• How might a refuge be designed to maximise benefit to salmon?







## **Question 2: Migrating salmon**

#### **Historical assessments**



Make inferences around HD-PTM linkage

#### **Current needs**



Specifically simulate HD-PTM linkage





# **Question 2: Migrating salmon**

#### The requirement

- · Particles are to respond to hydrodynamics
  - Swim against the current
- And also dynamically to
  - Local temperature gradients
- This will allow
  - Lateral deviation of upstream swimming to seek cooler waters
  - Assist in designing constructed refuges







# **Question 2: Salmon migration**









### **Question 2: Salmon migration**

Velocity vectors









### Summary

#### **Past and present**

- · Requirements are becoming more demanding
- Historical approaches are no longer sufficient

#### The future

- As a matter of course:
  - Two-way interaction of HD, PT, WQ
  - Cloud and GPU compute







### Summary

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