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Ecological risk assessment of nonylphenol in coastal waters of China based on species sensitivity distribution model

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HIGHLIGHTS

- The SSD model can be used for the derivation of PNEC for nonylphenol.
- We established the PNEC value of nonylphenol in both freshwater and seawater.
- Nonylphenol occurs ubiquitously in coastal waters of China with RQ values up to 70.

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ABSTRACT

Nonylphenol (NP) is an endocrine disruptor and causes feminization and carcinogenesis in various organisms. Consequently, the environmental distribution and ecological risks of NP have received wide concern. China accounts for approximately 10% of the total NP usage in the world, but the water quality criteria of NP have not been established in China and the ecological risks of this pollutant cannot be properly assessed. This study thus aims to determine the predicted no effect concentration (PNEC) of NP and to assess the ecological risks of NP in coastal waters of China with the PNEC as water quality criteria. To obtain the HC_5 (hazardous concentration for 5% of biological species) and PNEC estimates, the species sensitivity distributions (SSDs) models were built with chronic toxicity data of NP on aquatic organisms screened from the US Environmental Protection Agency (USEPA) ECOTOX database. The results showed that the PNEC for NP in freshwater and seawater was 0.48 μg L^{-1} and 0.28 μg L^{-1}, respectively. The RQ (risk quotient) values of NP in coastal waters of China ranged from 0.01 to 69.7. About 60% of the reported areas showed a high ecological risk with an RQ value $\geqslant$ 1.00. NP therefore exists ubiquitously in coastal waters of China and it poses various risks to aquatic ecosystems in the country. This study demonstrates that the SSD methodology can provide a feasible tool for the establishment of water quality criteria for emergent new pollutants when sufficient toxicity data is available.

1. Introduction

Nonylphenol (NP) in natural environment mainly originates from the breakdown of its parent compounds, nonylphenol ethoxylates (NPEO), a group of non-ionic surfactants widely used in industrial and household products such as detergents, emulsifiers, solubilisers and dispersing agents (Servos, 1999; Ying et al., 2002; Soares et al., 2008). NP is more persistent, lipophilic and toxic than its parent compounds (Ekelund et al., 1993; Ahel et al., 1994; Lee and Peart, 1995) and as an endocrine disruptor it causes harmful effects including feminization and carcinogenesis to various organisms (Capaldo et al., 2012; Chen and Yen, 2013). The environmental distribution and ecological risks of NP therefore receive wide concern. This pollutant was listed as a priority substance in the European Union (EU) Water Framework Directive in 2001. The production and usage amount of NP have been increasing exponentially since its first synthesis in the 1940s (Manzano et al., 1998). The annual production of NP was 31,434 tonnes in 2011 in China, which accounted for about 10% of the total world production according to the record of China Petroleum and Chemical Industry Federation (CPCIF). Consequently, NP is widely distributed in both freshwater and seawater systems related with the discharge of industrial wastewater and domestic sewage (Ahel et al., 1994; Hale et al., 2000). The wide distribution of NP in the natural environment and the associated adverse effects on wildlife necessitate the assessment of its ecological risks in the aquatic ecosystems.

Referring to the generic framework and guidelines of the USEPA, ecological risk assessment (ERA) is defined as a process that

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evaluates the likelihood of adverse ecological effects on ecosystems exposed to one or more stressors (US EPA, 1998). In this process, the first step is to derive the "predicted no-effect concentration" (PNEC), at which no harmful effects on the environment are expected. PNEC values are then compared with the "predicted environmental concentrations" (PEC) to calculate the "risk quotient" (RQ = PEC/PNEC), which is used as a measurement of the ecological risk (US EPA, 1998). PEC values can be obtained either by model prediction or through environmental monitoring. PNEC values are achieved mainly through two methods, the assessment factor (AF) method and the statistical extrapolation method based on species sensitivity distributions (SSD) (ECB, 2003).

The AF approach is simple to use and is feasible when toxicity data is limited. But the PNEC estimates with this method show great uncertainty since they are solely dependent on the minimum toxicity value and a certain factor. The SSD method provides more reliable and reasonable statistics since the PNEC estimates are based on an established distribution of a full of toxicity data set (Lei et al., 2012). The SSD methodology is therefore increasingly being used in ecological risk assessment procedures (Wheeler et al., 2002; Hickey et al., 2009).

To date, there have been several reports for PNEC or water quality criteria of NP the world. For example, the European Union (EU) published a risk assessment document for NP in 2001, which provided the PNEC in various environmental media (ECB, 2001). The US EPA also established the ambient water quality criteria for NP (Brooke and Thursby, 2005). The AF methodology was chiefly used in these reports (ECB, 2001, 2003), whereas the SSD method was rarely applied mainly due to the data limitation. In many countries, including China, however, no water quality criteria or PNEC for NP have been established, and this hinders the ecological risk assessment for this pollutant. This study therefore aims to build an SSD model for the determination of PNEC for NP and to assess the ecological risks of the pollutant in coastal waters of China.

2. Procedure and methods

The SSDs methodology assumes that the acceptable effect level (sensitivity) of different species in an ecosystem follows a probability function called "species sensitivity distribution" (Dowse et al., 2013). An acceptable effect level for all biological species can be estimated based on the assumption that a limited number of tested species is a random sample of the whole biological system (Van der Hoeven, 2004). The primary aim of SSD analysis is to determine hazardous concentrations (HCs) to protect most species in the environment. HCs are calculated by assuming a statistical distribution, for example, log-logistic or log-normal distribution, of species sensitivities expressed as the no observed effect concentration (NOEC) or least observed effect concentration (LOEC) values. HCs are thus developed as an analytical expression for the concentration associated with the pth percentile of the distribution, also referred to as the HC for p percent of the species (Kooijman, 1987; Van Straalen and Denneman, 1989). Currently, PNEC values are usually derived from a statistical cutoff value of 5% for p. This value of 5% is a practical choice but has been validated on the basis of field studies (Posthuma et al., 2002). The ecological risk assessment based on SSDs usually involves four steps: (a) screening toxicity data; (b) selecting distribution model and fitting SSD curves; (c) calculating values of HC_5 and PNEC; (d) describing the characteristics of ecological risks.

2.1. Screening toxicity data

The selection of toxicity data for SSD, usually expressed as NOEC, LC_{50} or EC_{50}, depends on the aim of study and the availability of data. Chronic data (NOEC or LOEC) was adopted in this study as they express the effects of long term exposure to organisms.

As toxicity data of NP testing with Chinese native species is very limited, the chronic toxicity data used in this study are mainly screened from the USEPA ECOTOX database (http://cfpob.epa.gov/ecotox). The selected data involve three taxonomic groups: algae, invertebrates and vertebrates, respectively. The screening criterion for test duration was $\geqslant$3 d, $\geqslant$7 d and $\geqslant$14 d for algae, invertebrate and vertebrate, respectively.

The selected toxicity data of NP for freshwater and seawater are listed in Tables 1 and 2, respectively. According to the EU Technical Guidance Document (ECB, 2003), the geometric mean is calculated if more than one N(L)OEC value is available for the same species and endpoint.

2.2. Selection of distribution model

For the construction of SSD models, it is generally assumed that the toxicity data fit a type of distribution, e.g., log-logistic, log-normal or log-triangular. The log-normal distribution recommended by US EPA and TGD of EU is most commonly used because of the available methodology for in depth analyses of various uncertainties.

In this study, log-normal distribution is adopted for constructing the SSD model. The probability distribution function (f) and cumulative distribution function (CDF) of log-normal distribution are as follows:

$$f(x;\mu,\sigma) = \frac{1}{x\sigma\sqrt{2\pi}} e^{-(\ln x-\mu)^2/2\sigma^2} \tag{1}$$

$$\mathrm{CDF}(x;\mu,\sigma) = \frac{1}{2} + \frac{1}{2} erf\left[\frac{\ln(x)-\mu}{\sigma\sqrt{2}}\right] \tag{2}$$

where the μ and σ are mean and standard deviation of the variable logarithm, respectively.

2.3. Calculation of HC_5 and PNEC

The HC_5 (hazardous concentration for 5% of species) is the estimated 5th percentile of the distribution, i.e., the concentration expected to be protective of the 95% of the species in an ecosystem (Wheeler et al., 2002). According to the assessment factor method provided by TGD of EU, the PNEC (predicted no effect concentration) is calculated by the following equation:

$$\mathrm{PNEC}_{\mathrm{water}} = \frac{\mathrm{HC}_5}{\mathrm{AF}} \tag{3}$$

where AF is an assessment factor between 1 and 5, reflecting the uncertainties of data (ECB, 2003). In this study, the value of AF is set as 3 based on the number of species tested, quantity and quality of toxicity data and model goodness of fit.

2.4. Characterization of the ecological risks

PNEC values are compared with the "predicted environmental concentrations" (PEC) to calculate the "risk quotient" (RQ = PEC/PNEC), which is used to determine the ecological risk (Cristale et al., 2013). Due to a shortage of detailed geographic distribution data for the usage and discharge amount of NP in China, the "measured environmental concentration" (MEC) was used to represent the exposure condition. The risk level can be ranked as low, medium and high if the RQ value is <0.1, 0.1–1.0 and $\geqslant$1, respectively.