Transactions of Azerbaijan Higher Technical
Educational Institutions
ISSN 1609-1620
Volume 22, № 3 (2020), 86-89
UDC 543.544

Efficient identification of complex mixtures of unknown composition

Metrology and instrument-making

Ibrahimova A.E., Mustafayeva S.E.
Azerbaijan State Oil and Industry University
E-mail: arzu21mk@gmail.com

The implementation of a proposed method of chromatography leads to the creation of universal intelligent chromatograph, that allows to receive information on qualitative and quantitative chromatographic analysis automatically regardless of the conditions of its conduct.

Key words: chromatograph, standard identification column, retention time, qualitative and quantitative analysis.

Introduction

One of the main modern methods of automatic analytical control of multi-component substances is chromatography [1, 2].

Interpretation of chromatographic information involves two rather complicated tasks. The first of theme – is the task of qualitative analysis, the solution of which is to recognize the components registered on the chromatogram. The second task is quantitative analysis, which consists in determining the concentration of the components of the chromatographic analysis.

There are currently a number of qualitative methods of chromatographic analysis. However, each of the existing methods has certain advantages and disadvantages, and at the same time, none of them meets modern requirements for identification:

1. Identification in a wide range of changes in chromatography parameters (temperature, pressure, carrier gas flow rate, property and type of sorbent in the column).
2. Identification of a wide class of substances.
3. Simplicity of metrological support.
4. Providing of standard reference data.
5. Automation of identification procedures.
6. High reliability, simplicity and reliability of identification results.

At present, in the world practice of chromatography for the purposes of qualitative analysis, used the method of identifying substances by retention time – the elution time of a component from the chromatographic column. This time is given in the reference literature for a number of components, as well as a number of substances [7], for specific columns filled with specially selected sorbent for a specific temperature of chromatographic procedure. However, when specified conditions are changed, using the deterministic tabular data of the retention times becomes impossible. In this case, the task of qualitative analysis is complicated, requires much time and need to have expensive and often deficit components or certified mixes.

As for the quantitative interpretation of chromatographic analysis, it is solved relatively easily, with a known qualitative composition of the analyzed mixture. When analyzing substances are with a known composition, their identification is carried out according to reference literature, in which the relative retention values of a number of components are given.

In case of chromatographing of substances of unknown composition (totally or partially), and if requires changes the conditions of chromatographic procedure, the problem of quantifying identification of composition of components cannot be solved without qualitative interpretation.

Statement of the problem

Based on the analysis of the different methods of identification, suggested to completely separate the identification procedures from the chromatographic procedure.

Solution of the problem

To solve this problem, it is proposed to chromatographic procedure realized on two serial connected columns.

First column is the main or principal, is intended for the direct separation of substances. The second, called identification (standard) column – is used to identify the components, beforehand separated into the main column. Chromatographic procedure (separation) on the main column can be made with any necessary conditions (temperature, length of columns, sorbent, carrier gas). The components, which divided into the main column, consecutively arrive at the identification column, which has a constant length, fill of the same sorbent and always is on the same temperature, which is higher than possible temperature of the main column. Then measuring retention time of pure standard components on identification column.

Definition of retention times is carried out on the signals of the two detectors installed on the inlet and outlet of the identification column.

The scheme of identification of components of the mixture using the identification column is shown in Fig.1.

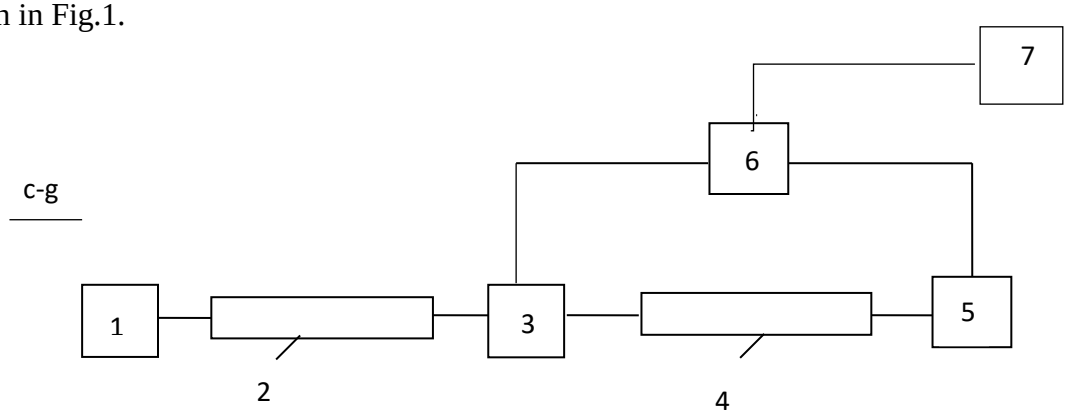

Fig.1. The scheme of identification using the standard column

Identification of components of the analyzed mixture is carried out in the following sequence. The mixture is entered in main chromatography column 2 through the dosing device 1, where it is separated into individual components that come in detector 3, and then, through standard column 4 - in detector 5. The components which through detectors 3 and 5 are registered on charts of self-recording devices in the form of a signal of measuring information as a sequence of chromatographic peaks, which arrive in normalize converter 6, then on computer 7. In Fig.2 represented signals U1,

U2 of component of researched a multi-component mixture, which are recorded on the detector 3 and 5.

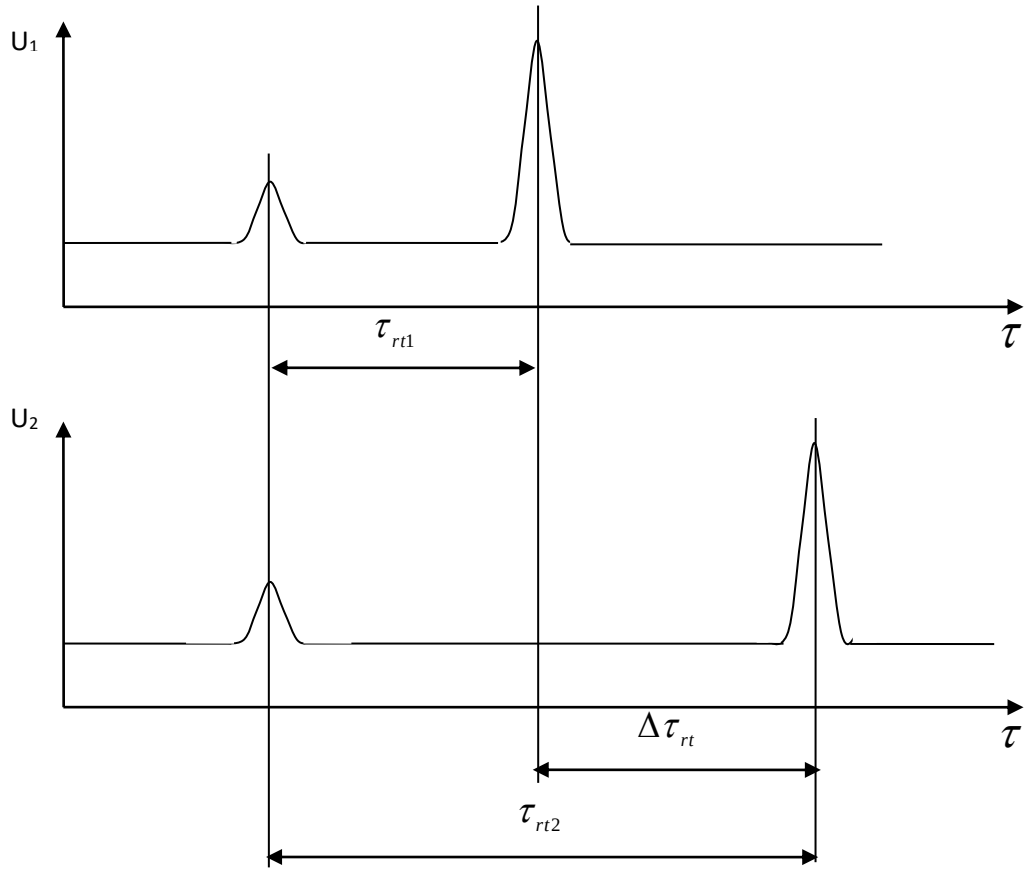

Fig. 2. The signals of components registered on detector 3 and 5

The interval τ_{rt1} corresponds to the time between entering the investigated mixture in the carrier gas flow and the moment of appearance of maximum peak of component i in the chart recorder of the detector 3, i.e. the retention time of component *i* in the first column, and the interval τ_{rt2} – the time between entering the investigated mixture in the carrier gas flow and the moment of appearance of maximum peak of the same component on a chart recorder of the detector 5, i.e. the retention time of the *i*-component on two columns.

Identification of component *i* is calculate as follow:

$$\Delta\tau_{rti} = \tau_{rt2} - \tau_{rt1} \quad (1)$$

The value $\Delta\tau_{rti}$ is represents as the retention time of the *i*-component on a standard column.

The determination can also be carried out according to an algorithm, where the counting of the retention time on the identifying column begins from the moment of the registration of the maximum of the *i*-th component peak by the detector 3 installed at the input of the standard column. The use of a specific retention time calculation algorithm depends on the placement of the detection devices.

Further identification procedure involves comparison of the founded values with the values obtained for standard-components on a standard identification column. Coincidence the value $\Delta\tau_{rti}$ with any table value, allow identify the *i*-component.

Considering the above identification scheme using standard columns, it should be noted that, the use of such columns brings significant benefits, as:

– does not restrict researchers in choosing a sorbent and parameters of chromatographic analysis;
– creates an opportunity to work with programming temperature;
– when you create an identity system, you must have a databank on the retention times on the standard column;
– the possibility to use databank for one standard columns and for one temperature allows to simplify the automation of experiment to identification.

Conclusion

Follows from the above we can say that the identification of components of the mixture based on the proposed methodology, using modern computer, allows to create an intelligent chromatograph. The retention time of component obtained on a standard column, which are written down in a databank of computer and calibration coefficients for pure components will display on screen of computer the name of components and their percentage. Databank in computer may constantly replenished through the Internet, where information will be collected from users applying similar technique of chromatographing.

References

1. Лейбниц Э., Штруппе Х.Г. Руководство по газовой хроматографии. – М.: Мир, 1988.
2. Царев Н.И., Царев В.И., Катраков И.В. Практическая газовая хроматография. – 2000. – С.97-108.
3. Вигдергауз М.С., Семченко Л.В., Езрец В.А., Богославский Ю.Н. Качественный газохроматографический анализ. – М.: Наука, 1978. – 244 с.
4. Сакодынский К.И. Аналитическая хроматография. – 1993.
5. Количественный анализ. – dic/academic.ru/dic.nst/ruwiki.
6. Столяров Б.В. Руководство к практическим работам по газовой хроматографии. – 1998. – С.412.
7. Chromatography coloumns and supplies. // Catalog 2005-2006/www.phenomenex.com.
8. Фарзане Н.Г. Автоматические детекторы газов. – anchem.nglib.ru/book_view.jsp.

Xülasə

İbrahimova A.E., Mustafayeva S.E.

Naməlum kompozisiyanın mürəkkəb qarışıqlarının effektiv identifikasiyası

Təklif edilən xromatoqrafiya üsulunun tətbiqi, xromatoqrafik təhlilin aparılma şəraitindən asılı olmayaraq, keyfiyyət və kəmiyyət analizi barədə məlumatı avtomatik olaraq əldə etməyə imkan verən universal intellektual xromatoqrafın yaradılmasına gətirib çıxarır.

Açar sözlər: xromatoqrafiya, standart identifikasiya sütunu, saxlanma müddəti, keyfiyyət və kəmiyyət təhlili.

Резюме

Ибрагимова А.Э., Мустафаева С.Э.

Эффективная идентификация сложных смесей неизвестного состава

Реализация предложенного метода хроматографии приводит к созданию универсального интеллектуального хроматографа, который позволяет автоматически получать информацию о качественном и количественном хроматографическом анализе независимо от условий его проведения.

Ключевые слова: хроматография, стандартная идентификационная колонка, время удержания, качественный и количественный анализ.