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Stationary and non-stationary autoregressive processes with external inputs for predicting trends in water quality

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A B S T R A C T

An autoregressive approach for the prediction of water quality trends in systems subject to varying meteorological conditions and short observation periods is discussed. Under these conditions, the dynamics of the system can be reliably forecast, provided their internal processes are understood and characterized independently of the external inputs. A methodology based on stationary and non-stationary autoregressive processes with external inputs (ARX) is proposed to assess and predict trends in hydrosystems which are at risk of contamination by organic and inorganic pollutants, such as pesticides or nutrients. The procedures are exemplified for the transport of atrazine and its main metabolite deethylatrazine in a small agricultural catchment in France. The approach is expected to be of particular value to assess current and future trends in water quality as part of the European Water Framework Directive and Groundwater Directives.

1. Introduction

The assessment and the prediction of trends in water quality is often a challenge when external inputs such as meteorological conditions influence the dissipation and transfer processes of pollutants, especially in situations where the observation period is short in comparison with the response time of the hydrosystems. This paper reports on the implementation of mathematical models also referred to as the autoregressive process with external inputs (ARX) that are devoted to transfer process characterization, prediction and control (Karacan, 2003). The method under consideration can be considered as a particular case of the widespread multivariate autoregressive analysis (from the Box and Jenkins approach, 1970; Berthouex et al., 1978) when the "feedback" is not observable, i.e. when the terms representing the influence of the output on the inputs are zero (Box and Jenkins, 1970).

New developments on stochastic recursions emphasize the remarkable stability of short- and long-term forecasting from autoregressive processes. Stochastic recursions appear in queuing theory (Baccelli and Brémaud, 2003), random walks in random environment or branching processes (Altman and Fiems, 2006) and the theory is being studied actively (Asmussen, 2003; de Saporta et al., 2004; de Saporta and Yao, 2005; Guivarc'h, 2006). The advantages of autoregressive processes within the context of the present study are that: i) the so-called 'tail' of the process, i.e. the extrapolation of the recursive process beyond the observation period, may be extended without an increase in random and systematic errors as time increases; and, ii) the calibration of the autoregressive process may be performed accurately using a time period which is short in comparison with the response time of the systems under study. This latter aspect distinguishes autoregressive processes from Kalman filtering techniques and neural network modelling.

In the present study, a "true" transfer model is presented which reports the results obtained using the ARX approach to assess and predict trends in the contamination of groundwater and surface water by inorganic or organic pollutants from monitoring data. The fact that these compounds are typically subject to chemically- or biologically-driven degradation processes means that fluxes of micropollutants in hydrological systems are typically non-stationary. Methodological developments are proposed to address the non-stationary nature of these processes and the procedures are applied to the investigation of

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trends in pesticide fluxes measured in spring water at the outlet of a small agricultural catchment in France. Two aspects of the ARX approach are investigated to characterize the natural processes of transfer and degradation of pesticides. First, the autoregressive approach is used for long-term forecasting while the initial conditions of the system have no longer influence on pesticide fluxes. Secondly, constrains are introduced into the model to account for mass conservation and the autoregressive term is weighted to take into account decay processes. The approach is demonstrated for concentrations of atrazine and its main metabolite deethylatrazine (DEA) in groundwater.

2. Materials and methods

Crop protection products are known to represent a potential risk for human and the environment (e.g. Birarder and Rayburn, 1995) and the presence of pesticides is therefore routinely monitored in environmental media such as groundwater, surface water (Gilliom et al., 2006) and, to a lesser extent, the atmosphere (Dubus et al., 2000; Shen et al., 2004; Yao et al., 2006). Most surveillance efforts are targeted towards investigating the spatial spread of the contamination of water resources by pesticides and/or detecting any positive or negative trends in concentrations (Gilliom et al., 2006). Monitoring programmes have demonstrated that the contamination of water resources by atrazine and its metabolites tends to be widespread (Thurman et al., 1991; Ritter et al., 1994; Tindall and Vencill, 1995; Goolsby et al., 2001; Kolpin et al., 1998; Clark et al., 1999; IFEN, 2006).

2.1. The context

The autoregressive approach is demonstrated for pesticide concentrations and fluxes measured in spring water for 7 years at an experimental site ca. 75 km north-west of Paris, France (Mouvet el al., 2004; Baran et al., 2005; Roulier et al., 2006; Morvan et al., 2006). The site is of particular interest because the use of atrazine on the catchment was discontinued in 1999 following concentrations of atrazine and its metabolite deethylatrazine (DEA) exceeding regulatory thresholds for drinking water. Concentrations of atrazine, DEA and major cations and anions have been monitored in the Bréville spring at a two-week interval from December 2000 to June 2004 and on a monthly sampling rate since (Fig. 1).

2.2. Transfer and degradation processes

The release of atrazine and DEA that is observed after 1999 while atrazine was no longer used on this catchment discloses the persistence of those pollutants (Fig. 1). Pesticides that are retained into the pores of the root zone are subject to degradation. The dissolved part of pesticides migrates through the vadose zone to the watertable. During wet years, atrazine and DEA are subject to quick transfer as a result of preferential flow paths in the limestone of both the unsaturated and the saturated zones. Subsequently, quick transfer through the macropores of the vadose zone is enhanced when the capillary pressure is high enough to establish a hydraulic continuity in preferential pathways.

2.3. Autoregressive process with external inputs

The autoregressive process with external inputs (ARX) may be regarded as a mathematical representation of the hydrosystem. It therefore gives more of a functional relationship which may or may not agree with other models obtained by utilizing the knowledge of the physical, chemical and biological mechanisms of the system.

The general expression for an ARX model can be written as:

$$F^{\mathrm{out}}(t_i) = (1-\omega)\left[\lambda_1 \Gamma_1 \cdot \mathbf{F}_1^{\mathrm{in}} + \cdots + \lambda_q \Gamma_q \cdot \mathbf{F}_q^{\mathrm{in}}\right] + \omega \Gamma_{\mathrm{out}} \cdot \mathbf{F}^{\mathrm{out}} + \varepsilon(t_i) \qquad (1)$$

q is the number of external inputs

$\mathbf{F}_k^{\mathrm{in}} = (F_k^{\mathrm{in}}(t_i), F_k^{\mathrm{in}}(t_{i-1}), \cdots)^T$, $\mathbf{F}^{\mathrm{out}} = (F^{\mathrm{out}}(t_{i-1}), F^{\mathrm{out}}(t_{i-2}), \cdots)^T$, are $p \times 1$ column vectors of observations at time t_i representing the inputs and the output of the transfer model (p is the order)

$\mathbf{\Gamma}_k$ and $\mathbf{\Gamma}_{\mathrm{out}}$ are $1 \times p$ line vectors, the so-called impulse responses

ε is the noise of the transfer model which represents erratic, complex, and usually short-term variability of the output which is not explained by the model whatever the underlying reasons might be (e.g. lack of or inadequate description of key processes, measurement error, inadequate sampling or modelling strategy).

In the actual case which concerns us additional conditions are required since fluxes are positive functions of time constrained by the mass conservation of the system.

series F_1^{in}, ..., F_q^{in} and F^{out} are assumed to be reduced to unit average

$\mathbf{\Gamma}_k$ and $\mathbf{\Gamma}_{\mathrm{out}}$ are unit impulse responses (area is unity) with the constraint $\Gamma(t_i) \geq 0$, $k = 1, \cdots, p$

λ_k, $k = 1, \cdots, q$ and ω are weighting factors such as $\lambda_1 + \cdots + \lambda_q = 1$

The weighting factor ω and the impulse response $\mathbf{\Gamma}_{\mathrm{out}}$ express the 'internal' functioning of the hydrosystem.

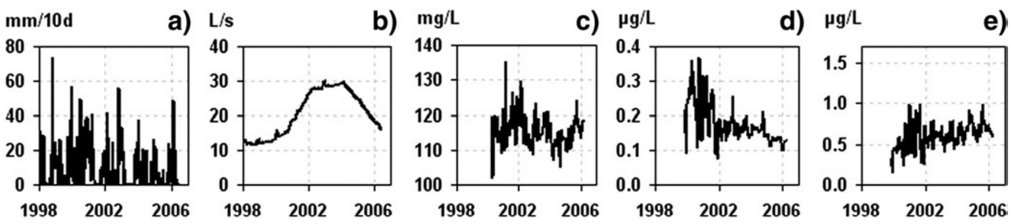

Fig. 1. Variables used in the modelling — a) effective rainfall — b) water flow at the spring — c) Ca concentrations in spring water — d) atrazine concentrations in spring water — e) deethylatrazine concentrations in spring water.