ITT6: Water Quality Testing with Bacteria V2.0

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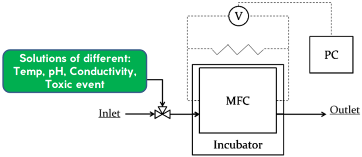
The Problem

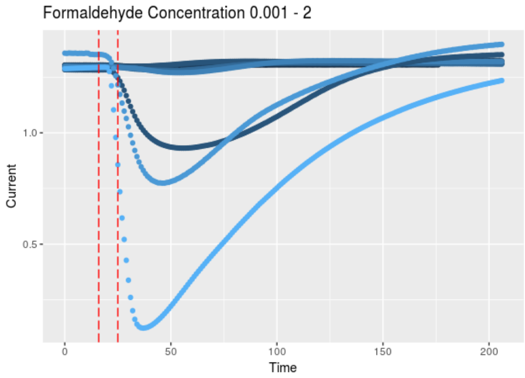
- Bacterial fuel cell in water : current is dependent on level of contaminant and environmental conditions.
- Current drops and recovers as bacteria recover after a toxic event.
- AIM: use data on the change in current (in the form of these *"current curves"*) to identify contaminants and safety of water.



[1]

[1] Chouler et al., Electrochemica, 192,89-98,(2016)

The Data

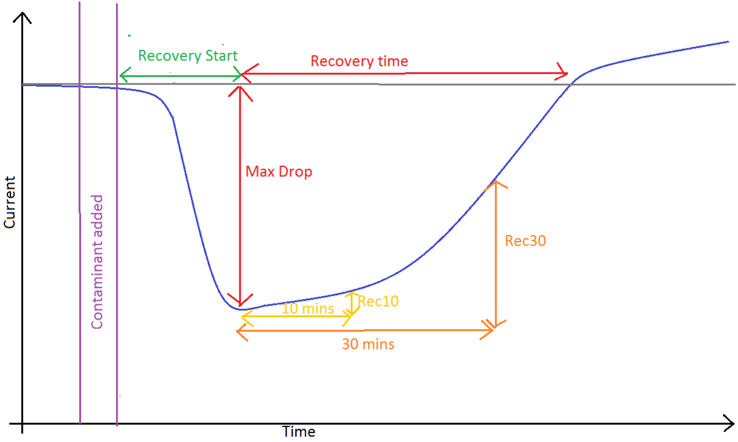


- Change in current from a biocell conditional upon the change in temperature, pH and a pollutant (formaldehyde).
- Plot shows current with addition of formaldehyde at different concentrations.

Modelling the concentration

- Initial data: formaldehyde pollutant in different concentrations with environmental conditions kept constant.
- We can view each varying current curve as a data point, varying with concentration.
- We treat characteristics of these curves as explanatory variables.

Characterising the curves



Fitting a model

This week...

- Linear Model with concentration response, and explanatory variables of characteristic measurements of curves.
- Backwards selection implies:
  $Conc. = \alpha_0 + \alpha_1 Maxdrop + \alpha_2 Rec10 + \epsilon$
- Possible extra nonlinear effects may be seen with more data.

The future...

- Further data would be needed to assess possible nonlinear effects
- Interaction terms with pH, temperature etc. may be included after experiments have been conducted.

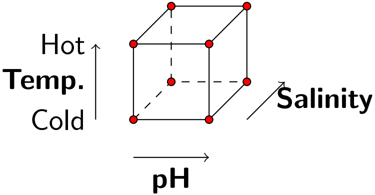
We need more data!

- Only one variable changed at a time: no interactions can be observed
- Very few data points: not enough power to detect effects, especially possible nonlinear ones.
- Different devices are used, yet not enough data for a mixed effects model

Experimental Design

Factorial Design:

- Consider each variable as a categorical variable with multiple levels.
- Experiments for every combination.



Practical Considerations:

- Random effects to account for different MFCs
- Washout necessary
- Further investigation into population changes to ensure independence.

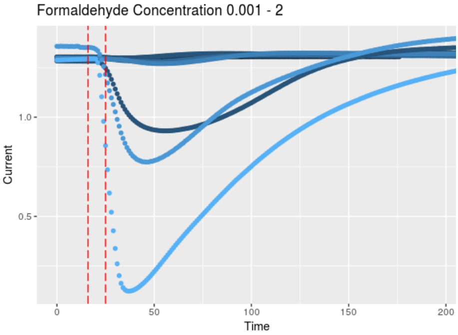
Modelling Bacterial Population

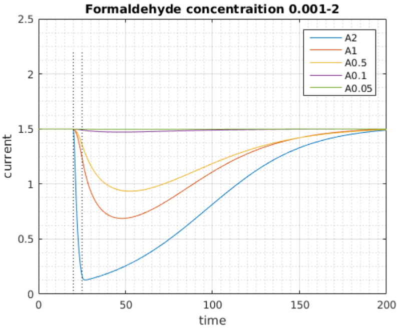
$$\frac{ds}{dt} = g_s \left(s - \frac{s+r}{K} \right) - d_s c(t) s$$
$$\frac{dr}{dt} = g_r \left(r - \frac{s+r}{K} \right) - d_r c(t) r$$
$$\frac{dc}{dt} = C_0 - d_c c$$

$$c(t) = \begin{cases} 0 & \text{if } t \in [0, t_s] \\ \frac{C_0}{d_c}\left(1 - e^{-d_c(t-t_s)}\right) & \text{if } t \in [t_s, t_f] \\ \frac{C_0}{d_c}\left(1 - e^{-d_c(t_f-t_s)}\right)\left(1 - e^{(-d_c(t-t_f))}\right) & \text{if } t > t_f \end{cases}$$

For $i \in \{s, r\}$, g_i and d_i are the growth and death rate (resp.) of bacteria i, k is the capacity of the system, C_0 is the addition of toxins to the system, d_c is the rate of diffusion of the toxins.

Modelling Bacterial Population





Next steps

- Obtain more data using factorially designed experiments.
- Identify possible non-linear effects #fitaGAM.
- Investigate the identification of multiple pollutants.
- Compare these statistical models with existing neural network techniques.

Any Questions?