Abstract

Health impact prediction by constituents and physicochemical properties of chemical mixtures

- focus on the chemical mixtures used in Marine Paint Plants -

Ki-Woong Kim, Yong Lim Won, Jeong Ho Ahn, Dong Jin Park, Ja Hoon Gu and Kyung Sun Ko

Occupational Health Research Department
Occupational Safety and Health Research Institute, KOSHA
400 Jongga-ro, Jung-gu, Ulsan 681-230, Korea

Objectives: In the marine paint companies, was generally used chemical mixtures such as cyclohexanone(CHnone), methyl ethyl ketone(MEK), styrene, toluene and xylene). Therefore, this study was designed to compare the experimental results of metabolic interaction in workers exposed to chemical mixtures and predicted results of toxicity using quantitative structure-property ralationships(QSPR).

Methods: A QSPR model for single substances and mixtures was analyzed using multiple linear regression (MLR) by taking into account the statistical parameters between the observed and predicted EC_{50}.

Results: Significant differences in physico-chemical properties such as boiling point (BP), specific gravity (SG), Reid vapor pressure (rVP) and

flash point (FP) were observed between the single substances and the mixtures. The EC_{50} value of the chemical mixtures contained CHnone and toluene were significantly lower than that of other chemical mixtures and morphological changes in HepG2 cell was marked cell necrosis in mixtures contained CHnone and toluene. The mixture toxicity was directly related to the mixing ratio of toluene and CHnone (MLR EC_{50} equationy=1.7409451+0.0833945*MEK+0.0632504*styrene-0.011699*toluene-0.15519*CHnone), as well as to BP and SG (MLR equation EC_{50}=48.406843-0.219267*BP-32.26887*SG+0.1776163*rVP+0.6068308*FP). It was found that metabolism of toluene (y=1.111+0.096*Toluene-0.689*CHnone) and MEK(y=2.982+0.728*MEK-0.322*CHnone) will be affected by the co-exposure to CHnone and toluene may inhibit the metabolism of styrene and xylene.

Conclusions: These results suggest that QSPR-based model can be used to quantitatively prediction of the mixtures toxicity in the field of occupational health.

Key words: Marine paint, Chemical mixtures, Mixture toxicity, QPAR, Metabolic interaction, Workers