Surface Measurement Systems
World Leader in Sorption Science

GLOSSARY OF SCIENTIFIC TERMS

SURFACE MEASUREMENT SYSTEMS

(Version 2)

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A

Absolute Zero

The lowest point in the Kelvin temperature scale. 0 K = - 459.67 °F or -273.15 °C.

Absorption

A process that occurs when a gas or liquid solute diffuses into a liquid or solid (adsorbents) to form a solution.

Activated Carbon

Charcoal is activated by heating to 800-900ºC to form a material of high adsorptive capacity for many gases, vapors, organics, etc. It has a large internal surface area, and it is commonly used in the pharmaceutical industry to remove organic contaminants. It can also be used as a filter media in a filtration device itself.

Acid-base Properties

Acid-base interactions can be considered in terms of the Lewis acid-base theory i.e. electron donor (base) and electron acceptor (acid) properties. For instance, dichloromethane is generally considered an electron acceptor (acid), and ethyl acetate is generally considered an electron donor (base).

Adhesion

Can be described as the interaction between two different materials. The thermodynamic work of adhesion can be determined from the dispersive (γ^d) and specific (γ^{sp}) surface energy values of the different components.

$$W_{AD} = 2\cdot(\gamma_1^d \cdot \gamma_2^d)^{1/2} + 2\cdot(\gamma_1^{sp} \cdot \gamma_2^{sp})^{1/2}$$

Adjusted Retention Time (t_r)

The adjusted retention time is the difference between the dead time (hold-up time for a reference gas through the column) and the retention time for a compound.

Adsorbate

A material that has been or is capable of being adsorbed; a substance adhered to a surface (the adsorbent).

Adsorbent

A material having the capacity or tendency to adsorb another substance; solid or liquid surface on which a gas or liquid (the adsorbate) adheres.

Adsorption

The adherence of molecules, ions, or atoms of a gas or liquid to the surface of another substance. The adsorbed species is thought to be adhered to the surface by weak physical or chemical forces.

Alkanes

Alkanes, also known as paraffins, are chemical compounds that consist only of the elements Carbon (C) and Hydrogen (H) (i.e., hydrocarbons), wherein these atoms are linked together exclusively by single bonds (i.e., they are saturated compounds) without any cyclic structure (i.e. loops) e.g. hexane, heptane, octane, etc.

Ambient

Refers to "common" environmental conditions in which the experiment is conducted. For example, 20º to 25 ºC and 30 to 40% RH (typical room conditions).

Amorphous

Lacking definite form; shapeless; of no particular type; anomalous; lacking organization; formless; lacking distinct crystalline structure; typically has higher surface area than crystalline form.

Amorphous Content

Describes the amount of amorphous versus crystalline material for a particular sample; for instance, an amorphous content of 10% means that 10% of the sample is in the amorphous form and 90% of the sample is in the crystalline form.

Amorphous Solid

A solid in which there is no long-range order; opposite of crystalline.

Aqueous

Similar to or resembling water. In reference to a solution made in water.

B

Backpressure

A backward surge of pressure from downstream to upstream of the filter.

Balance Purge

A flow of dry gas is used to keep the balance electronics dry and stable; typically set to one-third of the total flow rate.

Ballasting Oil

Cleaning the oil used in the rotary pump in the DVS Vacuum. The pump needs to be ballasted regularly when condensable vapors and gases are used.

Bar

A unit of pressure. One bar = 14.5 psi = 750 Torr = 1 atmosphere.

Baratron

A capacitance transducer which measures the true pressure of a gas, independent of the type of gas used.

Batch-to-Batch Variation

Refers to dissimilarities in different lots of the same material; dissimilarities may be due to impurities, different processing conditions, or different sample histories.

BET SSA (Brunauer-Emmett-Teller Specific Surface Area)

Refers to the surface area of a material estimated via the BET equation. If an experimental isotherm of a vapor or gas forms the type II or IV isotherms (-see `Isotherm curves`), the specific surface area of the adsorbent (sample) can be estimated via linear regression within the linear part of the graph p/po vs. 1/n[(p/po)- 1]. This linear part usually falls within the range $0.05 < p/po < 0.35$. (p: partial pressure; po: saturation pressure; n: amount of adsorbed gas)

Boiling Point (BP)

The temperature of a liquid at which the vapor pressure is equal to the pressure of the atmosphere above it.

Buoyancy Force

A force generated by gas flow that pushes up on a sample pan. It is dependent on the sample pan geometry and the rate of gas flow.

Butterfly Valve

A valve in the DVS Vacuum system that regulates the pressure inside the sample chamber by opening or closing to certain degrees.

C

Calibrate

To check, adjust, or determine by comparison with a standard.

Carrier Gas

The gas that flows through a separation column of a gas chromatograph and propels a sample to a detector.

Catalysts

A chemical substance that increases or decreases the rate of a chemical reaction; a catalyst is not consumed in the reaction; used in various industries including petroleum refining, automobile catalytic converters, and bulk chemical production.

Heterogeneous Catalyst: acts in a different phase than the reactants; mostly these are solids that are used for liquid or gas phase reactions.

Homogeneous Catalyst: acts in the same phase as the reactants; usually liquids.

CFR

The Code of Federal Regulations refers to an FDA regulation that was put in place to prevent fraud in the submission of electronic records. The common title of the regulation is 21 CFR Part 11, which means Title 21 CFR Part 11. Any company that submits electronic records to the FDA should comply with this regulation.

Chemisorption

Chemisorption (or chemical adsorption) is adsorption in which the forces involved are valence forces of the same kind as those operating in the formation of chemical compounds, a covalent bond between adsorbate and substrate.

Chromatography

The separation of substances in a mixture is based on their affinity for certain solvents and solid surfaces.

Clausius-Clapeyron Equation

When isotherms are measured at different temperatures the heat of sorption can be calculated using a Clausius-Clapeyron type Equation:

$$\left(\frac{\partial \ln p}{\partial T}\right)_{\theta} = -\frac{\Delta H_s}{RT^2}$$

where p is the partial pressure, T is temperature, R is the universal gas constant, and H_s is the heat of sorption.

Closed Loop

In a closed loop setting, the Speed of Sound (SoS) sensor constantly measures the actual vapor pressure and if it deviates from the target P/Po, will feed back to the MFC's to adjust the flow. Closed Loop is recommended for organic vapors and at temperatures where salt calibrations have not been performed.

Co-Adsorption / Competitive Adsorption

The DVS can be used to carry out a complete study of sample affinities towards a series of solvents as a single or multi-component sorption (competitive sorption) experiment. It can be done either by keeping one solvent at a constant concentration and increasing the other one or varying both Solvent concentrations.

Cohesion

Can be described as the interaction between two like materials. The thermodynamic work of cohesion can be determined from the dispersive (γ^d) and specific (γ^{sp}) surface energy values of the material.
$W_{COH} = 2\cdot(\gamma_1^d \cdot \gamma_1^d)^{1/2} + 2\cdot(\gamma_1^{sp} \cdot \gamma_1^{sp})^{1/2}$

Conditioning

To expose the column to conditions before starting the experiment. In IGC the conditioning method is saved as *.cnd extension and the data is saved during the conditioning method.

Contact Angle

The contact angle is the angle at which a liquid-vapor interface meets the solid surface and provides information on the interaction energy between the surface and the liquid; a common technique used to measure surface energies on homogenous, flat surfaces.

Control of Substance Hazardous to Health (COSHH)

United Kingdom Statutory Instrument that stipulates general requirements on employers to protect employees and other persons from the hazards of substances used at work by risk assessment, control of exposure, health surveillance, and incident planning.

Crystalline Solid

A solid in which it is arranged in an ordered repeating structure extending in all three spatial dimensions (aka ordered lattice structure); some materials may exist in more than one crystalline state, but there is typically one thermodynamically preferred orientation.

Crystallization

The (natural or artificial) process of formation of solid crystals; this can occur from a super saturated solution or the conversion from the amorphous solid.

Counterweight

The purpose of a counterweight is to make the measurement of a high-mass sample more accurate. It is used in a DVS system when high masses are being used. In a low-mass balance a counterweight is used for samples ±150 mg, in the high-mass balance samples ± 1 g require the use of counterweights.

D

DAT

All DVS instruments save raw data in a binary file with the extension .dat. These files are imported by the DVS Analysis macros and automatically converted to Excel files.

Data Sampling Rate

The data sampling rate determines how fast the computer reads a data point during the experiment.

DVS experiments: Data from the DVS instrument and it is used to analyze dm/dt and to update the sensor displays. Not the same as data saving rate

IGC experiments: Data sampling rate is same as data saving rate

Data Saving Rate

The data saving rate determines how often a data point is saved to a file. The data saving rate must be equal to or slower than the data sampling rate (DVS only).

Dead Time (t_m)

The dead time is the amount of time the non-retained compound spends in the column. Dead time is generally reported in minutes.

Dead Volume

In gas chromatography, it is usually taken as the retention volume of a completely un-retained solute.

Delay

During a delay, the IGC column will get to the conditions of the first step of the selected method and wait the entered time. The delay is another way to perform column conditioning without having to write a conditioning method; however, no data is collected during the delay time.

Deliquescence

When a material absorbs enough solvent (water or organic), that it begins to dissolve and liquefy.

Della Volpe Scale

A scale for the surface tension component of probes in iGC-SEA. The Della Volpe scale assumes water is more acidic in nature: $\gamma_l^+ = 10$ mJ m^{-2} and $\gamma_l^- = 65$ mJ m^{-2}.

Density

The mass of a substance divided by its volume.

Desorption

A process where molecules leave the surface of a material or are “given off”, into their surrounding environment. These could be molecules that were adsorbed or absorbed by the material earlier.

Detector

As compounds come off the column, they enter a detector. The compound and detector interact to generate a signal. The size of the signal corresponds to the amount of the compound present in the sample. Several different types of detectors that can be employed, depending on the compounds to be analyzed. These detectors can measure from 10^{-15} to 10^{-6} grams of a single component.

DI Water

Deionized water; water processed through an ion exchange process by passing through both cation and anion exchange resin beds, or a mixed resin bed to remove both positive and negative ions. The purity of water is measured by its electric resistance. High-quality DI water has a minimum resistance of 18 megohm per cm at 25ºC.

Dielectric Humidity Sensor

A humidity sensor that uses the electrical properties of a polymer as a way to calculate the relative humidity of a gas. These polymers swell in the presence of water. Rotronic sensors in SMS instruments use this type of sensor.

Diffusion

The motion of molecules through a material. For example, gas molecules moving through a plastic film or water molecules moving inside a cube of gelatine.

Diffusion Coefficient

This is a measure of how fast a molecule is moving inside another material. A common way to express this value is in cm^2/sec (centimeters squared per second).

Dispersive

The dispersive interactions also called London, non-specific or universal interactions, originate from the rapid electron density change hence, even nonpolar molecules such as alkanes are capable of undergoing dispersive interaction.

Dispersive Component of Surface Energy

To evaluate the dispersive interaction capacity, it can be expressed in terms of the dispersive component of the surface energy (γ^d_s in mJ/m^2).

Dm/dt

This is the change in mass in real-time. Mathematically it is the derivative of mass versus time. The DVS software monitors mass in real-time and uses this data to change RH steps if the program uses dm/dt steps.

Dynamic

Pertaining to or characterized by energy or effective action; vigorously active or forceful; in relation to SMS equipment, dynamic refers to the flow-driven flux of vapor or gas delivered to the sample; in contrast to static sorption.

> **Dynamic mode in DVS Vacuum:** The butterfly valve regulates the pressure in the chamber by opening or closing. The MFC pumps molecules into the chamber and the turbo pump pumps molecules out.

Dynamic Vapor Sorption

A term that was introduced by SMS to describe what our instruments do. The DVS instruments expose samples to vapor. The vapor is taken up by the samples and the change in sample mass is monitored in real-time (dynamic).

E

Effusion

This refers to gas molecules leaking through a small opening. Heavier molecules effuse or leak out more slowly.

Equilibrium

Meaning that there is little or no change. In DVS we mean that the mass of the sample is not changing.

Excipient

An inactive substance used in pharmaceutical formulation; can act as a carrier, stabilizer, controlled release agent, or diluent.

F

FDA

United States Food and Drug Administration; an agency of the United States Department of Health and Human Services and is responsible for regulating and supervising the safety of foods, dietary supplements, drugs, vaccines, biological medical products, blood products, medical devices, radiation-emitting devices, veterinary products, and cosmetics.

Filtration

A mechanical or physical operation that is used for the separation of one material (gas, liquid, or solid) from another material (typically liquids or gases) by interposing a medium to fluid flow through which the fluid can pass, but not the material being separated; filtration is important in air or water purification, separation of different materials in chemical production, fuel cells, and chemical sensing.

Flame Ionization Detector (FID) & FID Signal

The flame ionization detector uses a hydrogen flame to decompose organic species, which are then measured by electrodes near the flame; FID cannot detect compounds that do not contain carbon-hydrogen bonds e.g. H_2O or CO.

Fowkes Theory

An approximation for surface energy, made from two components, a dispersive (γ^d_s) and acid-base (γ^{ab}_s) component.

$$\gamma_s^T = \gamma_s^d + \gamma_s^{ab}$$

Frontal

Continuous injection of vapor; resultant chromatograph is a solvent front or breakthrough curve.

G

Gibbs Free Energy

Also known as Free energy. The maximum amount of non-expansion work that can be extracted from a closed system under ideal reversible conditions. It is also a quantitative measure of the feasibility of a chemical reaction.

Glass Transition

Where an amorphous solid, such as glass or a polymer, becomes brittle; more specifically it defines a second-order phase transition in a material that goes from the glassy to rubbery state; increasing temperature or vapor pressure can cause a glass transition.

Good Van Oss Scale

A scale for the surface tension component in iGC-SEA probes. The Good Van Oss scale considers the acid-base surface tension of water to be equal: $\gamma_l^+ = \gamma_l^- = 25$ mJ m^{-2}.

Gravimetric Vapor Sorption (GVS)

Another name for Dynamic Vapor Sorption; does not convey the ability to take data in real-time.

H

Heat of adsorption

The heat of (ad)sorption for a particular vapor solid system can describe the sorption mechanism between the two, indicating the level of thermodynamic affinity between the vapor and substrate; also called enthalpy of (ad)sorption.

Heat of Vaporization

The heat energy needed to transform one mole of a substance from the liquid phase to the gas phase at one atmosphere of pressure.

Henry Constants

The ratio of the aqueous phase concentration of a substance to its equilibrium partial pressure in the gas phase.

Heterogeneous

Object or system consisting of multiple items having a large number of structural variations; for instance, a heterogeneous surface would have localized variations in structure, chemistry, or reactivity.

High Throughput

Allows a researcher to quickly conduct several tests simultaneously; this is accomplished by measuring samples in parallel, not series; can be accomplished by the DVS-HT or by using multiple DVS-Intrinsic units.

High Mass Balance

The High Mass Balance measures changes in mass in the dynamic range of ±1.0 g without counterweights. With counterweights, this mass is 5.0g in total.

Homogeneous

Being similar throughout; for instance, a homogeneous surface is the same throughout the entire material.

Hydrate

A material that has one or more water molecules for each one of its molecules. The water is held by chemical bonds. This is not the same as water sorbed on the surface or in pores of a material. This water becomes part of the chemical equation of the material.

Hydration

The process of water uptake by a material. When talking about waters of hydration, this means how many water molecules per molecule of solid material.

Hydrocarbon

An organic compound that contains both carbon and hydrogen in its molecular structure, e.g. benzene or methane.

Hydrophilic

Displaying an affinity for water.

Hydrophobic

Displaying an aversion for water.

Hygroscopicity

The rate at which a material adsorbs and absorbs water.

Hysteresis

The difference between the forward-going and reverse-going phases of a process. In the case of DVS, it's the variance between the sorption and desorption isotherm plots.

I

iGC-SEA at Infinite Dilution Conditions

Experiments where very small amounts of probe molecules were injected; no probe-probe interactions; only interactions are between solid and probe; in the Henry's (or linear) portion of the sorption isotherm; values obtained are representative of interactions with the highest energy sites.

iGC-SEA at Finite Concentration Condition

Higher injection concentrations; outside of Henry's portion of isotherm; values obtained are representative of interactions with higher surface coverages.

Inert

Chemical inactivity; totally unreactive.

Inert Gas

A gas that is considered stable and does not react with other materials at normal temperatures and pressures.

Inorganic Compounds

Substances that do not contain carbon in their molecular structure.

Inverse Gas Chromatography (iGC)

Inverse of traditional analytical gas chromatography; reverts the roles of stationary and mobile phases; vapors or gases are used to characterize a solid material; IGC is concerned with the physic-chemical characterization of powders and films. In order to characterize it, solutes of known properties are injected.

Inverse Gas Chromatography – Surface Energy Analyser (iGC-SEA)

It is an inverse gas chromatography system that is specially designed to determine the surface energy and the surface properties of the solid and semi-solid samples

Isobaric Process

Is a process during which the pressure ***P*** remains constant.

Isochoric (or Isometric) Process

Is a process during which the specific volume ***V*** remains constant.

Isolated System

Is a closed system in which energy is not allowed to cross the boundary.

Isotherm

Equilibrium amount of vapor or gas sorbed as a function of pressure.

> ***iGC-SEA experiments:*** The peak height measured in the chromatograph is related to pressure in the column and retention volume is related to the amount sorbed.
>
> ***DVS experiments:*** The plot of sample mass versus RH (or P/Po). The sample mass should be at a steady value, equilibrium, for the isotherm to be accurate. The DVS software uses the last n points of data (user selected) in a step and takes the average of these values.

Isotherm Curves

There are several isotherm shapes, Types I, II, III, IV, and V, as described by the BDDT theory. These different shapes can be useful in determining how vapors are sorbed by a material.

Isothermal Process

Is a process during which the temperature ***T*** remains constant.

J

K

Kinetics

Investigations of how different experimental conditions can influence the speed of a chemical reaction to yield information about the reactions' mechanism; Chemical kinetics, also known as reaction kinetics, is the study of rates of chemical processes; in DVS experiments the kinetic data is the mass change with time.

Knudsen Cell

A container made of metal or high-temperature resistant material, with a small opening on the cover. It is used to test or control the evaporation of samples placed inside the cell.

Knudsen Effusion Method

A dynamic gravimetric technique to measure the vapor pressure of a substance. The sample is placed in a Knudsen Cell which has an orifice of known dimensions, allowing vapor molecules to escape into a vacuum at a known temperature.

L

Limit of Detection on Chromatography

The amount of sample in a stream necessary to produce a peak height of two to three times the baseline noise height.

Low Mass Balance

The High Mass Balance measures changes in mass in the dynamic range of ±150 mg without counterweights. With counterweights, this mass is 1.0 g in total.

M

Mass

Usually, we think of mass as the weight of a material expressed in milligrams, grams, or kilograms. But in physics, mass is used to measure the amount of matter in a material. It is not the same as weight because weight depends on gravity. Mass does not change, regardless of where it is measured, on Earth or somewhere else.

Mass Flow Controller (MFC)

A device used to measure and control the flow of gases; designed and calibrated to control a specific type of gas over a particular range of flow rates.

Material Characterization

The use of external techniques to probe into the internal structure and properties of a material; analysis techniques are used simply to magnify the specimen, visualize its internal structure, and gain knowledge as to the distribution of elements within the specimen and their interactions.

> ***Particle Characterization***: The use of external techniques to probe into the internal structure and properties of a powder; typical parameters measured include: vapor and gas sorption properties, particle size/shape, surface area, porosity, density, and particle chemistry
> ***Surface Characterization***: The use of external techniques to probe into the surface properties of a material; involves both physical and chemical analysis techniques; typical parameters measured include: surface energy, surface area, porosity, surface chemistry, chemical composition, reactivity, and surface orientation.

Material Safety Data Sheet (MSDS)

A data sheet for a particular substance describing the characteristics and hazards associated with the handling and use of this product.

Membranes

Layer of material which serves as a selective barrier between two phases and remains impermeable to specific particles or groups of particles or substances when exposed to the action of a driving force.

Method

A programmed set of conditions or steps used for a single experiment.

DVS Method: A small program that the DVS user can create to control the instrument and perform an experiment. Methods can be used to control vapor generation or the pre-heater. Humidity (or P/Po) methods have a *.sao extension and preheat methods have a *.pre extension.

IGC Method: A small program that the IGC user can create to control the instrument and perform an experiment. Methods can be used to control injection probe molecules, temperature, flow rate, humidity, and concentration. Pulse methods have a *.sen extension; conditioning methods have a *.cnd extension; purge methods have a *.prg extension; frontal methods have a *.fba extension; and preheat methods have a *.pre extension.

Microbalance

A balance capable of measuring very small mass values; typical resolutions are 1 microgram or less.

Mo

The mass of a sample at time zero, or at the beginning of the experiment. The DVS user has the option of setting the sample mass as Mo at other points in the experiment.

Metal Organic Framework (MOF)

Porous materials containing metal ions coordinated with organic ligands to form single or multidimensional structures.

Monolayer Adsorption

In monolayer adsorption, all the adsorbed molecules are in contact with the surface layer of the adsorbent.

Monomer

A simple compound whose molecules can join together to form polymers.

Multi-component

More than one component in a system. A gas stream is multi-component if it has more than one gas or vapor present.

Multilayer Adsorption

In multilayer adsorption, the adsorption space accommodates more than one layer of molecules and not all adsorbed molecules are in contact with the surface layer of the adsorbent.

Multisampler

A system that can sample multiple different samples in parallel for high throughput experiments. The DVS Discovery is a two-sample system, while the DVS Endeavour is a five-sample system.

N

NIR Spectroscopy

Near infrared spectroscopy; a spectroscopic method utilizing the near infrared region of the electromagnetic spectrum (from about 800 nm to 2500 nm); applications include pharmaceutical, medical diagnostics, food, and agrochemical quality control, as well as combustion research.

Nonpolar Compound

A compound composed of molecules that possess a symmetric distribution of charge, so that no positive or negative poles exist, and that are not ionizable in solution, e.g., straight-chain alkanes (n-alkanes).

O

Open Loop

A configuration for the Speed of Sound (SoS) sensor where vapor generation is dictated by the saturated salt solution calibration. There is no feedback system to adjust the %RH if the actual %RH deviates from target %RH.

Organic Vapor Sensor

Detects the concentration of organic vapor; has a maximum threshold level when reached will activate a switch to shut down flow and/or power to the instrument.

P

P/Po (%)

The pressure of a vapor relative to its saturated vapor pressure at a given temperature; values will range from 0 (no vapor) to 100 (completely saturated vapor); for water % P/Po is equivalent to % relative humidity.

Partial Pressure

For an ideal gas in a mixture, it is equal to the pressure it would exert if it occupied the same volume alone at the same temperature.

Payne Cell

A cup-like device used in DVS to measure the permeability of a film sample. The cup can be filled with water to measure the loss of water through the film, or zeolite to measure the ingress of water through the film sample.

Permeation

The penetration of a gas, liquid, or vapor across or through another material.

Pharmaceutical

Drug or medicine that is prepared and used in medical treatment.

Phase Separation

When a mixture separates into two or more phases.

Phase Transition

A phase transition is the transformation of a thermodynamic system from one phase to another.

> ***First-order phase transformations***: those that involve latent heat; examples include melting of a solid or boiling of a liquid.

Second-order phase transformations: those that do not involve latent heat; examples include glass transitions.

Physico-Chemical Properties

Also called physical chemistry properties; incorporates macroscopic, microscopic, atomic, subatomic, and particulate phenomena in chemical systems.

Physisorption

Physisorption (or physical adsorption) is adsorption in which the forces involved are intermolecular forces (Van Der Waals forces) of the same kind as those responsible for the imperfection of real gases and the condensation of vapors, and which do not involve a significant change in the electronic orbital patterns of the species involved. The term Van Der Waals adsorption is synonymous with physical adsorption.

Polar Compound

A compound whose electrons are not shared equally in chemical bonds, resulting in a positive and negative pole. A polar compound is not necessarily ionized; water is a polar compound.

Polar Probes

Gases or vapors used in determining the acid-base properties in IGC.

Polymers

Relatively large molecule (macromolecule) composed of repeating structural units (monomers) typically connected by covalent chemical bonds; in popular usage suggests plastic; proteins are also generally considered polymers.

Polymorphism

The ability of a solid material to exist in more than one form or crystal structure.

Polymorphs

Materials with the same chemical composition, but different crystal orientation; hydrates or solvates are not technically polymorphs because they have the addition of a water or solvent molecule in the crystal structure, respectively.

Porosity

A measure of the void spaces in a material.

Micro Porosity: pores smaller than 2 nm in diameter
Meso Porosity: pores greater than 2 nm and less than 50 nm in diameter
Macro Porosity: pores greater than 50 nm in diameter

Pressure Drop

The difference between the inlet pressure and outlet pressure in the column.

Prime

The process in which a gas line is preconditioned with a gas or the vapor of a solvent. This process assures a constant pressure (stable amount) of the vapor or gas throughout the line.

Probes

Gases or vapors used for surface characterization study in IGC.

PT100

A platinum resistance thermometer: temperature sensor that exploits the predictable change in electrical resistance of platinum with changing temperature; has a nominal resistance of 100 ohms at 0 °C.

Pulse

A single injection of vapor or gas.

Purge

The process in which a gas line is cleaned. This prevents cross-contamination that may be caused by the presence of residues of any other solvent or gas.

Q

R

Raman Spectroscopy

A spectroscopic technique used in condensed matter physics and chemistry to study vibrational, rotational, and other low-frequency modes in a system; relies on inelastic scattering, or Raman scattering, of monochromatic light, usually from a laser in the visible, near-infrared, or near ultraviolet range.

Relative Humidity

This is a measure of the humidity in air (or in a gas stream) using as a reference the fully water-saturated air, at the temperature being measured. It is expressed in percent RH, where 100% RH is 100% humid air, or fully saturated.

Retention Time

It is the elapsing time between the injection of a solvent and the detection of its related time to the peak (Max FID signal or Centre of Peak Mass) on a time (t) vs. signal (I(t)) graph. Net Retention Time: The retention time which is corrected with the time of a compound used to determine the dead time (tm) – usually methane.

Retention Volume

The volume of the carrier gas needed to push the solute through the column.

Reservoir

The container holding a solvent, from which its vapor will be taken by the carrier gas (inert gas, e.g. Helium), and transported to where the sample is located.

RH Generation

The ability of the system to generate a target %RH. The RH generation ability is temperature dependent, as at higher temperatures lower %RH is required for condensation. Therefore between 5-60°C 0-98%RH can be achieved while between 60-85°C, only 0-85%RH can be achieved.

Rotary Pump

The rotary pump is used to achieve vacuum conditions of approximately 10^{-3} Torr.

Rotronic Probe

The Rotronic Relative humidity probe measures the %RH being delivered to the sample chamber. It has an accuracy of ± 0.5% between 5-60°C and an accuracy of ± 1% between 60-85°C.

S

Sequence

A group of methods run in order. Up to 10 methods can be run in one sequence for the IGC and DVS instruments. DVS sequence methods have a *.seq extension.

Silanized Glass Columns

Silanized glass columns are used to reduce the adsorption of compounds onto the surface of the glass.

Semi Static

This is a mode in the DVS Vacuum. It is similar to True Static, however similar to closed loop configuration in DVS flow systems, the MFC regulates the pressure in the chamber until the sample mass has reached equilibrium.

Solute

The dissolved substance in a solution; the component of a solution that changes its state; a solute dissolved in another substance, known as a solvent to form a solution.

Solvate

A material that has one or more solvent molecules for each one of its molecules; the solvent is held by chemical bonds which is not the same as solvent sorbed on the surface or in pores of a material. The solvent molecule(s) becomes part of the chemical equation of the material; a hydrate is a type of solvate with water as the solvent molecule.

Solvation

Commonly called dissolution, is the process of attraction and association of molecules of a solvent with molecules or ions of a solute; as ions dissolve in a solvent they spread out and become surrounded by solvent molecules.

Sorbate

A material that has been or is capable of being taken up by another substance by either absorption or adsorption.

Sorption

Encompasses both adsorption and absorption processes.

Specific

Specific interactions include all types of interactions except dispersive interactions. IGC allows the estimation of the specific interaction of a polar solid surface by injecting polar probes (such as ethanol, acetone, etc.) of known characteristics.

Speed of Sound Sensor

The speed of sound (SoS) sensors measures the concentration of vapor in a DVS system. The SoS sensor measures the time of flight of an ultrasonic wave through an organic vapor. The time of flight is directly proportional to the speed of sound through the vapor which is related to the concentration of the vapor.

Speed of Sound Calibration

When starting an experiment at a different temperature it is recommended to do a speed of sound calibration on the DVS. The Speed of Sound sensor also needs to be calibrated when a new Carrier Gas + Solvent combination is used. This is an automatic process using the DVS control software.

Standard Cubic Centimetres per Second (SCCM)

Also, the same as ml/minute.

Static Electricity

The build-up of electric charge on the surface of objects. The static charges remain on an object until they bleed off to ground or are quickly neutralized by a discharge; static can typically be discharged in a DVS by raising the humidity to 90% RH.

Static Vapor Sorption

Pertaining to or characterized by a fixed or stationary condition; static sorption refers to techniques that simply expose a sample to an environment without a

steady driving force of gas/vapor; static sorption techniques include desiccator jars and traditional vacuum sorption equipment.

Surface Area

How much exposed area a material has; is typically described in units of m^2/g; also called specific surface area. BET is the most common model for the calculation of surface area.

Surface Chemistry

Roughly defined as the study of chemical reactions at interfaces; also, can be used to describe the functionality of a material's surface (i.e. is it acidic or basic).

Surface Energy

The amount of energy required to create a unit area of a solid surface; analogous to the surface tension of a liquid; typically dived into two parts, the dispersive component, and the specific component.

Surface Tension

The force per unit length used to overcome the microscopic forces between molecules at the liquid-air interface.

T

Target Versus Actual

In DVS control software, a target RH or P/Po value is set. This is the RH or P/Po we want the instrument to generate. The sensor detects this change and reports a value, which we call the Actual value. The sensor must be calibrated for this value to be accurate.

TEWL

Transepidermal Water Loss or moisture flux across skin.

Thermoconductivity Detector (TCD) and TCD signal

One of the universal detectors used in gas chromatography. This detector senses changes in the thermal conductivity of the column effluent and compares it to a reference flow of carrier gas. Since most compounds have a thermal conductivity

much less than that of the common carrier gases of helium, when an analyte elutes from the column, the effluent thermal conductivity is reduced and produces a detectable signal called TCD signal.

Thermocouple

A kind of thermometer consisting of two wires of different metals that are joined at both ends; one junction is at the temperature to be measured and the other is held at a fixed lower temperature; the current generated in the circuit is proportional to the temperature difference.

> ***Type K****:* made from an alloy of chromel–alumel; is the most commonly used for general purpose thermocouple; available in the −200 °C to +1350 °C range.

Thermodynamics

The study of the conversion of heat energy into different forms of energy (i.e. mechanical, chemical, and electrical), different energy conversions into heat energy, and its relation to variables such as temperature, pressure, and volume; Chemical thermodynamics is the study of the interrelation of heat with chemical reactions or with a physical change of state within the confines of the laws of thermodynamics.

True Static

A mode in the DVS Vacuum. In true static mode, the butterfly valve is closed into the vacuum. MFC pumps molecules in to reach a certain Torr and then stops to obtain equilibrium. During desorption, the butterfly valve opens to reduce pressure to desorb.

Turbo Pump

The turbo pump allows vacuum conditions of approximately 10^{-9} Torr to be reached.

U

V

Vacuum Sorption

The sorption of gases or vapors on solids at very low overall pressures.

Vapor Pressure Analyzer (VPA)

The Vapor Pressure Analyzer (VPA) system can be used to determine the vapor pressure of different materials using the Knudsen effusion method.

Vapor Generator Instrument (VGI)

A microscope accessory for advanced environmental control (i.e. temperature and humidity); can be interfaced with optical, Raman, and IR microscopes.

Vapor Pressure

The pressure exerted by the vapor above a liquid when the two phases are in equilibrium.

Volatile

Evaporates easily and converts easily from liquid form to gas.

W

Water Activity

This is a different way to express relative humidity (discussed above). Instead of using percent RH, the decimal equivalent is used, for example, 50% RH is written as 0.50 Water Activity. This terminology is commonly used in the food industry.

Water Content

The amount of water present in a material usually expressed as a percentage of its dry weight.

Wet and Dry Flow

SMS instruments generate the desired vapor concentration by mixing two carrier gas streams: the wet flow is bubbled through the solvent of interest to completely saturate the carrier gas, and the dry flow is the pure carrier gas; these flows are controlled by electronic mass flow controllers; these flows are mixed in different proportions to generate a total flow rate with the desired relative vapor pressure.

Wettability

The wettability of a material is related to the tendency of water to spread on its surface. It's related to the surface energy of the material and can be measured by iGC-SEA.

X

X-Ray Diffraction (XRD)

Finds the geometry or shape of a molecule using X-rays based on the elastic scattering of X-rays from structures that have long-range order.

Y

Z

Zeolite

A class of microporous aluminosilicate minerals. Commonly used as absorbents and catalysts in industry.