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Integrated hydraulic and organophosphate pesticide injection simulations for enhancing event detection in water distribution systems

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ABSTRACT

As a complementary step towards solving the general event detection problem of water distribution systems, injection of the organophosphate pesticides, chlorpyrifos (CP) and parathion (PA), were simulated at various locations within example networks and hydraulic parameters were calculated over 24-h duration. The uniqueness of this study is that the chemical reactions and byproducts of the contaminants' oxidation were also simulated, as well as other indicative water quality parameters such as alkalinity, acidity, pH and the total concentration of free chlorine species. The information on the change in water quality parameters induced by the contaminant injection may facilitate on-line detection of an actual event involving this specific substance and pave the way to development of a generic methodology for detecting events involving introduction of pesticides into water distribution systems. Simulation of the contaminant injection was performed at several nodes within two different networks. For each injection, concentrations of the relevant contaminants' mother and daughter species, free chlorine species and water quality parameters, were simulated at nodes downstream of the injection location. The results indicate that injection of these substances can be detected at certain conditions by a very rapid drop in Cl_2, functioning as the indicative parameter, as well as a drop in alkalinity concentration and a small decrease in pH, both functioning as supporting parameters, whose usage may reduce false positive alarms.

1. Introduction

A water distribution system (WDS) is a fundamental infrastructure in modern society and the necessity to connect to all consumers causes it to be spatially dispersed. The vulnerability of such systems is in their accessibility such that a contamination in the network can risk many lives within minutes. This underlines the importance of gaining knowledge regarding detection of such events within the WDS. Intentional injection of contaminants can be carried out with relatively simple equipment, the only constraint being to overcome the pressure in the network, while the consequences caused by such an event may be dramatically harmful.

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The simulations presented in this study are of injections of two organophosphates. The first is the commonly used pesticide chlorpyrifos (CP) and the second is the potent insecticide parathion (PA). (Parathion FAO CORPORATE DOCUMENT REPOSITORY). Simulations are conducted at certain nodes within an example network and the resulted output comprises concentrations of the relevant chemical species as the contaminant flows through the system and reacts with components in the aqueous phase. The concentration of the byproducts formed by these reactions and their effect on measurable parameters within the distribution system are taken into account as well.

CP is recognized as a moderately toxic organophosphate insecticide (toxicity category 2), and in the presence of free chlorine (Duirk and Collette, 2006), oxidizes to chlorpyrifos oxon (CPO) and undergoes hydrolysis to 3, 5, and 6 trichloro-2-pyridinol (TCP). Consumption of CP causes malfunction of the nervous system and, at large volumes, may result in death. The acute and chronic reference doses of CP are (Smegal, 2000) 0.005 mg/kg/day and 0.0003 mg/kg/day, respectively, and the oral LD50 is 50–250 mg/kg/day (chlorpyrifos technical fact sheet).

Studies inconclusively indicate that women and neonates are more sensitive to chlorpyrifos than other subpopulations, hence their hazardous doses are lower. CP has a solubility limit of 2 mg/l (Singh, 2009), indicating that injection of this specific contaminant at a concentration higher than this level will be visible in the water, thus irrelevant as a contaminant simulation herein. This value limits the simulations to events which do not cause life threatening conditions but will result in invertible health effects to the consumers.

Unlike CP, PA is recognized as a highly toxic organophosphate insecticide (toxicity category 1), and in the presence of free chlorine (Duirk et al., 2009), oxidizes to paraxon (PAO). Consumption of extremely small volumes of PA (3–5 mg/kg body weight) will result in death. The oral LD50 of PA is 2 mg/kg body weight (FAO corporate document repository). PA has a solubility limit of 20–25 mg/l, indicating that simulations with this contaminant may result in death with concentrations which are significantly lower than the solubility limit.

The conducted simulations provide data on the concentrations and other water components formed downstream of the contaminant injection location. This information should mitigate immediate response actions, and the identification of the intruded contaminant.

Current event detection models (Oliker and Ostfeld, 2014; Arad et al., 2013; CANARY, 2013; Perelman et al., 2012) utilize data series analysis based on machine learning and statistical inference methods. Those methodologies learn the behavior of each water quality parameter time series. Then the expected measured value of the next time step is predicted. That way, the models identify deviations from anticipated behavior and classify measurement outliers. Finally, fusion of all the generated time series data is conducted for assessing the probability of an event occurrence. Event detection was also studied by Helbling and VanBriesen (2009) who explored the changes in chlorine residual as an indicator for microbial contamination based on a limited number of batch experiments. The chlorine degradation in Helbling and VanBriesen relates directly to the stoichiometric equations of the relevant organophosphate. This method calculates the exact volume of free chlorine which takes place in each reaction. In addition, constant first order degradation is assumed for natural chlorine reactions which aren't caused by the presence of the injected contaminant.

More generally, event detection is part of the broad problem caused by contamination intrusions into water distribution systems. Models on enhancing the security of water supply as a result of contamination intrusions, include studies on sensors placement (Kessler et al., 1998; Ostfeld and Salomons, 2004; Berry et al., 2006; Guan et al., 2006; Krause et al., 2008; Ostfeld et al., 2008; Preis and Ostfeld, 2008a), source identification (Preis and Ostfeld, 2006; Skadsen et al., 2008), and response modeling (Xu et al., 2008; Preis and Ostfeld, 2008b). Bayesian network (BN) methodologies were also proposed for detecting contamination events (Dawsey et al., 2006; Xu et al., 2010). These three stages of sensor placement, source identification, and response modeling are commonly solved separately, but all together form the solution to the entire problem. Event detection is related to triggering an event occurrence. With that respect it is associated with all three stages.

Unlike all event detection models available to-date for water distribution systems, which do not take advantage of the water quality of the system in the decision process, this study considers the interrelated change in the values of several water quality components such as pH, alkalinity, acidity, total free chlorine concentration emanating from the reactions and injected organophosphate species occurring on top of background events such as normal chlorine decomposition, blending of different water qualities in nodes, etc.. These reactions are further related to the changes over time as means of identifying actual contamination events by these organophosphates. In order to strengthen the identification of an OP contamination event we chose to simulate the changes in acid-base water quality parameters (particularly pH and alkalinity). Measuring small variations in these parameters constitutes a challenge with the respective analytical devices, nevertheless highly accurate and sensitive analytical methods have already been developed, and can be used also in the context of distribution systems.

The simulation outputs of these substances are a step towards creating a database of potential hazardous substances and their influences on water quality parameters when injected at given locations and concentrations. CP was selected as a contaminant representative of the organophosphate group. The choice of PA is due to its high toxicity and consequently its substantial damage potential in contamination events.

Simulations were performed using the EPANET-MSX (Shang et al., 2008) program, an extension of EPANET (Rossman, 2000), which can model the reaction and transport of multiple interacting chemical species. To run the MSX, differential equations, which describe the degradation and formation of all the relevant species and water quality parameters, had to be defined.

The simulated network case study comprises two sources of different water types and water quality parameters. The simulations begin, prior to the contaminant injection, with a period of time where the water types blend and reach a steady state point at which the water quality parameters remain