CHEMOMETRIC CLASSIFICATION OF ADVANCED OXIDATION PROCESSES FOR THE DEGRADATION OF PHARMACEUTICALS AND PERSONAL CARE PRODUCTS

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Abstract

The present study was focused to classify various advanced oxidation processes (AOPs) to degrade sixteen common pharmaceuticals and personal care products (PPCPs). The classification was based on the degradation rate constant (h⁻¹). Chemometric techniques like principal component analysis (PCA) and cluster analysis (CA) were used to classify AOPs which can efficiently degrade a certain class of PPCPs. The bipolt based on first two principal components (PCs) of PCA model identified two distinct groups of PPCPs. The first group was comprised of the PPCPs which were effectively degraded by UV based AOPs methods whereas second group was composed of those PPCPs which were degraded by ozone based AOPs more efficiently. Tendency in two groups of PPCPs was also disclosed in correlation coefficient matrix of PPCPs on the basis of chemical structure. The same groups of PPCPs were identified in a dendrogram from CA. Within second group of PPCPs, a subgroup was pointed out by CA that was effectively removed by combination of ozone and UV methods; O³/UV and O³/UV/TiO₂. The score plot and the dendrogram also highlighted the tentative identification of employed AOPs. Both the chemometric techniques could classify all the investigated PPCPs properly.

Key words: advanced oxidation processes, classification, cluster analysis, degradation rate constant, pharmaceuticals, principal component analysis

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