# Insights from dynamical physics-based models of contaminant transport in river flow

ITT 19: Wessex Water Challenges 2 and 3

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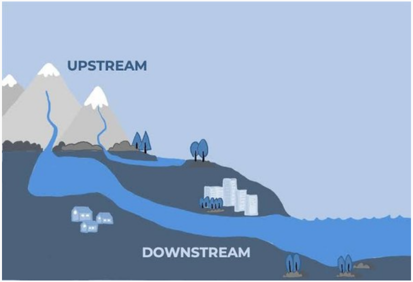
# Motivation and challenges

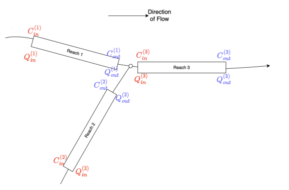
Wessex water is interested in understanding:

- **Effects/predictions of velocity**: velocity is a key ingredient in predictions; how can it be better estimated?
- **Source apportionment**: how can we attribute original upstream sources of contaminants from downstream measurements.
- Effects of UV exposure on transport and decay

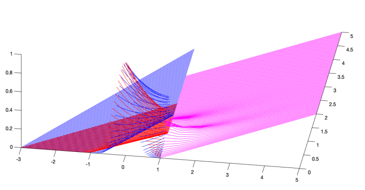
**Our approach:** develop dynamic mathematical models



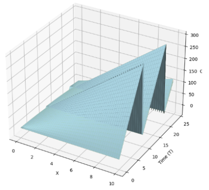
# Overview of approaches



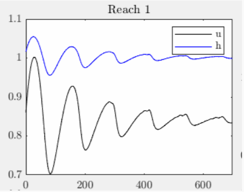

**(a)** Simplified network model of contaminants



**(b)** Dynamic network model of contaminants




**(c)** Exploring functions influencing the concentration profile

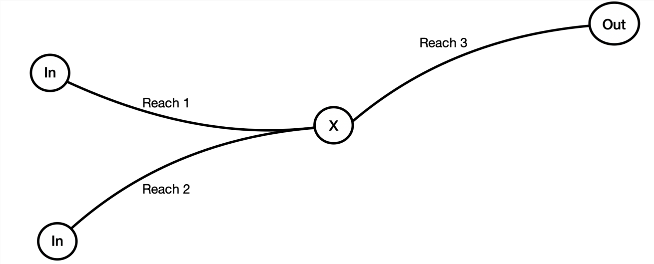



**(d)** Varying velocity and flow rates

## Toy setup: the 3-reach geometry

We consider a simplified geometry divided into three river sections (“reaches”).

- Contaminants injected (or measured) in Reach 1 and Reach 2 (“in”)
- Key downstream measurement at Reach 3 (“out”)



1D physics based model for bacteria concentration, $c_i(x_i, t)$, and velocity, $u_i(x_i, t)$, $i = 1, 2, 3$.

- **Concentration:** advection-diffusion-reaction equation in each reach:

$$\frac{\partial c_i}{\partial t} + \underbrace{u_i \frac{\partial c_i}{\partial x_i}}_{\text{advection}} = \underbrace{k \frac{\partial^2 c_i}{\partial x_i^2}}_{\text{diffusion}} + [\text{source terms}] + [\text{decay terms}],$$

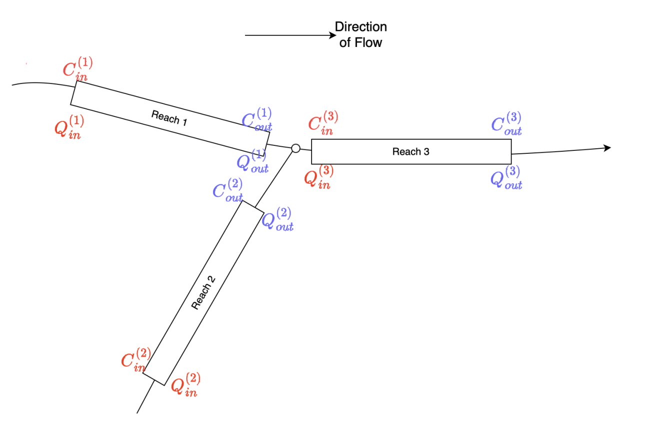
  where $x_i$ is the arc length coordinate along the river.

- **Velocities:** determined using the St. Venant shallow water equations describing river flow:

$$\underbrace{\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x_i}}_{\text{acceleration}} + \underbrace{g \frac{\partial h_i}{\partial x_i}}_{\text{pressure}} = \underbrace{g \frac{S_f}{h_i}}_{\text{friction}} - \underbrace{g S_0}_{\text{gravity}},$$

$$\frac{\partial h_i}{\partial t} + \frac{\partial (h_i u_i)}{\partial x_i} = [\text{source terms}].$$

# Developing a simplified graph-based model I




River network with 3 segments.

Red: inputs of the reach models. Blue: outputs of the reaches.

# Developing a simplified graph-based model II

In each reach model, we assume

- No internal mass change within the reach
- Reach flows are constant and governed by a law:

$$\mathbf{F}(Q_1, Q_2, \ldots, Q_N) = 0 \implies Q_{\text{in}} = Q_{\text{out}}.$$

  *We assume the flows are known in the procedure; either approximated via simple mass balance or simulated via PDE models*

- Contaminants obey a mass balance law:

$$\mathbf{G}(\mathbf{C}; \mathbf{Q}) = 0 \implies C_{\text{in}}^{(3)} = \frac{Q_1 C_{\text{out}}^{(1)} + Q_2 C_{\text{out}}^{(2)}}{Q_1 + Q_2}.$$

- Velocities assumed known via empirical law: $v = aQ^b$, after which travel time in each reach determined via $\tau = \text{length}/\text{velocity}$.
- Once travel time is known, contaminant concentration can be predicted.

# A simple decay law I

- Let us assume the decay rate is constant and contaminants obey

$$\frac{\partial C_i}{\partial t} = -k_i C_i.$$

$\implies C_i = C_{i0} e^{-k_i t}$ for each reach.

- Then the output concentration at reach 3 is

$$C_{out}^{(3)} = \Gamma_1 e^{-\Lambda_1} + \Gamma_2 e^{-\Lambda_2},$$

where $\Gamma_i(C_{in}^{(i)}, Q_i)$ and $\Lambda_i(k_i, L_i, Q_i)$ are completely known.

- For example, concentration behaviour is **strongly dominated** by the Lambda-functions:

$$\Lambda_1 = k_1 \frac{L_1}{Q_1} + k_3 \frac{L_3}{Q_1 + Q_2}$$

*i.e. decay dictated by reach properties.*

# A simple decay law II

*Simplicity of such approximate decay laws facilitate intuition of processes.*

- Consider the effect of erroneous prediction of a flow measurement, $Q_1 \mapsto \overline{Q}_1 + \delta Q$. It can be verified this modifies decay prediction:

$$\log\left(C_{out}^{(3)}\right) \propto (-\bar{\Lambda} - \mathcal{P}\delta Q)t$$

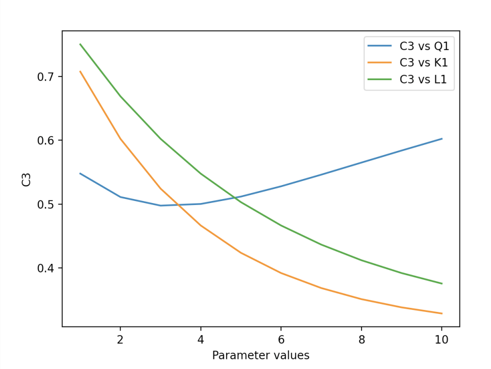



**Figure 2:** Parametric sensitivity analysis

# Dynamic decay laws I

Now including transport/velocity, the 1D advection-diffusion-reaction equations can be solved in closed form.

- Concentration $C(x,t)$ in each reach follows

$$\frac{\partial C^{(j)}}{\partial t} + u(Q_j)\frac{\partial C^{(j)}}{\partial x} = -k(t)C^{(j)}$$
$$\text{I.C.} \quad C^{(j)}(x,0) = C^{(j)}_{\text{in}}(x), \quad j = 1,2$$
$$C^{(3)}(x,0) = 0$$

- Concentration at the junction

$$C_i^{(3)}(t) = \begin{cases} 0 & t < t_1^* \\ \frac{Q_1 C^{(1)}_{\text{out}}(L_1, t_1^*)}{Q_1+Q_2} & t_1^* \le t < t_2^* \\ \frac{Q_1 C^{(1)}_{\text{out}}(L_1, t_1^*) + Q_2 C^{(2)}_{\text{out}}(L_2, t_2^*)}{Q_1+Q_2} & t \ge t_2^* \end{cases}$$

# Dynamic decay laws II

- In each reach, solution is combination of wave and decay:

$$C(x,t) = \underbrace{C_{\text{in}}(x-ut)}_{\text{wave phenom}}\,\underbrace{e^{-K(x,t)}}_{\text{decay}},$$

$$K(x,t) = \int_{t-x/u}^{t} k(t')\,dt'$$

where all three solutions must be matched at the junction.

- Example diurnal effects: $k(t) = A\cos(\pi t/12) + B$

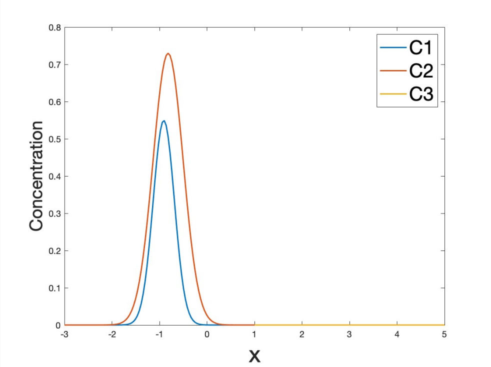
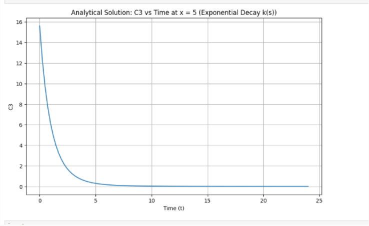


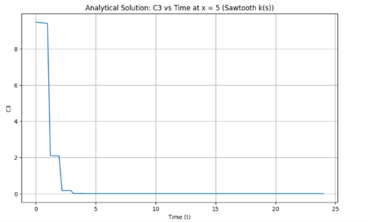

**Figure 3:** I.C. for first two reach models

**Conclusion:** highly-efficient formulae for concentration decay and transport

# Exploring suitable functions for k(t')



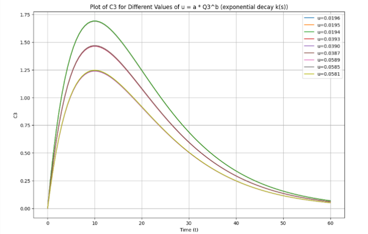

**(a)** Exponential decay for smooth behaviour



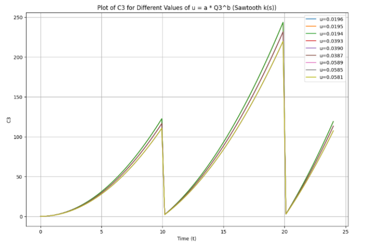

**(b)** Sawtooth function for periodic decay

- Exponential Decay: $k(t') = e^{-at'}$ - continuous decay patterns.
- Sawtooth function: $k(t') = \text{mod}(s, \text{period})$ - periodic/cyclic decay processes.

# Influence of u and k(t) in the analytical solution



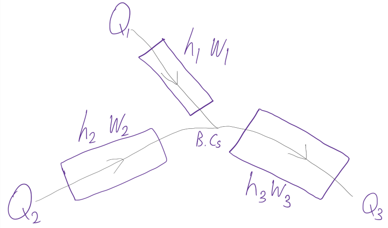

**(a)** Exponential decay(u values)



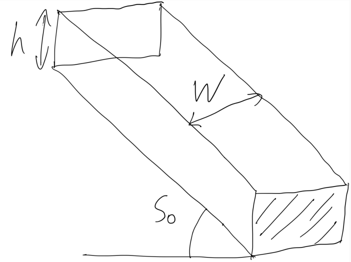

**(b)** Sawtooth function(u values)

- High Q(flux) - Steeper slopes and faster rate of decay
- Low Q(flux) - gentler slopes and lower decay rates over time

- **Challenge:** Can we use a PDE model to develop dynamic (spatial-temporal-varying) river velocities?




**(a)** 3 rivers catchment




**(b)** Cuboid shape for a river

- Assume cuboid river. Width ($w$), energy slope ($S_0$) and initial heights are known

# Model setup

Find $u_i$ and $h_i$ from the St. Venant (shallow river) conservation of momentum and conservation of mass equations ($i = 1, 2, 3$):

$$\underbrace{\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x_i}}_{\text{acceleration}} + \underbrace{g \frac{\partial h_i}{\partial x_i}}_{\text{pressure}} = \underbrace{g \frac{S_f}{h_i}}_{\text{friction}} - \underbrace{g S_0}_{\text{gravity}},$$

$$\frac{\partial h_i}{\partial t} + \frac{\partial (h_i u_i)}{\partial x_i} = [\text{source terms}],$$

where $S_f$ is found using Manning's Law,

$$S_f = \frac{{u_i}^2 n^2 (2h_i + w_i)^{4/3}}{(h_i w_i)^{4/3}}.$$

Equation for the flow, $Q_i$, linking $u_i$ and $h_i$:

$$Q_i = w_i h_i u_i.$$

# Boundary conditions

- For reaches 1 and 2, we specify $Q$ at the upstream end $(x = 0)$.
- Modelled $Q_i = A_i \sin(\omega_i t)$ to reflect the diurnal flow variation.
- At the river junction, require continuity of momentum/mass:

$$Q_1 + Q_2 = Q_3,$$
$$h_1 w_1 + h_2 w_2 = h_3 w_3.$$

- Imposed simplified boundary conditions on reach 3:

$$Q_3 = \frac{Q_1 + Q_2}{2}, \qquad h_3 = \frac{h_1 + h_2}{2}.$$

# Gif Animation!

# Conclusions and future work

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- Simplified network models can provide **powerful machinery** for intuition and approximation.
- Sensitivity analysis and optimisation is possible within simplified physics-based frameworks.
- Physics-based PDE models for river flows can provide detailed predictions of transport phenomena.

# Conclusions and future work

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- Physics-based PDE models for river flows can provide detailed predictions of transport phenomena.

## Next steps

- Develop framework for **data-driven simulations**: *Can we couple uncertainties with physics-based modelling?*
- **Upscaling**: Incorporate realistic river geometries, source effects, storm overflows.
- Can we augment a network model with PDE behaviours?
- Combine varying velocity field with simplified concentration models.
- Source apportionment: Inverse problem for unknown concentrations.


"That's all Folks!"

# References