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Fast and accurate numerical method for predicting gas chromatography retention time

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Highlights

- â€¢ Retention time can be predicted with high accuracy and reduced computational time.
- â€¢ Retention time predicted by the proposed method could be used to reach a solution that is as close as possible to the exact one.
- â€¢ The proposed method is suitable for use to test the accuracy of other methods of retention time prediction.

Abstract

Predictive modeling for gas chromatography compound retention depends on the retention factor (k_i) and on the flow of the mobile phase. Thus, different approaches for determining an analyte k_i in column chromatography have been developed. The main one is based on the thermodynamic properties of the component and on the characteristics of the stationary phase. These models can be used to estimate the parameters and to optimize the programming of temperatures, in gas chromatography, for the separation of compounds. Different authors have proposed the use of numerical methods for solving these models, but these methods demand greater computational time. Hence, a new method for solving the predictive modeling of analyte retention time is presented. This algorithm is an alternative to traditional methods because it transforms its attainments into root determination problems within defined intervals. The proposed approach allows for t_r calculation, with accuracy determined by the user of the methods, and significant reductions in computational time; it can also be used to evaluate the performance of other prediction methods.

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Keywords

Gas chromatography; Prediction; Retention time; Programmed temperature gas chromatography (PTGC); Thermodynamic properties; Numerical method

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