7.1 END POINT SUMMARY

Chapter : 4

Remark : 2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO3), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO3 in equilibrium with the atmosphere (pCO2=3x10-4 atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water (Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability : (1) valid without restriction

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