

# On the fate of micropollutants in the environment: Dynamic modelling of Bisphenol A and heavy metals in wastewater treatment plants

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SIDISA.08

International  
Symposium on Sanitary &  
Environmental Engineering

Firenze, Italy

25 June 2008



Canada Research Chair  
on Water Quality Modelling



## modelEAU: its logo ...

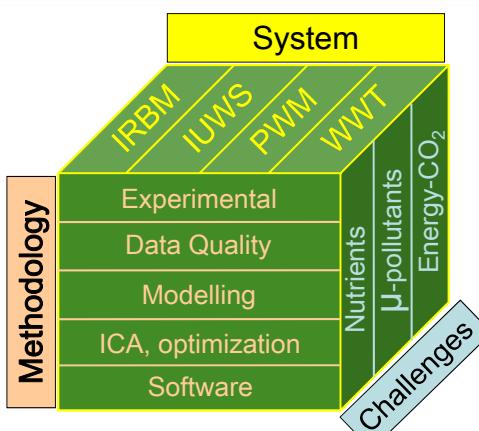
- Location
  - Québec, along a river
- Relation with our long term objectives
  - Data collection
  - Urban waters
  - Continuous (automated)
  - Data quality
- Its name : Modelling water systems



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## 3D schematic of modelEAU's research ("cubEAU")



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## Overview

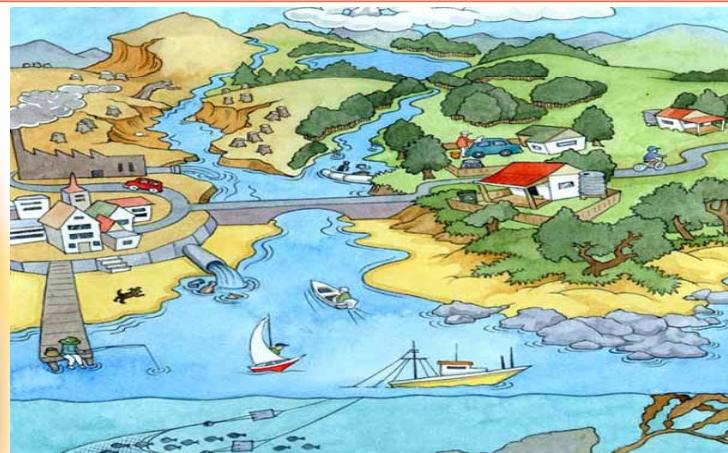
- Problem statement
- Objectives
- Materials and methods
- Modelling
- Results
- Conclusion



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## Problem statement

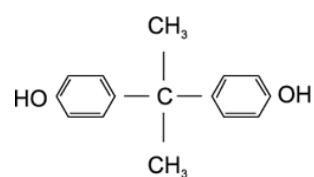


## Problem statement

### ■ Example: Bisphenol-A (BPA)

#### ▪ Use

- Polycarbonates (Bottles, CDs)
- Epoxyresins (canned goods)



## Problem statement

- Example: Heavy metals
  - Origin
    - Tires (Zinc, Copper, Chrome)
    - Car parts (Lead, Cadmium)
    - Roofs (Zinc, Copper)



## Problem statement

- Protect the environment:



## Problem statement

- Influent of a WWTP:

- Traditional pollutants:

- Organic matter (excrements, kitchen, shower, leaves)
    - Nitrogen (urine, fertilizer)
    - Phosphorus (detergents, fertilizer)

- Toxic products

- Xenobiotic organic compounds (perfumes, detergents)
    - Heavy metals

Micropollutants  
Emerging pollutants  
Priority pollutants



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## Problem statement

- Effluent of a WWTP

- A certain amount of pollutants will be rejected

- Which fraction?

- How can we improve the situation?

- Limit the use of certain products

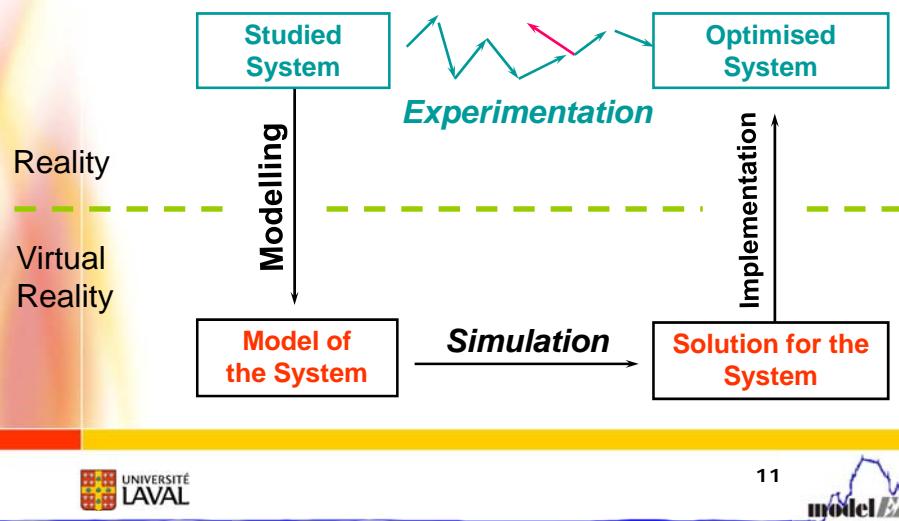
- Modify the configuration/operation of the WWTP



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## Problem statement: Why modelling ?



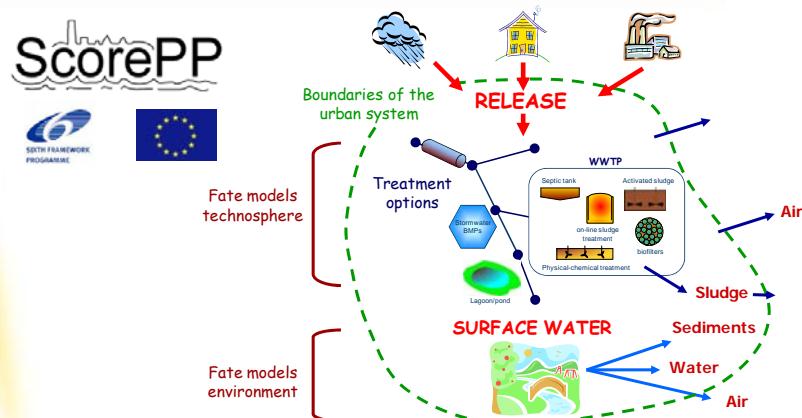
## Overview

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- Modelling
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## Objectives

- Develop a model able to describe the fate of micropollutants on top of traditional pollutants in a WWTP  
*(and in the sewer system and the river)*
- Score-PP
  - Source Control Options for Reducing Emissions of Priority Pollutants

## Objectives



## Overview

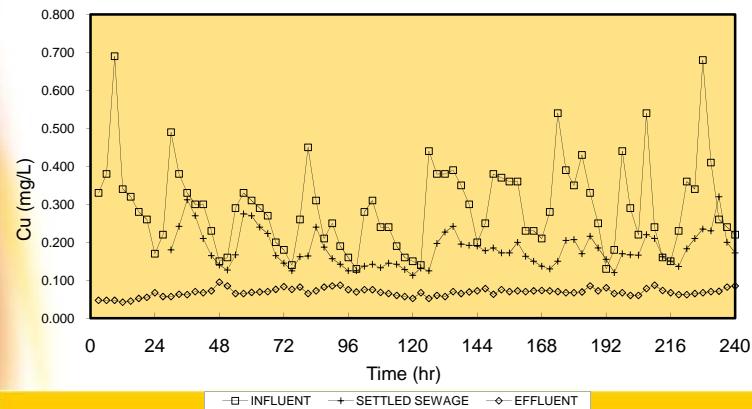
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## Materials and methods

- WWTP of Norwich, UK
- Activated sludge with anaerobic digestion
- Data collected in 1986
  - COD, SS,  $\text{NH}_4$ , 6 heavy metals
  - 10 days, 3h interval
  - Different sample locations in the WWTP
  - Unique data set in the world

## Materials and methods

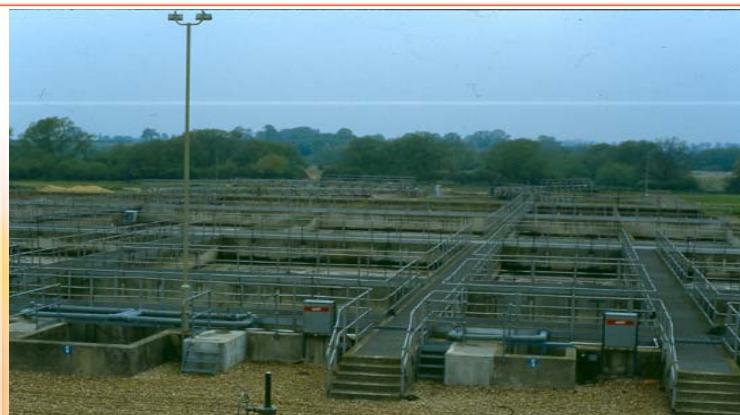
### ■ Example of data series: Copper



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## Materials and methods



Source: Paul Lessard



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## Materials and methods



Source: Paul Lessard



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## Materials and methods



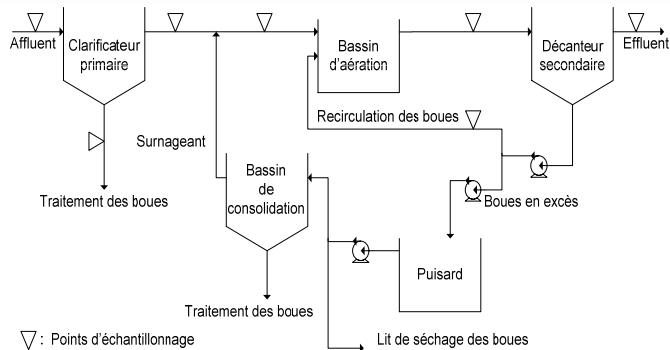
Source: Paul Lessard



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## Materials and methods



Activated sludge system at the Norwich WWTP  
(Lessard and Beck, 1993)



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## Materials and methods

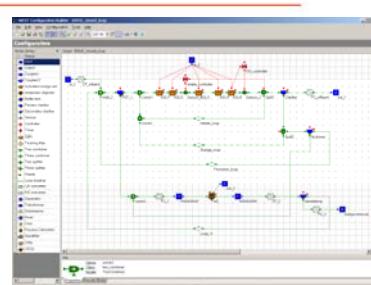
### ■ WEST® simulator

#### ▪ Developed by:



#### ▪ Functionality:

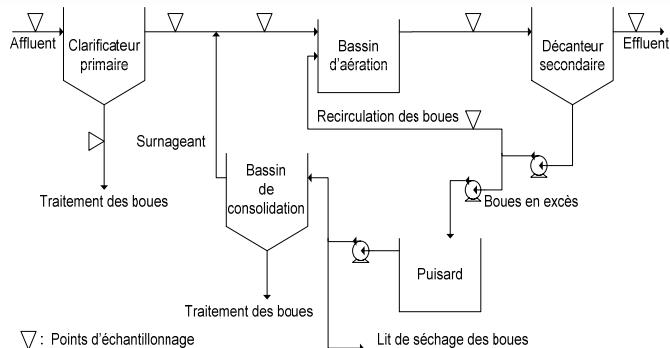
- Dynamic simulation
- Add/extend models yourself
- Extensions for sewers (KOSIM) and rivers (RWQM1)



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## Materials and methods



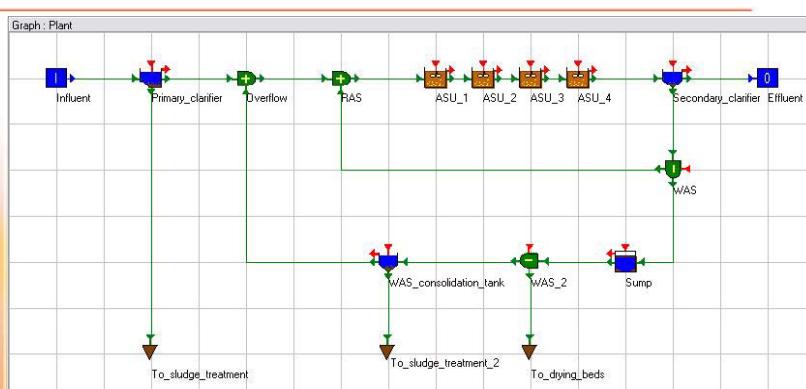
Activated sludge system at the Norwich WWTP  
(Lessard and Beck, 1993)



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## Materials and methods



The Norwich WWTP in the WEST simulator



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## Overview

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## Modelling

- Mass balance

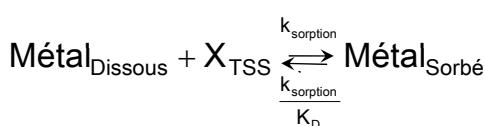
$$\frac{d\text{Métal}}{dt} = \frac{Q_{in}}{V} (\text{Métal}_{in} - \text{Métal}_{out}) - \text{Dég. bio.} - \text{"Sorption"} - \text{Volatilisation}$$

Transport

Reactions

## Modelling

- Describe sorption:



$$K_D = \frac{k_{\text{sorption}}}{k_{\text{désorption}}}$$

$$\text{Rate} = k_{\text{sorption}} \cdot \left( S_{\text{Métal}} \cdot X_{\text{TSS}} - \frac{X_{\text{Métal}}}{K_D} \right)$$

## Modelling

Transport

Reactions

- Mass balance

$$\frac{d\text{Métal}}{dt} = \frac{Q_{\text{in}}}{V} (\text{Métal}_{\text{in}} - \text{Métal}_{\text{out}}) - \text{Dég. bio. - "Sorption" - Volatilisation}$$

$$\frac{dS_{\text{Métal}}}{dt} = \frac{Q_{\text{in}}}{V} (S_{\text{Métal,in}} - S_{\text{Métal,out}}) - k \cdot \left( S_{\text{Métal}} \cdot X_{\text{TSS}} - \frac{X_{\text{Métal}}}{K_D} \right)$$

$$\frac{dX_{\text{Métal}}}{dt} = \frac{Q_{\text{in}}}{V} (X_{\text{Métal,in}} - X_{\text{Métal,out}}) + k \cdot \left( S_{\text{Métal}} \cdot X_{\text{TSS}} - \frac{X_{\text{Métal}}}{K_D} \right)$$

Transport

Sorption/Desorption

## Modelling

- Importance of TSS:

$$\frac{dS_{\text{Métal}}}{dt} = \frac{Q_{\text{in}}}{V} (S_{\text{Métal,in}} - S_{\text{Métal,out}}) - k \cdot \left( S_{\text{Métal}} \cdot X_{\text{TSS}} - \frac{X_{\text{Métal}}}{K_D} \right)$$

$$\frac{dX_{\text{Métal}}}{dt} = \frac{Q_{\text{in}}}{V} (X_{\text{Métal,in}} - X_{\text{Métal,out}}) + k \cdot \left( S_{\text{Métal}} \cdot X_{\text{TSS}} - \frac{X_{\text{Métal}}}{K_D} \right)$$

- We need good quality TSS simulations!
- We need a model that describes growth/decay of biomass and the accumulation of org. matter

ASM1  
(Activated Sludge Model No.1)

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## Modelling

- Importance of TSS – WWTP

- Primary clarifier

- $r_H [\text{m}^3/\text{g}] = 0.00026$  (0.00019) ← Hindered sedimentation
    - $r_P [\text{m}^3/\text{g}] = 0.00054$  (0.00070) ← Individual sedimentation
    - Average waste flow [ $\text{m}^3/\text{d}$ ] = 201.5 ← Not constant

- Aeration tanks

- $k_L a [\text{j}^{-1}] = 220, 60, 14, 12$
    - $K_S [\text{g/m}^3] = 20$  (130)

- Secondary clarifier

- Average waste flow [ $\text{m}^3/\text{d}$ ] = 575.5

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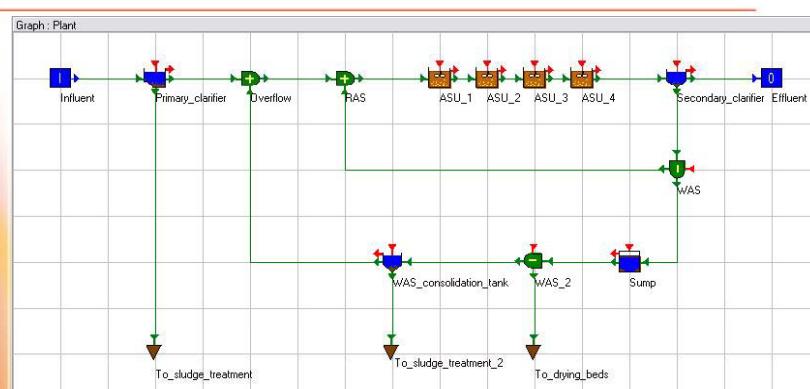
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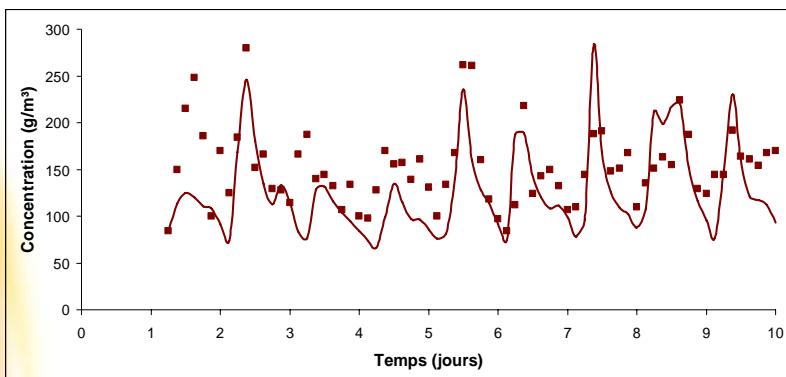
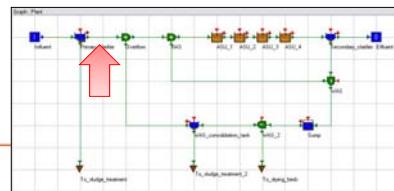
## Results



The Norwich WWTP in the WEST simulator

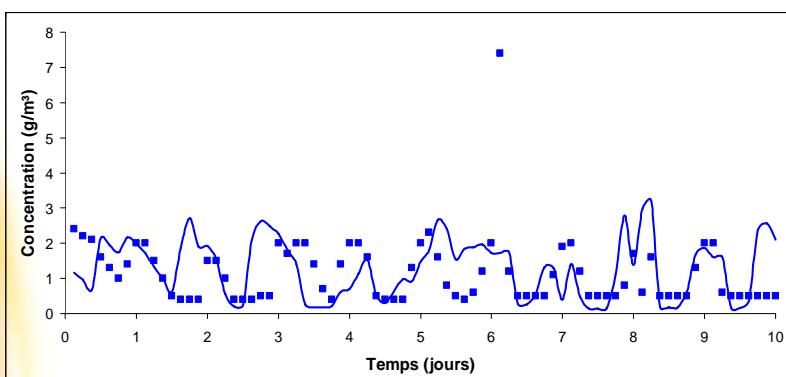
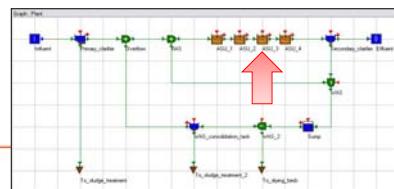
## Results

### ■ TSS in PC effluent



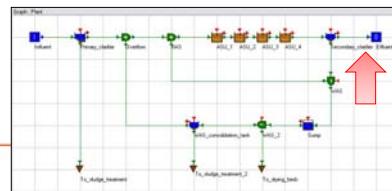
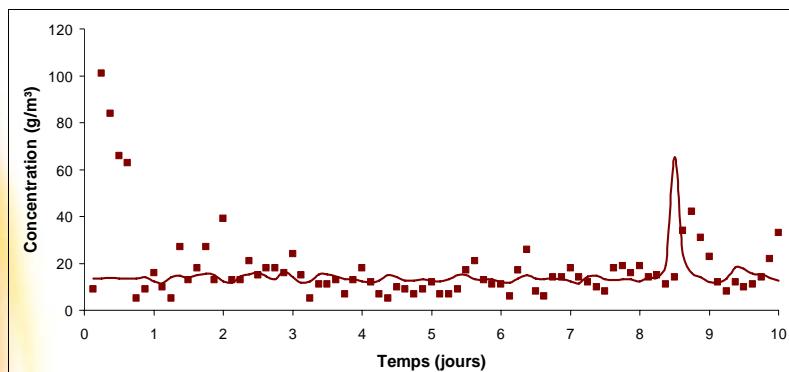
## Results

### ■ Dissolved oxygen



## Results

### ■ Effluent TSS



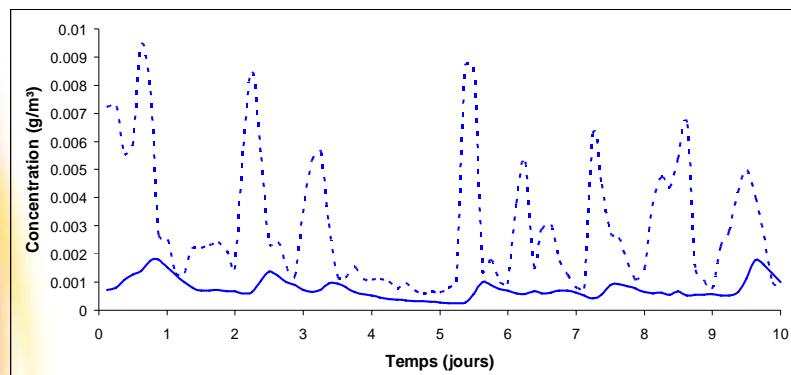
## Results

### ■ Studied heavy metals

Parameters	Units	Copper	Zinc	Lead	Cadmium	Chrom e	Nickel
$k_{\text{sorption}}$	L/mg.d	0.0008	0.0001	0.0023	0.0002	0.0015	0.0008
$\text{Log}(K_D)$	L/kg	4.0 (3.1 – 6.1)	5.1 (3.5 – 6.9)	4.6 (3.4 – 6.5)	4.6 (2.8 – 6.3)	4.6 (3.9 – 6.0)	3.9 (3.5 – 5.7)
Removal	%	90.2	80.1	93.3	75.6	86.5	71.6

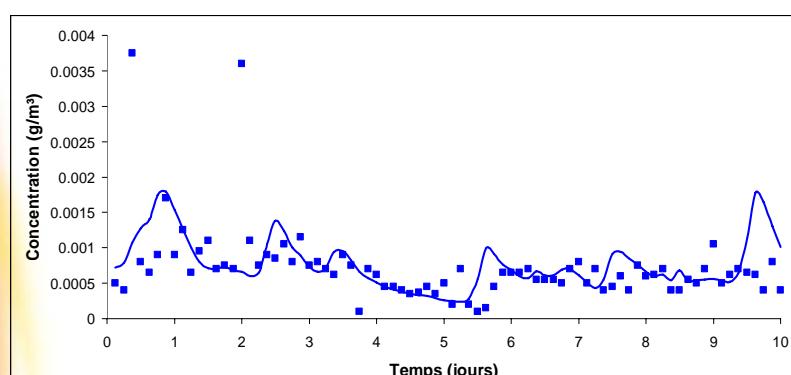
## Results

### ■ Cd: Influent - effluent



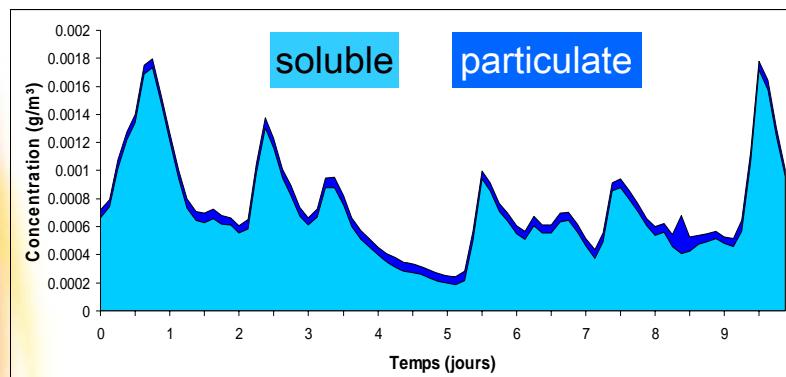
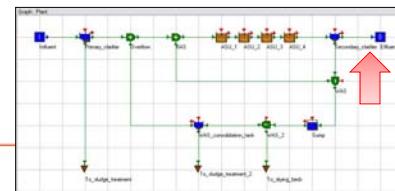
## Results

### ■ Cd: Effluent



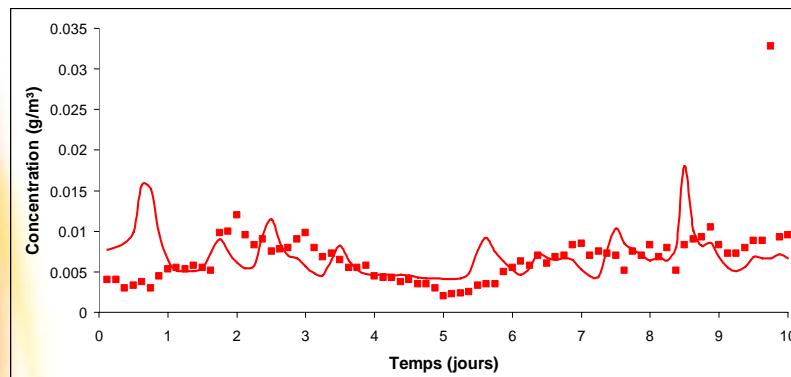
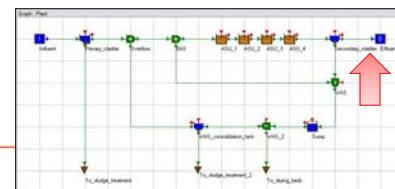
## Results

### ■ Cd: partitioning



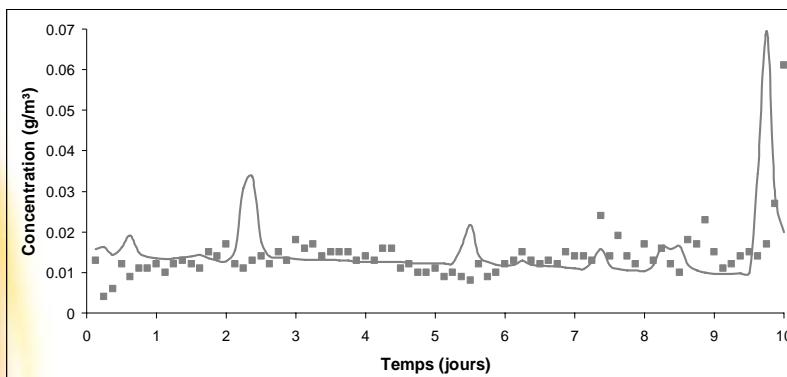
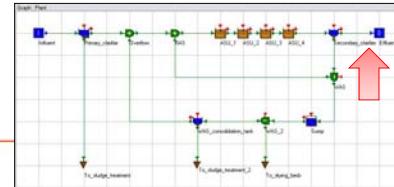
## Results

### ■ Cr: Effluent



## Results

### ■ Pb: Effluent



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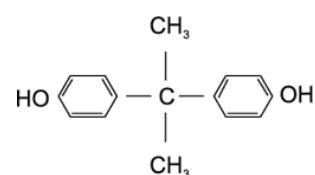
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## Problem statement

- Example: Bisphenol-A (BPA)

- Use

- Polycarbonates (Bottles, CDs)
    - Epoxyresins (canned goods)

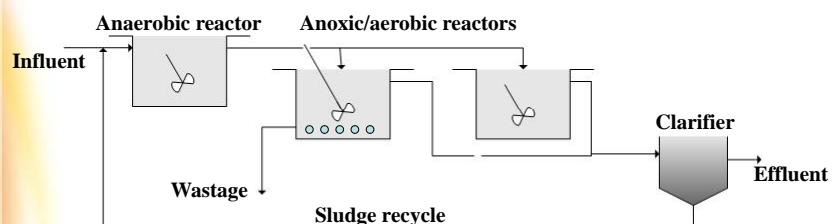


## Problem statement

- Example: Bisphenol-A (BPA)
  - Endocrine disruptor
    - Modifies the hormonal equilibrium of an organism
  - Is extracted from materials, especially when:
    - Cleaned with strong detergents
    - Heated to high temperatures
    - Contacted with strong acids
  - Typical concentration in wastewaters:
    - between 5 and 10 µg/L

## Materials and methods

- Pilot plant at Copenhagen (Denmark)
  - WWTP Lynetten
  - Biodenipho™ process
  - Total volume of the reactors: 11.6 m<sup>3</sup>



## Materials and methods

- Pilot plant at Copenhagen (Denmark)



## Materials and methods

- Pilot plant at Copenhagen (Denmark)



## Modelling

$$\frac{dXOC}{dt} = \frac{Q_{in}}{V} (XOC_{in} - XOC_{out}) - \text{Dégradation biologique} - \text{Sorption} - \text{Volatilisation}$$

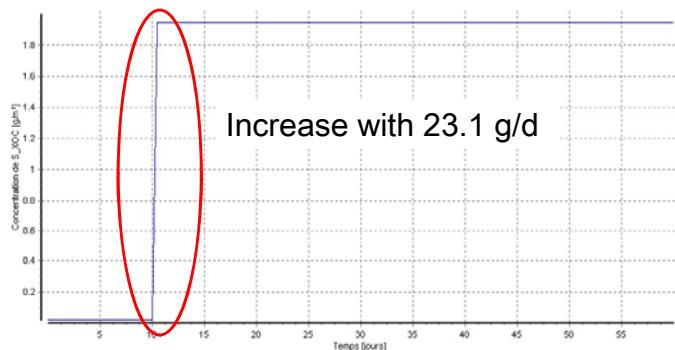
- Bisphénol A is non-volatile
- Biodegradation by a specialised bacterium
- Biodegradation only in presence of O<sub>2</sub>

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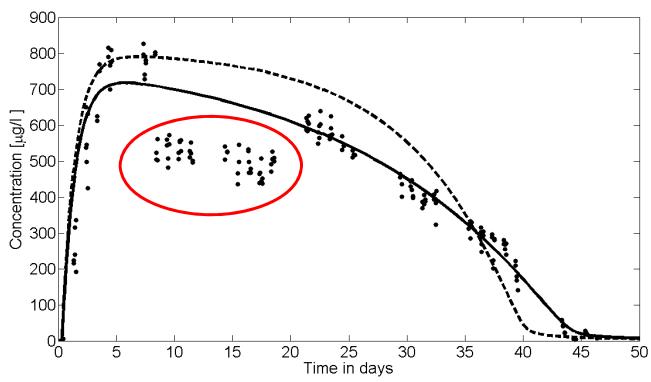
## Results

- Experiment: Step load change to BPA



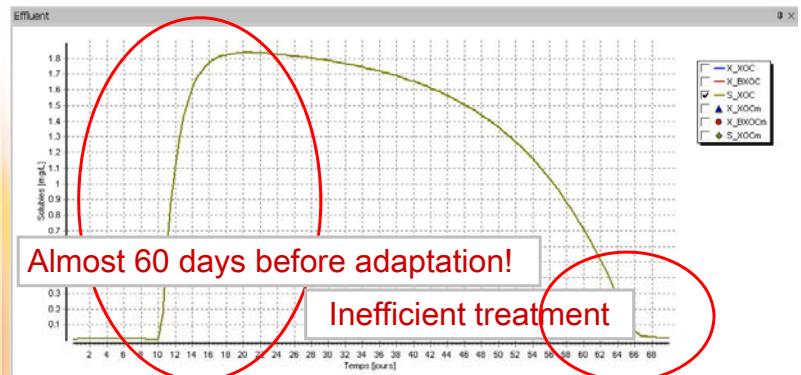
## Results

- Case study Lynetten (Injection of 10 g/d of BPA)



## Results

### ■ Effluent BPA concentration

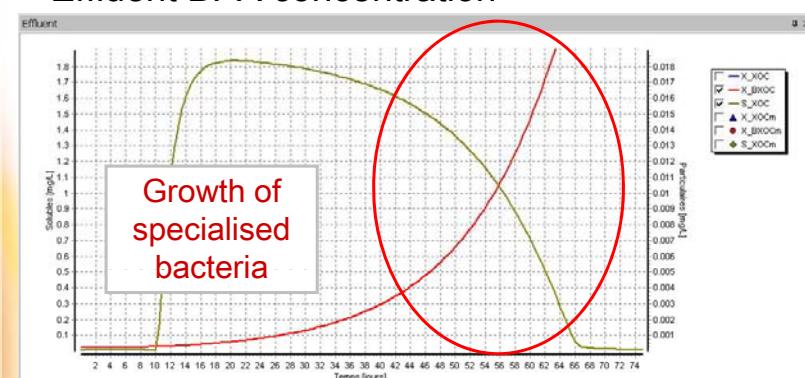


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## Results

### ■ Effluent BPA concentration



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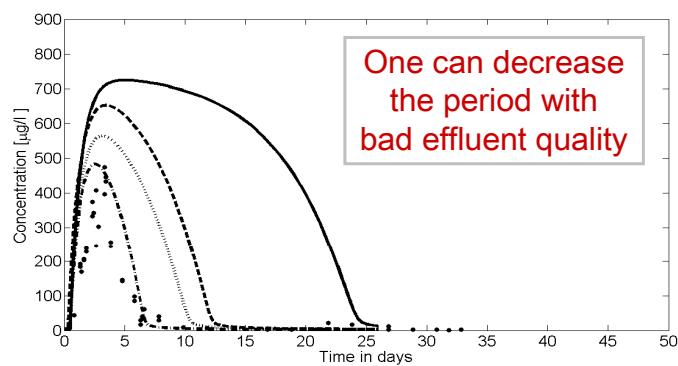


## Results

- Use of the model:  
Effect of operational parameters:
  - Increase temperature and aeration
  - Injection of 1 g/d of BPA for 60 days in order to adapt the biomass to the new pollutant
  - No injection for 14 days
  - Injection of 10 g/d of BPA

## Results

- Effect of operational parameters



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## Conclusion

- Case studies:
  - Xenobiotic Organic Compounds (XOC)
  - Heavy metals
- Development of a model that deals with:
  - Traditional pollutants
  - Heavy metals
  - Bisphenol A
- Potential of the model
  - Optimising the design/operation of WWTPs

$$k_{\text{sorption}} \cdot \left( S_{\text{Métal}} \cdot X_{\text{TSS}} - \frac{X_{\text{Métal}}}{K_D} \right)$$

## Conclusion

### ▪ Acknowledgement



*Canada Research Chair  
in Water Quality Modelling*

- Frédéric Cloutier
- Guillaume Jalby
- Paul Lessard
- Erik Lindblom
- Peter Steen Mikkelsen



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