Calibration & sensitivity analysis of a 1D model of pollutant transport & degradation in maturation ponds

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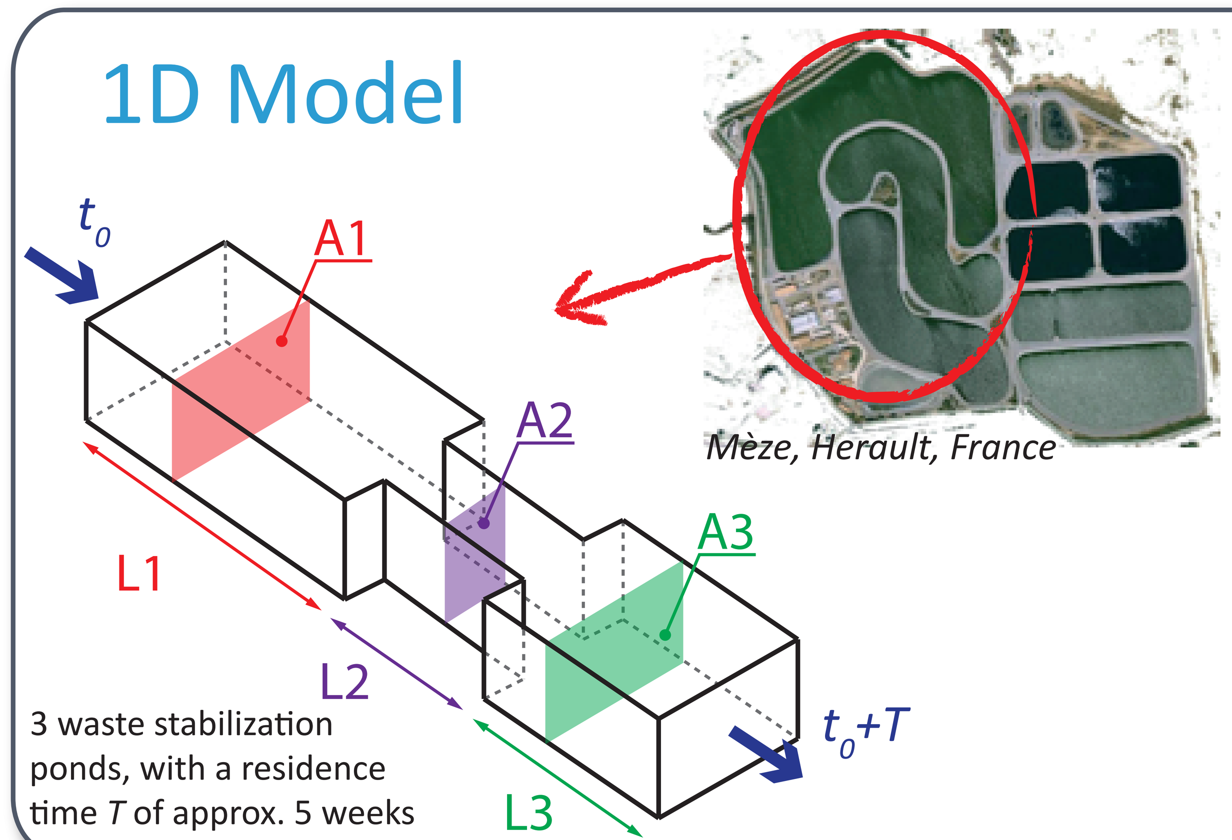
Context and Objective

A simple 1D model of transport and degradation is proposed for a maturation ponds system. A sensitivity analysis of the model output with respect to different parameters is performed in the aim of:

- Assessing the precision required for the main parameters measurements or calibration (section, discharge, degradation coefficient) .
- Calibrating the contaminant degradation coefficient $k(t)$ (depending on time)

1D Model



Continuity and transport/degradation equations:

$$\frac{\partial A(x,t)}{\partial t} + \frac{\partial Q(x,t)}{\partial x} = 0$$

$$\frac{\partial AC(x,t)}{\partial t} + \frac{\partial QC(x,t)}{\partial x} = -k(t)AC(x,t)$$

A: section
Q : discharge
C : Chemical Oxygen Demand
k : degradation coefficient

Simplified system

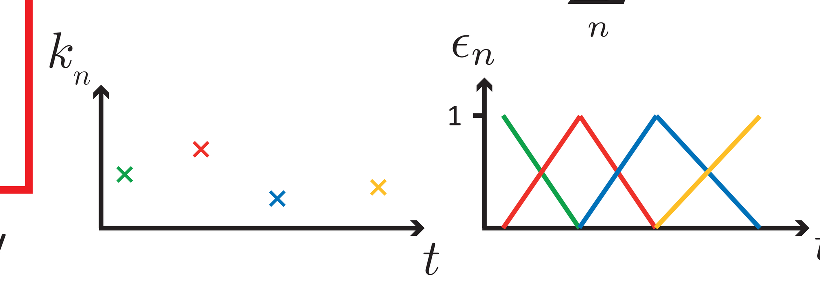
$$\boxed{\frac{\partial C(x,t)}{\partial t} + u(x,t)\frac{\partial C(x,t)}{\partial x} = -k(t)C(x,t)}$$

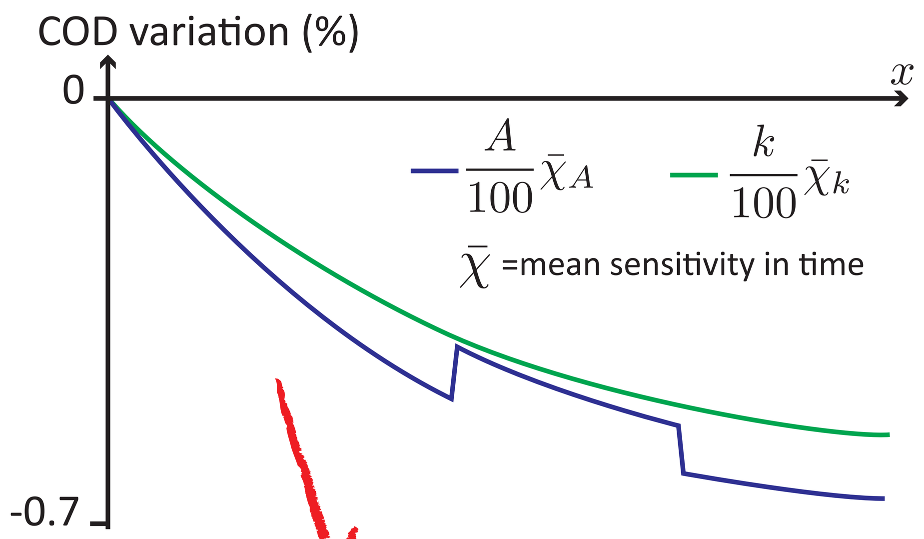
u=Q/A: flow velocity

Solved with a finite volume approach and a Godunov scheme

Hypotheses:

- Water elevation controlled so that A is independent of time => Q independent of space
- $k(t)$ piecewise linear: $k(t) = \sum_n k_n \epsilon_n$





- A variation of 1% in A implies a variation of ≈0.7% in COD
- The influences of k and A on the solution are equivalent

Sensitivity analysis

- Solve the sensitivity equation with $\chi = \frac{\partial C}{\partial \psi}$ | ψ: A, Q, k_n

$$\frac{\partial \chi(x,t)}{\partial t} + u(x,t)\frac{\chi(x,t)}{\partial x} = -k(t)\chi(x,t) - \epsilon_n C(x,t)$$

if $\psi = k_n$

$$\left.\begin{array}{l}\chi(0,t) = 0 \\ \chi(x,0) = 0\end{array}\right\}$$ null sensitivity when initial and boundary conditions are known

- When ψ is discontinuous (such as A), C is not differentiable and an extra source term must be added to avoid locally infinite sensitivity [2].

Calibration process

- Calibration with respect to the output concentration
- Difficulties encountered with classical distance-based objective functions (DOF) because of local minima.

=> use of weak form-based objective functions (WOF) [3,4]

- WOF are monotone *wrt* k => change the optimisation problem into a root finding problem (avoid local minima)

=> calibrate n values of k_n : find the intersection beetween n WOF i.e. solve $W_{pn}(k_n)$=0 for n values of p using *e.g.* Newton-Raphson's algorithm :

$$\mathbf{k}^{i+1} = \mathbf{k}^i \mathbf{J}^{-1}\mathbf{W} \qquad \begin{pmatrix} k_1 \\ \vdots \\ k_n \end{pmatrix} \qquad \begin{pmatrix} W_{p1} \\ \vdots \\ W_{pn} \end{pmatrix}$$

$$\mathbf{J}^{-1} = \begin{pmatrix} \frac{\partial W_{p1}}{\partial k_1} & \dots & \frac{\partial W_{p1}}{\partial k_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial W_{pn}}{\partial k_1} & \dots & \frac{\partial W_{pn}}{\partial k_n} \end{pmatrix}$$ with $$\frac{\partial W_{pi}}{\partial k_j} = p|e|^{p-1}\frac{\partial C}{\partial k_j}$$

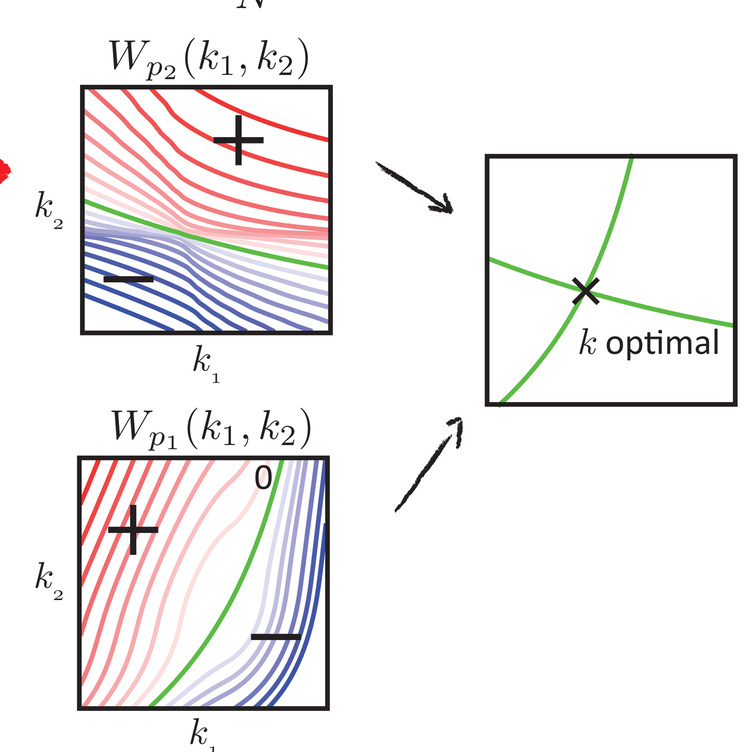
error = simulations - measurements

$$e = C_s(L,t) - C_m(L,t)$$

$$D_p = \sum_N |e|^p$$

$$W_p = \sum_N e|e|^p$$

- Big values of p: give more weight to the higher values of e
- Small values of p: come closer to the measurements in average



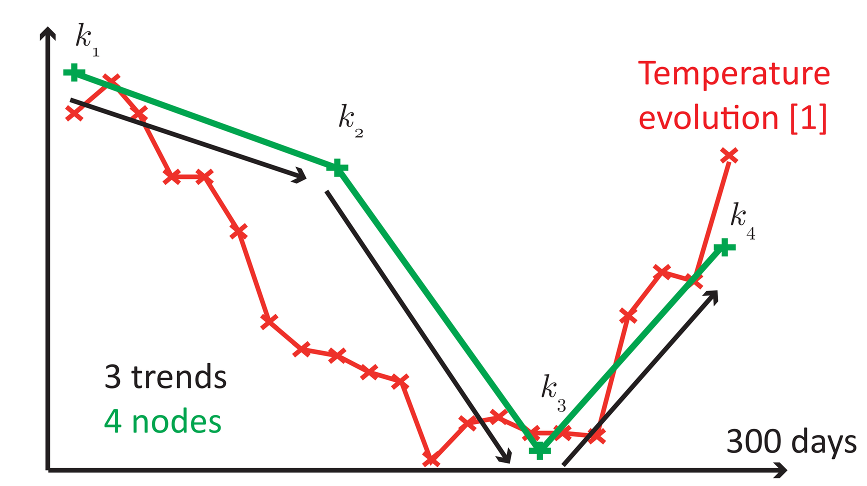
Application

Measurements [1]:

- ≈ each 15 days during 1 year: inlet and outlet COD and discharge, with an uncertainty of at least 15%

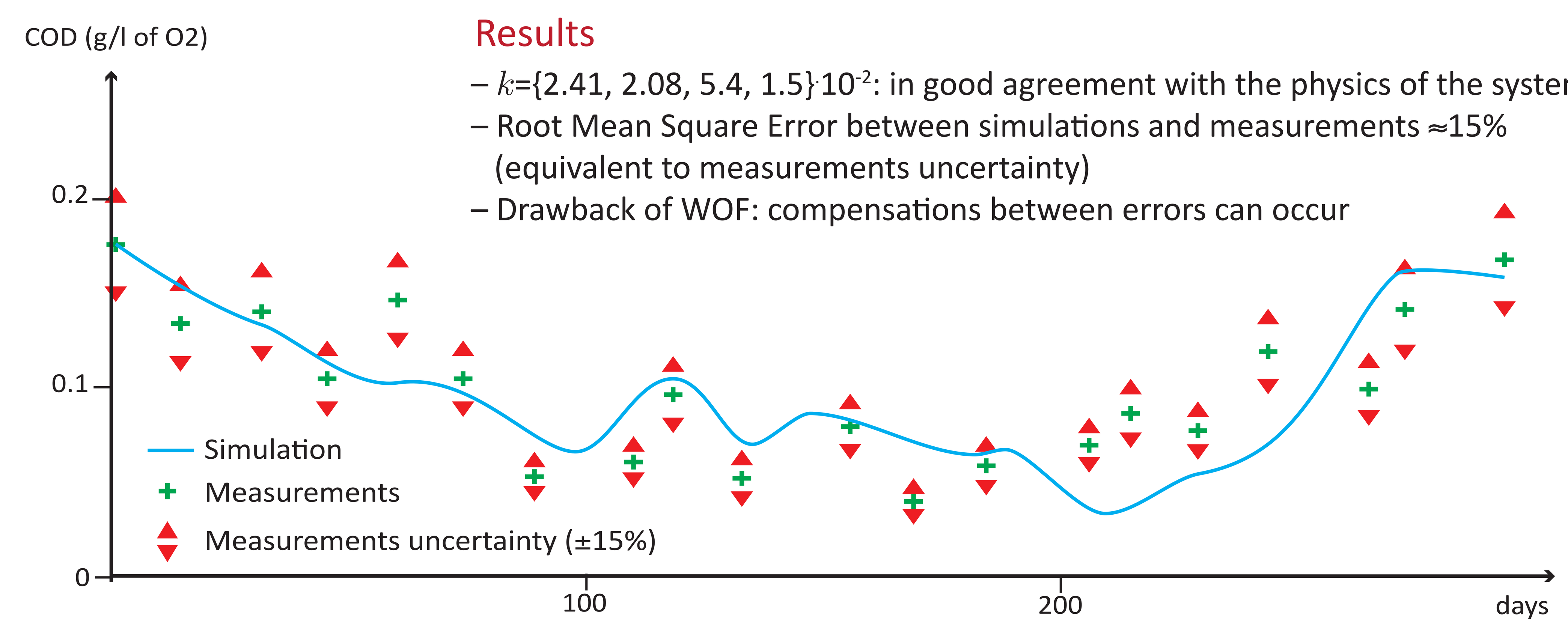
Model:

- Input: $C_m(0,t)$ and $Q_m(0,t)$ (linear interpolation of measurements)
- 3 trends for k acording to the temperature evolution
- p={0, 0.3, 0.6, 1}
- Output: $C_s(L,t)$ compared to $C_m(L,t+T)$ including retention time of T≈30days



Results

- k={2.41, 2.08, 5.4, 1.5}$\cdot 10^{-2}$: in good agreement with the physics of the system.
- Root Mean Square Error between simulations and measurements ≈15% (equivalent to measurements uncertainty)
- Drawback of WOF: compensations between errors can occur



Conclusions & Perspectives

- Correct estimation of the output COD according to measurements uncertainty

Further research are ongoing to enhance the results:

- use both WOF and DOF to avoid error compensation
- use a variable retention time T
- describe the degradation coefficient by a function of the temperature
- collect more measurements and use data assimilation

References

[1] T.R. Andrianarison. *Traitement d'effluents urbains dans un système de 11 lagunes. Décontamination microbienne et élimination de l'azote.* PhD thesis, Université Montpellier 2, 2006.
[2] V. Guinot, An approximate Riemann soverf for sensitivity equations with discontinuous solutions. *Advances in Water Resources*, 30, p.1943-1961, 2007.
[3] V. Guinot, B. Cappelaere, C. Delenne and D. Ruelland, Towards improved criteria for hydrological model calibration: theoretical analysis of distance- and weak form-based functions, *Journal of Hydrology*, 401, p.1-13, 2011.
[4] C. Delenne, V. Guinot, B. Cappelaere, Weak form-based objective functions in hydrology, application to a 1D transport/degradation model, EGU 2010, poster A198.

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