

industrial sectors. The produced and industrial applied NPEOs consist of a technical mixture of nonylphenol isomers (NP, C₉H₁₉C₆H₄OH) (Wheeler et al., 1997) and the ethoxy (C₂H₄O) units. As proposed transformation process in the previous reports (Ahel et al., 1994; Ying et al., 2002), the biodegradation of NPEOs under aerobic or anaerobic conditions leads to a shortening of the polyethoxylate chain (hydrolytic cleavage of the ethoxy units). The resulting nonylphenol monoethoxylate (NP₁EO, C₉H₁₉-C₆H₄-OC₂H₄-OH), diethoxylate (NP₂EO, C₉H₁₉-C₆H₄-(OC₂H₄)₂-OH) and nonylphenol (NP) are more resistant to microbial degradation than higher ethoxylated compounds (Heemken et al., 2001). NP, the main metabolite of NPEOs, is toxic to both marine and fresh water species (Servos, 1999; Ahel et al., 2000). Concern over their possible environmental effects has led to the phase-out of NPEOs from household cleaning products in West European countries since 1992, but they are still used as industrial detergents in metal and textile processing (Field and Reed, 1996). In 1995, alkylphenol consumption in Germany amounted to about 20,000 t, of which approximately 14,000 t was NP. The rest of 6000 t consisted of octyl-, butyl-, and other alkylphenols (Maguire, 1999).

Dachs et al. (1999) reported concentration ranges of NP between 2.2 and 70 ng m⁻³ in the coastal atmosphere of the New York–New Jersey Bight. They concluded that the occurrence of NP in the atmosphere might be an important human and ecosystem health issue in urban, industrial and coastal-impacted areas receiving treated sewage effluents. Besides, Jahnke et al. (2004) have recently reported concentration ranges between 140 and 242 ng l⁻¹ for NP and 8–19 ng l⁻¹ for *t*-OP in the effluent of the sewage treatment plant of Hamburg, in Germany. Van Ry et al. (2000) further studied the seasonal trends of NP and *t*-OP in the atmosphere of the Lower Hudson River Estuary (USA). Concentrations of NP in gas phase at a coastal site Sandy Hook (USA) ranged from below the limit of detection (LOD) to 56.3 ng m⁻³, while the concentrations at a suburban site New Brunswick (USA) ranged from 0.13 to 81 ng m⁻³. Gas phase concentration of OP ranged from LOD to 1.0 ng m⁻³ at Sandy Hook and from 0.01 to 2.5 ng m⁻³ at New Brunswick. NP and *t*-OP exhibited seasonal trends with higher gas phase concentrations during summer than during fall and early winter. The estimation for the air/water exchange of NP in the lower Hudson River estuary indicates that the atmosphere is a significant sink for the NP in the contaminated area, and NP can be transported to the shallow aquatic environment by the atmosphere via the air/water exchange.

The Henry's law constant (HLC) of a compound determines its vapor exchange across air/water interfaces and can be used as an indicator of its persistence in the aquatic environment (Rice et al., 1997). The HLC can be

defined as

$$\text{HLC} = \frac{[X]}{P_X} \quad (1)$$

where $[X]$ is the aqueous-phase concentration of the substance X (mol l⁻¹) and P_X is its partial pressure in the air (atm). The inverse value H (Pa m³ mol⁻¹) is also widely used in multiphase modeling. The relation between H and HLC is the following:

$$H(\text{Pa m}^3 \text{ mol}^{-1}) = 101.325/\text{HLC}(\text{M atm}^{-1}) \quad (2)$$

For compounds that are slightly soluble, the HLC can be calculated from the ratio of the saturation vapor pressure (P_{sat}) and water solubility (S_{w}):

$$\text{HLC} = \frac{S_{\text{w}}}{P_{\text{sat}}} \quad (3)$$

However, literature values of P_{sat} and S_{w} for a particular substance often vary over a range of several orders of magnitude (Bruhn et al., 2003). Consequently, a need for measuring the HLC remains both for direct use in air/water exchange estimates and for developing numerical models. Several methods can be employed to measure HLCs, e.g. head-space sampling (Yin and Hassett, 1986; Murphy et al., 1987), wetted wall column technique (Fendinger and Glotfelty, 1988; Fendinger et al., 1989; Shepson et al., 1996; Rice et al., 1997), gas stripping (Mackay et al., 1979; Kucklick et al., 1991; Alaei et al., 1996; Jantunen et al., 2000), fog chamber (Fendinger et al., 1989), thermodynamic method (Brunner et al., 1990; Altschuh et al., 1999), and dynamic equilibrium system (Treves et al., 2000; Gautier et al., 2003).

For technical NP, the reported values of HLC are $4.08 \times 10^5 \text{ M atm}^{-1}$ (25°C) (Hellmann, 1987), $25\text{--}33 \text{ M atm}^{-1}$ (25°C) (Dachs et al., 1999) and 121 M atm^{-1} (20°C) (Lalah et al., 2001). These values are estimated from NP's P_{sat} and S_{w} and vary over 5 orders of magnitude. The main reason for the lack of experimental data on NP is its low solubility and its low vapor pressure making it difficult to deal with. Additionally, NP consists of isomers containing different branched nonyl chain that has been previously highlighted with high-resolution gas chromatography coupled to mass spectrometer (GC-MS) (Wheeler et al., 1997) and high-performance liquid chromatography (HPLC) equipped with graphitic carbon column (Gundersen, 2001). Recently, eight major components of NP isomer have been fractionated with HPLC from the NP mixture, and identified using GC-MS and nuclear magnetic resonance spectroscopy (NMR) (Kim et al., 2004). Study on the individual isomers indicated that the estrogenic activities were varying from each other for their different physicochemical properties, e.g. S_{w} , P_{sat} , octanol-water partitioning coefficient ($\log K_{\text{ow}}$) and their HLC (Lalah et al., 2001, 2003a, b).