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## ABSTRACT:

European policies (European Framework Directive: Water 2000/60/CE, Directive 76/464/CE) impose to reduce the releases of about a hundred substances in surface water. In the last years, the AQUAPOLE has been involved in two studies related to this matter.

First, on the request and with the financial support of both the French Ministry of Environment and ONEMA ("Office National de l'Eau et des Milieux Aquatiques"), INERIS ("Institut National de l'Environnement Industriel et des Risques") drew up the guidelines of a methodology allowing fixing the local Limit Values to Emission so as to abide by the quality standards on the whole watershed. Within this context, INERIS wishes to test the use of pollutant transfer models on pilot sub-basins. The PEGASE model has been used to simulate micropollutants on two concrete use cases (1):

- in the Meuse sub-basin, managed by the French Water Agency Rhine-Meuse, for simulations concerning cadmium and zinc;
- in the Adour sub-basin, managed by the French Water Agency Adour-Garonne, for simulations applied to cadmium and copper.

The choice of each substances and sub-basins was made by mutual agreement between INERIS, the concerned Water Agencies, and the AQUAPOLE. A major selection criterion for the substances and the sub-basins was the availability of data (sources and in situ measurements).

For the second study, the PEGASE model has been adapted to describe the cocaine's behaviour (using a stable metabolite of the cocaine in the environment: the benzoylecgonine (BZE)) in waste water, waste water treatment plants (WWTP) and surface water (2). The cocaine is newly described in the model as an additional micropollutant (PEGASE already treats numerous heavy metals), thanks to the implementation of new state variable equations and their specific parameterizations. Simulations of BZE have been done in the Walloon and Flemish regions, where many measurements from the COWAT project (3) were available.

The first results are showing good agreement between calculated and measured values. The ability of the model to simulate the fate of studied micropollutants (cadmium, zinc, copper, and the cocaine derivatives) in surface waters should be enhanced and extended to other substances and basins. Moreover, additional data still have to be collected and measured.

## A modelling study of heavy metals within two French basins

The PEGASE micropollutant (Cd, Cu, Zn, Pb, As, Ni, Cr, Ag, and Hg) sub-model includes:

### Mechanisms:

- transport by water (liquid phase)
- transport by the suspended matters (solid phase)
- adsorption of the micropollutants from the liquid phase on the solid phase
- adsorption of the micropollutants on the bottom sediments
- desorption of the adsorbed micropollutants
- sedimentation of the micropollutants adsorbed in the solid phase of the water column
- possibly, linear degradation

### Sources:

- diffuse loads of micropollutants from the watershed, as a result of the global erosion (use of statistical soil loads functions)
- pressure data (urban, industrial, waste water treatment plants and livestock discharges)

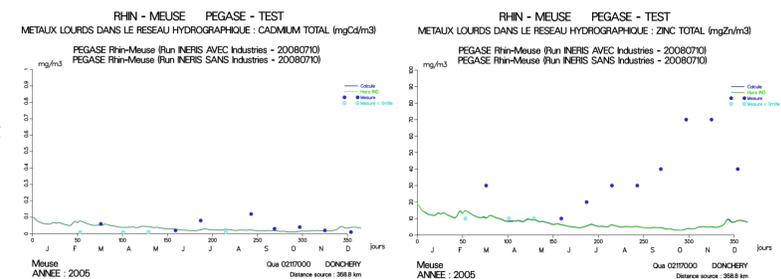
### General conclusion:

- improvement of release data (industries) seems necessary

### The Meuse sub-basin (French Water Agency Rhine-Meuse), Cd and Zn simulations

#### Conclusions:

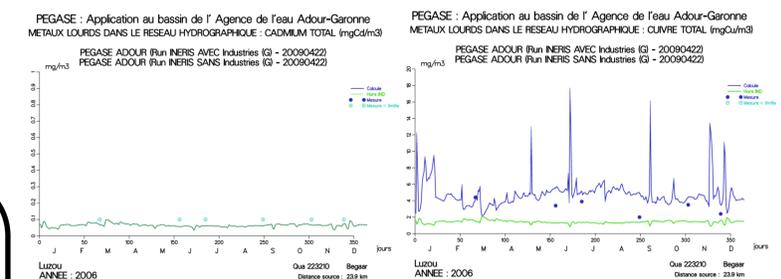
- the influence of the industrial loads on Zn and Cd concentrations in surface water of the Meuse basin is weak and strictly local
- it seems that important sources of Zn are not identified in the basin
- measurements are still to be improved (many points + detection limit) to be able to validate this kind of simulation



### The Adour sub-basin (French Water Agency Adour-Garonne), Cd and Cu simulations

#### Conclusions:

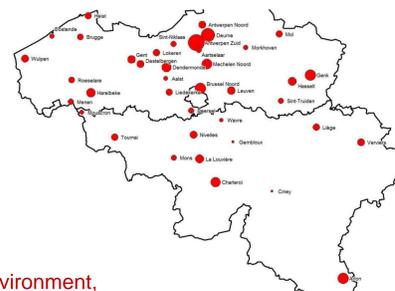
- the influence of the industrial loads on Cu and Cd concentrations in surface water of Adour basin is weak and strictly local
- it is difficult to make simulations of scenarios without improvements of input data



## A test application to cocaine in Belgium

### The COWAT (COcaine in WATER) study:

- Quantification of cocaine (COC) and its main metabolite (benzoylecgonine, BZE) in waste water, waste water treatment plants and in surface water in Belgium
- Estimation of the average consumption of cocaine per inhabitant: variations in - space - time



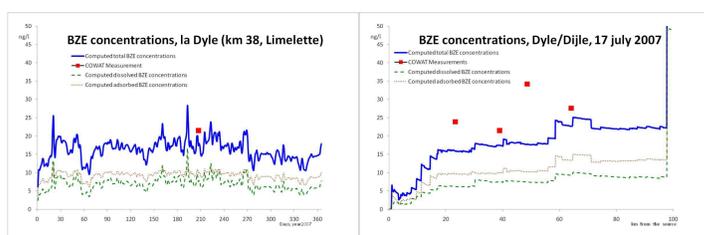
### PEGASE and cocaine:

- +- 45% of the Cocaine is metabolized in BZE and BZE is quite stable in the aquatic environment, → it is a good candidate to be modeled (as a state variable).
- The BZE has been represented in the PEGASE model as a micropollutant (such as heavy metals), with specific parameterization

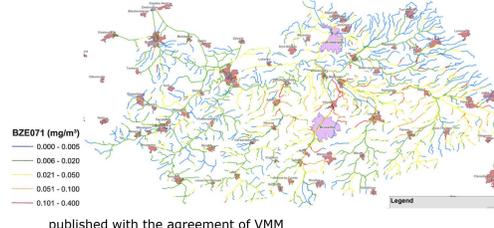
**Releases:** only urban releases (consumption by inhabitants) were considered; industrial releases and soil loads were assumed to be negligible

#### Assumptions:

- urban releases : constant value of 0.15 mg BZE/ie.day (median value measured in the COWAT study)
- rate of reduction of BZE in WWTP: 95% (mean value measured in the COWAT study)
- rate of degradation : the BZE has been supposed non degradable
- adsorption/desorption processes on suspended matter have been parameterized with "typical values" used for other micropollutants



### Simulated BZE concentrations, Belgian Scheldt basin, 27 June 2007



### Discussion:

This test study has shown:

- the ability to simulate with the PEGASE model the fate of the cocaine derivative in surface waters
- the consistency of cocaine and its metabolite measurements made in the framework of the COWAT study
- the ability to estimate through measurements in rivers and use of modeling, the consumption of cocaine (and its evolution in time and space)

A better knowledge of cocaine sources could be obtained using the model in reverse mode

- following improvements: - use of a PEGASE population equivalent "variable" in space (large cities) and time (Week-end, ...)
- use of better data (numerous measurements spots and frequencies) for calibration / validation

An extension of the model to other metabolites (drug residues, Pharmaceuticals as endocrine-disrupting contaminants ...) will be considered in the coming years

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- (3) VAN NUIJS, A., B. PECCEU, L. THEUNIS, N. DUBOIS, C. CHARLIER, P. G. JORENS, L. BERVOETS, R. BLUST, H. NEELS, A. COVACI (2009), Cocaine and metabolites in waste and surface water across Belgium, *Environmental Pollution 157, 123-129* (<http://hdl.handle.net/2268/6092>).

