Application of Unsupervised Chemometric Analysis and Self-organising Feature Map (SOFM) for the Classification of Lighter Fuels

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Abstract
A variety of lighter fuel samples from different manufacturers (both unevaporated and evaporated) were analysed using conventional gas chromatography-mass spectrometry (GC-MS) analysis. In total 51 characteristic peaks were selected as variables and subjected to data pre-processing prior to subsequent analysis using unsupervised chemometric analysis (PCA and HCA) and a SOFM artificial neural network. The results obtained revealed that SOFM acted as a powerful means of evaluating and linking degraded ignitable liquid sample data to their parent unevaporated liquids.