APPLYING VECTOR SOFTWARE CONCEPTS TO THE QUANTITATION OF POLYMER SYSTEMS

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ABSTRACT

In the application of today’s FT-IR systems to polymer science, the ease and the success of that application oftentimes is not the result of a benefit purely derived from Fourier transform infrared. Often the benefit to the analysis results from the ability to use some new accessory or the ability to apply an analytical concept to better advantage in conjunction with FT-IR. So too can there be new benefits and new improvements to methods through software and applied mathematics. Such is the basis for this description of vector concepts applied to the quantitation of polymer samples.

INTRODUCTION

For nearly four and a half decades, since the earliest infrared instruments, infrared analysis has contributed strongly to quantitation and control within the polymer science. At times, adequate answers have resulted merely from ratioing pairs of absorbance bands to measure relative amounts within copolymer systems or within polymer blends. In more traditional spectrophotometric quantitation, absorbance bands within an analyte spectrum are chosen for selectivity, sensitivity, and a linear response of intensity versus changing concentration. Measurements of these bands’ net absorbances, relative to a calibration made across known concentration changes, have been the means, therefore, of producing a quantitative answer from an infrared spectrum. Employing the relationship of the Beer-Lambert law (A=abc) enabled the analyst to determine concentration using simple mathematics. When more than one analyte is to be determined a selective absorbance band for each analyte is chosen, and the measured,
Multiple net-absorbances are fitted to the simultaneous solution of multiple equations. With the addition of computational capabilities, and by applying matrix algebra to the solution of the multiple equations, computerized infrared speeds a complex analysis and permits quantitative schemes requiring only one careful calibration and the storage of essential factors in a calibration matrix. Mathematics employing matrix concepts have, therefore, become common to infrared quantitative software, and there has been a growing tendency to apply other useful forms of mathematics. A more rigorous treatment of all these fundamentals is not intended here, since there are numerous texts to which one may refer [1-4].

FT-IR QUANTITATIVE ANALYSIS

These same traditional quantitative schemes have been carried forward into FT-IR instrumentation. Also, because quantitation in the infrared region is routinely practiced, an FT-IR without quantitation software would be considered incomplete. The fact is that FT-IR systems will benefit all areas of science bringing quantitative abilities to work in unusual sampling situations—as within hyphenated technologies, or in time-dependent studies, and in all applications demanding high signal-to-noise and speed. Speed is not always a consideration in the development of a quantitative method, but sample throughput (analyses per minute) may be important to a given experiment.

Applying multicomponent quantitative analysis methods directly to problem mixtures can save considerable time and speed throughput, because time-consuming separation steps can be avoided or minimized. But too often, today's analyst may lack complete familiarity with the capabilities of multicomponent quantitative analysis using matrix concepts or those concepts extended through the use of vectors. Our work actually began with applying vector mathematics to dispersive infrared data. The targeted use was always intended for FT-IR data, for as you will see, the Fourier transform plays an important part in our derivation of a vector. Vector concepts have been a natural extension of the application of mathematics to infrared analysis, and one reason for the pursuit of vectors has been for analytical speed.

As stated earlier, a complete definition of the fundamentals of multidimensional vector analysis [5-7] is beyond the scope of this paper, but suitable references will be listed to each topic area mentioned. The fitting of spectral information to vector space has been under investigation within our areas of product research for a number of years, and other groups have published vector concepts obviously from parallel but totally independent studies [8,9]. The mathematical basis is similar in nature to factor analysis applied to spectra, and a number of papers have