Introduction

In regards of increasingly stringent rules on toxicity, prediction engines for potable water treatment have become a necessity. This particularly applies to oxidation steps, where micropollutants should be removed and where potentially harmful by-products may be formed, and has therefore lead to the building up of a new simulator for both chlorination and ozonation.

Importance

The number of factors to be considered for the management of oxidation steps is increasing.
The points below can be highlighted:

- Three objectives have to be reached on an oxidation stage:
  - an effective disinfection based on the c*t criteria,
  - the generation of the least possible amount of disinfection by-products (e.g. bromates, THMs…)
  - evolution of micro pollutants in terms of removal but also in terms of by-products, these compounds being taken into account in the drinking water norm.
- An increasing number of micropollutants have to be considered.
  There is already quality objectives for PAH, pesticides and by-products, and since 2001 an objective of 1 µg/L for microcystin. But the general context is moving and great families of compounds as endocrine disruptors, pharmaceuticals… can be considered as emerging parameters. And in the future, it could be necessary to get information about treatability,
- Each site is a different case in terms of water quality, nature and concentration of micropollutants, reactor geometry…

So, such a tool could be useful to manage oxidation steps in different situation taking into accounts these points altogether.

Approach

Knowledge required for a simulation model and knowledge on site are quite different.
For simulation, initial conditions needed are hydrodynamic of the reactor, the reactional mechanisms and kinetic parameters and the knowledge of the whole operating conditions.
But on site, only some parameters are known, but not all, on the water quality, the reactor geometry and the outlet oxidant concentration. So the idea is to develop a strategy based on the 3 main following points:

- Simulation with an inverse method
  From the residual of oxidant and the limited available parameters on site we propose to build up an innovative simulator adapted to on-site conditions: simple and effective, provided only with few measurements (from the system boundaries: inlet and outlet), its indications should insure a good level of disinfection combined with an acceptable by-products formation rate.

- Micropollutant Data base

  This base will contain kinetic constants for ozone (K_d, K_{id}) and chlorine of compounds chosen among pharmaceuticals, endocrine disruptors, pesticides (and by-products when known), natural compounds (algae toxins for instance), gasoline compounds (e.g. MTBE)…This part will be develop in close cooperation with EAWAG,
- Simplification of the hydrodynamic of the reactors

  Determination of complex schemas for reactors with simulating procedures such as Fluent, CFX… are time consuming and often only valid for the reactor considered in precise conditions. So it seems interesting to test the sensibility of the response of the simulation to bring out a restricted number of standard systemic schemas corresponding to the different reactors on site.

Results

The first 18 months lead to a bibliographic report and at this time no experimental or modelised results are available. Nevertheless the first findings and actions to be taken that can be drawn from our study are the following:

- Preliminary contacts to build up a common TECHN'EAU modelling platform were taken with the teams of WRc and TU Delft.
- The first simulations have highlighted the difficulties of our approach :
  - choice of the numerical method (relaxation or shooting),
  - choice of the C language rather than Matlab which remains a too limited tool for such a problem,
  - direct implementation of the equations governing the physico-chemical laws of oxidation on an available solver is not suitable. One should first try to transform such equations in order to elaborate a simpler problem for the computer to solve.
- It appears that:
  - Chemical phenomena as instantaneous ozone demand and NOM implication are only partially understood and will be probably modelled via semi-empirical, empirical-statistical tools or artificial ased methods. These tools could also be used to provide initial guesses for the solver.
  - Chemical pathways will have to be selected. This task does not represent a major challenge for ozonation given the existing literature; it seems however more difficult in the case of chlorination. We shall hence rather opt for a semi-mechanistic model for chlorination.

- Next task in simulator development will be hence to reprogram the calculation engine ($SimO_3$) and to incorporate a BVP (boundary value problem) solving specific module in it. Further, the data collected (physico-chemical constants) will be implemented in the simulator and comparisons between micropollutants removal experiments done at various scales (ranging from the lab to the water treatment works) shall be compared to simulation results

More information

The overview and results can be found in deliverable D.2.4.2.6. The author is Pierre Mandel (Anjou Recherche).
Further information about contacts are given in the table below.

TECHNEAU kill requirement; No/low energy requirement; No/low chemical requirement; No/low sludge production; Developing world location.

Note that only the lowest level classification needs to be checked, e.g. Point-of-use (POU) in the above example.

Meta data can be included under the 'More Information' section of the Executive Summary Report, i.e. Author(s), Organisation(s), Contact details (name and email), Quality controller (name and organisation) and Date prepared. (The TKI administrator can enter Source (= TECHNEAU), Date submitted (TKI) and Date revised (TKI)).