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Optimization

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I. INTRODUCTION

The problem of optimization can be traced back to the advent of chromatography as an analytical method. Separation optimization is related to the proper choice of the parameters influencing the separation. Optimization is treated separately by every chromatographic method, taking into account the specific problems encountered in the fields of gas and liquid chromatography. Even in liquid chromatography, the subject of optimization is different in planar chromatography (1,2) from that involved in column liquid chromatography (3,4), and only a few authors have approached this subject as a general case (5). Simultaneously with the widespread use of computers in analytical laboratories, the topic has attracted more and more attention, and a great number of software packages have been developed to help the analyst in the optimization separation parameters (6–8). Some forms of optimization are generally necessary in planar chromatography if the separation of all compounds is required, especially when the number of components is larger than a small fraction of the spot capacity of the system.

In thin-layer chromatography, only a few factors need be taken into consideration for optimization, because most of them are fixed for theoretical or practical reasons even though the system is complex. The most important factors are the solvent system and its composition, the optimum time, the temperature, and, in some cases, the relative humidity. Temperature is not used as an optimizing factor because in most cases the variation of temperature in the normal temperature work range has no influence on the minimum time of analysis necessary to obtain a defined value of resolution. Relative humidity is an experimental variable difficult to change within narrow ranges, and therefore its use is not recommended in optimization. In conclusion, the most important factor that must be taken into account in the optimization of a thin-layer chromatography system is the composition of the mobile phase, which is often the only component seriously considered.

This chapter describes the methods used for mobile-phase optimization, including not only those developed for thin-layer chromatography but also those developed for liquid chromatography and applied to thin-layer chromatography. These methods are applied in both one- and two-dimensional TLC. Furthermore, the chromatographic response functions used to reflect the quality of separation are reported. Automated multiple development is described as a method for separation optimization.

II. CHROMATOGRAPHIC RESPONSE FUNCTION

Simple optimization methods are used for the separation of simple mixtures. In the case of complex mixtures, some sophisticated strategies have been developed to optimize the mobile-phase composition. These methods are intended to find the maximum or minimum of an "objective function" called the chromatographic response function (CRF) or criteria function, which ex-