

SOFTWARE

CHROMATEC ANALYTIC

BUILD 4.0

USER MANUAL

214.00045-51I

GLOSSARY

TERMS AND ABBREVIATIONS

Revision 15.11.2023

TABLE OF CONTENTS

A 3
C 3
D 3
E 4
F 4
G 4
H 5
I 5
J 5
L 6
M 6
N 6
P 6
R 7
S 7
T 8
W 8

A

Absolute Retention Time. This term is sometimes used for the time elapsed between the inlection of the sample and the appearance of the maximum concentration of the zone of the substance. This time is more often and correctly called Retention Time. In some cases, it is defined as the center of mass or the first moment of concentration distribution. For non-symmetrical peaks, these two definitions differ.

Absolute Retention Volume. True retained volume. This is the volume of gas corresponding to the absolute retention time. For this reason, the use of these two terms should be avoided.

Absorbent. A solid or liquid sorbent that dissolves gases, vapors or components of liquid mixtures in its volume.

Adsorbent. A solid sorbent that concentrates gases, vapors or dissolved substances on its surface.

Adsorption. A physicochemical process in which there is a difference in concentration at equilibrium in the bulk phase (gas or liquid) and at the interface between this phase and another phase. Adsorption can occur at the gas—solid, liquid–solid, or gas–liquid interface. In all cases, such adsorption leads to some retention of the substance. This is a significant or only contribution to gas adsorption chromatography, but in gas–liquid chromatography, adsorption on the gas—liquid or liquid—solid interface, or on both of these interface surfaces, can make a significant contribution to retention.

ADVIS. Ion source for the Chromatec mass spectrometric detector.

C

Carrier gas. Mobile phase in gas chromatography. Gas adsorption chromatography. A type of chromatography in which a gas is used as a mobile phase, and an adsorbent is used as a stationary phase.

CCD. Catalytic Combustion Detector.

Chromatography. Physico-chemical method of separation of mixtures of substances or particles based on the difference in the speed of their movement in a system of immiscible and moving relative to each other phases.

The science of intermolecular interactions and the transfer of molecules or particles in a system of immiscible and moving relative to each other phases.

The process of differentiated multiple redistribution of substances or particles between immiscible and moving relative to each other phases, leading to the isolation of concentration zones of individual components of the initial mixtures of these substances or particles.

In gas chromatography, a gas called a carrier gas is used as the mobile phase. The stationary phase can be either a solid (adsorbent) or a liquid (in the form of a film deposited on the surface of a solid carrier).

D

DAD. Diod-array detector.

DFC. Digital flow controller.

Docker. Software for automating application deployment and management in containerization-enabled environments, application containerizer. Allows you to "package" an application with all its environment and dependencies into a container that can be deployed on any Linux system.

E

ECD. Electron capture detector.

Eddy diffusion. Contribution to the broadening of the zone due to the uneven distribution of linear flow velocities around the filler particles in the nozzle column. The molecules move along the column, following paths of different length, at different speed. This determines the contribution to the dispersion of their residence time in the column, which depends not on the nature of the substance and its retention, but on the particle size and particle size distribution, and probably on the quality of the packing, although this latter factor has never been properly investigated.

Eluat. The dissolved substance that is moved along with the eluent.

Eluent. Mobile phase, a flow of liquid or gas that moves the components of the separated mixture along the stationary phase.

Elution. The process of moving a sample with an eluent.

Ethernet. A family of packet data transfer technologies between devices for computer and industrial networks. The name "Ethernet" (literally "ether network" or "network environment") reflects the original principle of operation of this technology: everything transmitted by one node is simultaneously received by all the others (that is, there is some similarity with radio broadcasting). Currently, almost always the connection takes place via switches, so that frames sent by one node reach only the addressee (with the exception of transmissions to the broadcast address) – this increases the speed and security of the network.

External standard. A pure substance or calibration mixture introduced from time to time into the column between the sample analysis sequences of the controlled product flow.

F

FID. Flame ionization detector.

FPD. Flame photometric detector.

G

Gas-liquid chromatography. A type of chromatography in which a gas is used as a mobile phase, and a non—volatile liquid is used as a stationary phase.

GC. Gas chromatography, Gas chromatograph.

GC-MS (GC-MS). An analytical instrument and the methods that use it. This is a combination of a gas chromatograph separating the components of the mixture and a mass spectrometer analyzing the column eluate and giving mass spectra for the separated substances.

H

Headspace analysis. Vapor phase analysis. Analytical technique for volatile substances contained in a complex matrix, such as biologicalfluids, food or beverages. It consists in the analysis of the aliquot of the gas phase in equilibrium with the sample contained in a closed vessel. This eliminates rapid contamination and destruction of the column by repeated injection of non-volatile substances contained in these samples, which means it requires less experimental work than solvent extraction, and involves less risk of contamination. Calibration is an important task, since the solubility of the analyzed substances in the matrix is often very different from their solubility in pure water.

Height of the peak. The maximum difference between the detector signal and the background during peak elution. The distance between the peak maximum and its base, measured along the signal axis.

Height of the plate. The length of the column corresponding to one theoretical plate. The height equivalent to the theoretical plate. Symbol: H.

Height equivalent to the theoretical plate. A measure of the efficiency of the column. The value obtained by dividing the column length by the number of theoretical plates. Symbol: HETP or N.

HPLC. High-performance liquid chromatography.

HID. Helium ionization detector.

I

Integration events. Fine-tuning parameters for marking peaks on the chromatogram. Most often they act in a certain specified time interval.

Internal standard. A substance added in a known amount to the aliquot of the analyzed mixture. After proper calibration, the quantitative composition of the mixture is obtained from the ratio of the peak areas of the substances of interest and the internal standard. The substance (substance) used as an internal standard should be chemically similar to the analyzed substances, eluted fairly closely, but well separated from all other components.

IP-address. A unique numeric identifier of a device in a computer network.

IQ-OQ-PQ. Qualification of installation (installation, IQ), operation (OQ), operation (PQ). The qualification of laboratory equipment and software guarantees their "validity", i.e. suitability for the implementation of user tasks.

J

JSON. JavaScript Object Notation. A text-based data exchange format used most often by web applications, which also includes Chromatec Analytic 4.

L

LIMS. Laboratory Information Management System) — software designed to manage laboratory work flows and documents. It optimizes the collection, analysis, return and reporting of laboratory data.

M

Method. A method is a set of settings that describes the conditions for analysis, features of processing results and generating reports. The method consists of three parts (see below).

- **Injection method.** The status of the parameters of the sample input devices.
- **Instrumental method.** The state of the parameters of the internal chromatograph devices, as well as some external ones, such as a mass spectrometric detector. The parameters can have a constant value during the analysis or change according to a certain program.
- **Processing method.** The state of the parameters for processing measurement results.

Modbus. An open communication protocol based on a client-server architecture. It is widely used in industry for the organization of communication between electronic devices. It can be used for data transmission via serial communication lines RS-485, RS-422, RS-232, as well as TCP/IP networks (Modbus TCP).

Moxa. Moxa Ethernet adapters. Previously, they were used with processor modules PM2 and PM31 to connect the chromatograph to a local computer network.

MSD. Mass spectrometric detector.

N

NetCDF. An open machine-independent binary file format that is a standard for the exchange of scientific, including chromatographic and mass spectrometric data. It is used for exporting/importing data, transferring them between different chromatographic programs.

NIST. The National Institute of Standards and Technology. Developer of the largest library of mass spectrometric data.

NPD. Nitrogen-phosphorus detector.

P

PDD Pulsed discharge ionization detector.

Peak asymmetry. The ratio of the front and rear peak widths measured at 10% of the height.

PLOT. Quartz capillary columns, on the inner walls of which an adsorbent layer, molecular sieves or porous polymers are applied. The thickness of the sorbent layer is significantly higher than the thickness of the stationary phase in WCOT columns. Most often it is 10-40 micrometers. Such columns are used to separate highly volatile substances and permanent gases.

PM1, PM2, PM3, PM 31. Processor module of chromatographs "Crystal", "Chromatec-Crystal" and "Chromatek Gasochrome".

PR. Pressure regulator.

PS. Pneumoresistance**.**

R

Retention time

- Absolute or total: the time elapsed between sample insertion and peak peak elution.
- Adjusted: absolute holding time minus dead time or "air" retention time.
- Corrected: absolute retention time, corrected for gas compressibility.
- Effective: absolute retention time corrected for both the compressibility of the mobile phase and the gas retention time in the column; also called fully corrected retention time.
- Specific: effective retention time at standard temperature and pressure divided by the amount of liquid phase in the column or the total surface area of the adsorbent.
- True: a synonym of the adjusted.
- Full: see absolute.

S

SIM. Selected Ion Monitoring. Special operating mode of the mass spectrometric detector. Used for quantitative analysis. The search for known substances by selective ions with maximum sensitivity is carried out. Concentrations from 0.05 ppb can be determined. Only selected ions are scanned. Thus, the analysis of the target components is performed with maximum sensitivity. One or two confirming ions are usually selected to confirm the identification of the component.

Sorbate. The analyzed mixture of substances converted into a liquid or gaseous state.

Sorption. The process of absorption of gases, vapors or liquids by absorbers (sorbents). The reverse process is called desorption.

Sorption can be carried out in two ways:

- static sorption – the process proceeds at relative rest of both phases and ends with the establishment of an equilibrium distribution of substances between the phases.
- dynamic sorption is a process in which there is a directional movement of the mobile phase relative to the stationary one.

SPME. Solid-phase microextraction is a method of concentrating the sample, involves sorption of the analyte onto a layer of sorbent deposited on the surface of a thin quartz fiber, followed by desorption in a chromatograph inlet. This approach allows you to achieve high sensitivity and abandon the use of organic solvents.

Stationary phase. It can be either a solid, then the main process for establishing equilibrium is the adsorption process.

If the stationary phase is a liquid, then in order to avoid convective mixing and ensure rapid mass transfer between the two phases, the stationary liquid phase is applied to a solid carrier.

This carrier should be inert with respect to the components of the analyzed mixture, so as not to affect the establishment of equilibrium between the mobile and stationary phases. Otherwise, there will be a distortion of the peaks, a strong broadening of the chromatographic zone, a decrease in both the height and the area of the peak, or the desired peak will not be recorded at all on the chromatogram.

T

TCD. Thermal Conductivity Detector.

TIC. Total Ion Current. The mass spectrometric detector sequentially scans all the masses in a given range. At each moment of time, called a scan, a spectrum is built. The TIC chromatogram is similar to the chromatogram of a conventional detector. It consists of interconnected points, scans. The intensity of the point is obtained by summing the intensities of all the ions of the spectrum in this scan.

W

WCOT. Hollow capillary columns in which a thin film of the stationary phase is applied directly to the inner surface.