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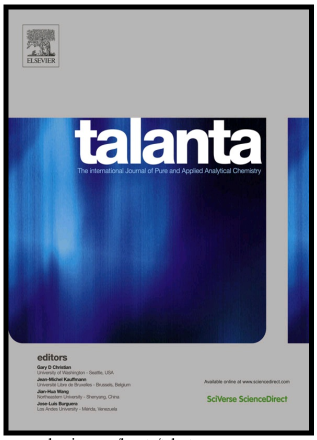

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A Chemometric Approach for the Prediction of the Aging Levels of Automatic Transmission Fluids by Mid-Infrared Spectroscopy

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Abstract

Automatic transmission fluids (ATF) are highly complex multi-component systems with a variety of different additive packages which suffer from manifold aging processes due to interfering factors. This work describes the development of a straightforward approach to model the aging effects by means of Fourier Transform Infrared (FTIR) spectroscopy combined with multivariate data analysis. Therefore, ATF samples were artificially aged under defined conditions by considering effects of product type, temperature, storage time and exposure to metallic materials, yielding 144 samples. For multivariate data analysis, three different approaches have been applied and compared: supervised Fisher's Linear Discriminant Analysis of principal components (PCFDA), regularized FDA (RFDA) of variables, and unsupervised PCA after orthogonalization using Error Removal by Orthogonal Subtraction (EROS + PCA). All methods worked well in reducing unwanted effects and transforming the relevant information to the first components. Combined with k-Nearest-Neighbor (kNN) prediction, RFDA leads to the best model, improving the accuracy ratios by 13%, 41%, and 12% in comparison with direct kNN classification for the target classes storage temperature, additional material and aging level, respectively. These results suggest that RFDA is highly suitable for the reduction of unwanted effects in a dataset with manifold perturbation influences. The model also predicted a correct aging level ranking when applied to unknown field samples.

Keywords: Spectroscopy, Classification, Automatic Transmission Fluid, Fisher's Linear Discriminant, Orthogonalization

1. Introduction

Automatic transmission fluids consist of base oil blended with various additive packages depending on their specific duty [1]. The main task of lubricants and in particular ATFs is to reduce friction between moving and fixed parts, thereby reducing wear on the components in the gearbox during operation, which is achieved by using specific molecules that apply a film of material to surfaces and form tribological layers [2]. There are additional additive packages which are supposed to prevent oxidation or foaming, to lower the pour point, to act as dispersant or detergent and to reduce metallic contamination [1].

The degradation of lubricants is mainly caused by the chemical breakdown and decrease of additives and the subsequent formation of undesired substances [3].

L'Hostis et al. have shown that the lubricant formulation and the degradation of additives have an enormous impact on contact fatigue and fatigue cracks in gears [4]. Used oils distinguish themselves by much greater water and sediment level, relatively higher concentrations of organic compounds (oxidation products) and relatively higher amount of metals such as Fe, Cd, Cr, Pb [1] compared to fresh oils. These materials could also act as catalysts that accelerate the degradation of lubricants during operation, implying a relationship between metallic particle content and oxidation [5].

Popular methods for the analysis of lubricant-like fluids are the comprehensive mass spectrometry (MS) [6], liquid chromatography (LC) [7], nuclear magnetic resonance (NMR) [8] and inductively coupled plasma emission spectrometry (ICP-OES) [9] but it is also well known that the differentiation between degradation stages of lubricants can be observed by means of absorption spectroscopy[1] [10]. Since optical sensors are suitable for industrial applications, the focus in this work is on the evaluation of FTIR transmission spectra [11]. We show that PCFDA, RFDA, and EROS + PCA work very well to transform the relevant information onto a subspace of two axes while eliminating unwanted perturbation. Subsequent classification models can easily predict the class membership concerning the

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