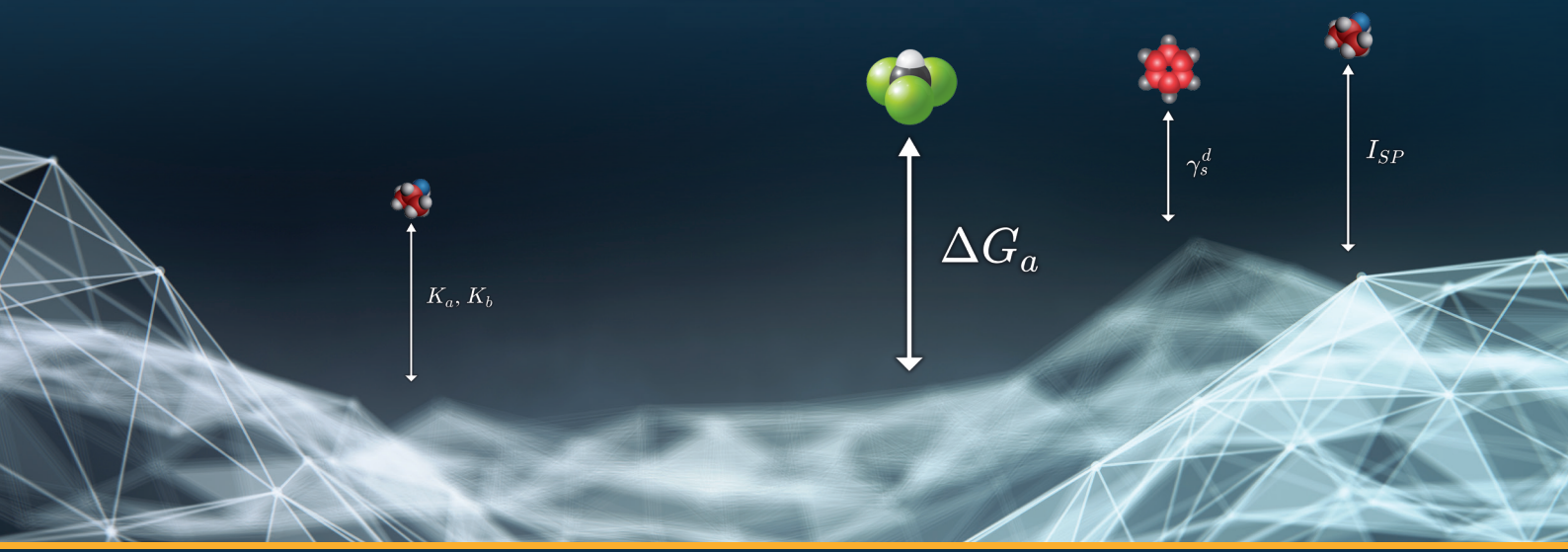
Physicochemical Analysis of Surface and Material interactivity by Molecular Probes

A Flexible Turnkey Solution for Commercial GC-to-Inverse GC Conversion that adapts to your budget and evolves with your needs



Adscientis' modular approach is adaptable to multiple GC platforms and can evolve from manual to fully-automated injections of up to 45 probes

GC instrument

Choose a compatible GC from Thermo, Agilent, or alternate GC supplier

Robotic Probe Handler

Enhance productivity with Industry standard PAL-RSI to automate injections of up to 45 probes in 2 parallel channels

IGC software suite

Employ Adscientis' NUCLEUS control software to automate GC+PAL robot and select custom IGC analysis modules

Expertise and support

Select support package for on-site install/training, protocol development and on-going scientifific support

Applies for powders, fibres, plates, films and liquids

Solves common questionings like:

- Same specifications but behave differently, why?
- What are the impacts of the grinding method, chemical treatment, heat treatment on my samples?
- Are my powders stable over time and if not, what has changed?
- What are the effects of a change in the manufacturing process on my product?

Adscientis
Smart Inverse Chromatography

neuronIC: the new standard in IGC science

- Built on 2 decades of IGC Consulting Experience
- Application Driven Software Developed by IGC Experts
- Guaranteed Reliable, Productive and Accurate Data
- Adaptable High-Throughput Smart Automation

Application-specific software

- Nucleus: the CORE Conductor of neuronIC Instrumental Automation
- Automates all GC and AutoSampler Operations
- Comprehensive Database Management
- Smart Peak End Detection
- Supports High-Throughput Dual-Channel (Parallel) Injections

- SolID: Data treatment for infinite dilution measurements
- Surface Energy
- Nanoroughness Indexing
- Polarity and Acid-Base Character
- Sorption/Desorption Isotherms

- InPulse: Data treatment for finite concentration
- Thermal Desorption Isotherms
- Specific Surface Area
- Adsorption Energy Distribution Function (AEDF)
- Diffusion Coefficients and HSP

Reliable, productive and accurate instruments

Gas Chromatography, both "standard GC" and "Inverse GC", requires high-quality GC hardware components and accessories to insure high-quality, accurate, and repeatable data. Nucleus provides bi-directional digital communications compatibility with Thermo Fischer Scientific's TRACE 1610 (released in 2022) and prior TRACE 1310 models with alternate GC platform compatibility under development and available via special request.

- One or Two analytical channels running simultaneously
- Operating T° range: ambient +3°C to 450°C
- Modular and scalable (see options page for details)

You will benefit from the modularity and flexibility of the neuronIC with a multitude of options available (ie TCD and other interchangeable detectors, headspace or liquid injectors, ss or glass column options with custom sizing options to minimize dead volume) to adapt to your available budget and vendor preferences with upgrade paths available on-demand as your needs change.

Adapted and smart automation: PAL RSI

Nucleus drives the industry standard PAL RSI AutoSampler, the most widely used in the industry (more than 50'000 users)

- Adaptable for both Headspace and Liquid Injections
- Pulse (100 µL/s) or Frontal injections (0.042µL/s)
- Concentration range: 0.1 to 1.5 10^8 nmol (n-octane)
- Standard configuration with 45 molecular probes
- Modular and scalable (see options)

Skilled know-how

Adscientis scientists use their collective knowledge and experience to offer specific advice pertinent to your objectives and dedicated to your materials and applications focus

- Protocol development
- Teaching
- Consulting

Modular and customizable, neuronIC solutions:

AVAILABLE PACKAGES	Productive	Explorer	"À la carte"
Adscientis Software Modules			
Nucleus Conductor	●	●	●
SolID Analysis	●	●	○
InPulse Analysis	●	○	○
Compatible GC/AutoSampler			
TRACE 1610 or 1310 GC*	●	●	*GC of your choice***
Single Channel (FID)	●	●	●
Dual Channel (FID)	●	○	○ *
PAL RSI AutoSampler	●	○	○
NI DAQ (A/D Convertor of GC analog signal)	–	–	●
On-Site Support			
Training using customer samples	●	○	●
Training using standard samples	○	●	○
Expert hardware/software Installation	●	●	○
Scientific Support			
Protocol development	●	●	●
Confirmation measurements	○	○	○
On-Going Consulting Support	○	○	○
IGC Starter Kit			
Required starter accessories	●	●	●

● included ○ optional *: Full Digital Communication **: ask for compatibility

Scalable Options

Items	Applications
Relative humidity generator	Measurements under controlled background humidity conditions
Flat surface device	Analysis of plates, sheets and films
TCD detector	Plug-and-Play swap for FID Detector when using water as a probe molecule
Miscellaneous specialty detectors	For specific applications
Secondary oven	Increase your productivity with a pre-conditioning elevated temp oven
Cryogenic options	Minimum temperature: -100 °C with liquid N_2 ; -50 °C with liquid CO_2
ZLC capabilities	Determination of diffusion coefficients via Zero Length Column Option Kit
Injection loops	Analysis using gaseous molecular probes (Ethane, Propane, CO_2, ect.)
PAL heating module	Analysis using low vapour pressure molecular probes
HSPIP software	Hansen Solubility Parameter and related computations

Adscientis' fully-automated IGC Solution: the world's most advanced IGC technology & software

FRONTAL

Some µL of liquid
up to 10^6 nmoles
Injection speed : down to 0.042 µL/s

FAST PULSE

Typically diluted vapour
Down to 1 nmole
Injection speed : up to 100 µL/s

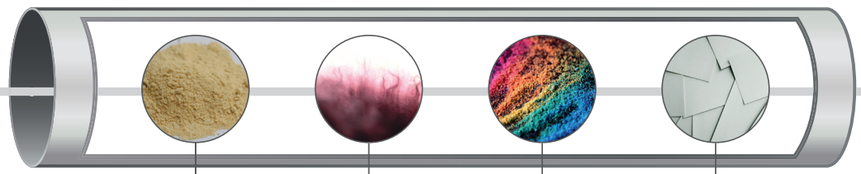
TWO INJECTION MODES

Up to 45 available molecular probes

- N-akanes (C_1 to C_{14})
- Branched alkanes (C_4 to C_8)
- Cyclic alkanes
- Alkenes and alcynes
- Aromatics
- Organic solvants (all kind of chemical functions)
- Water
- PDMS oligomers
- ...

YOUR SAMPLE

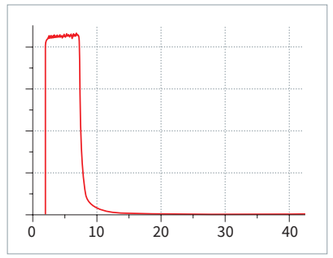
Column length: 0 – 1m or more



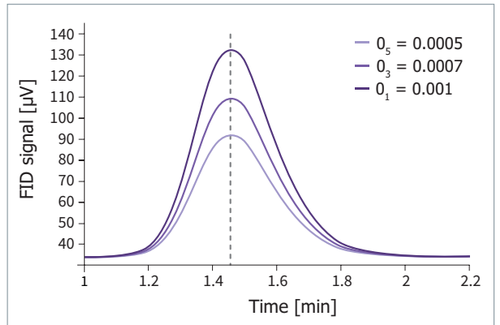
Powders	Fibers	Liquid films	Flat surfaces
(<1- 2000 µm) - Organic - Inorganic - Modified - unmodified	(no size limits) - Organic - Inorganic - Modified - unmodified	deposited on suport - Organic - Inorganic	(Sheets) - Plates - Films - Special device

FINITE CONCENTRATION CONDITIONS (IGC-FC)

- Sorption/Desorption Isotherms
- Specific Surface Area (BET)
- Surface Heterogeneity (AEDF)
- ZLC (diffusion coefficient)



Adsorption Energy [kJ/mol]



Measure Retention times using up to 45 well-defined/ targeted molecular probes

INFINITE DILUTION (IGC-ID)

- Dispersive Surface Energy
- Polar Surface Energy
- Surface Polarity (ISP)
- Surface Acidity/Basicity (Ka, Kb)
- Nanoroughness (IM, RIM) Index
- Diffusion Coefficient
- Hansen Solubility Parameters
- ΔGa, ΔHa, ΔSa

neuronIC

Based on 20 years utilizing IGC for practical

Introduced in 2017

Application-driven analysis software

Compatible with multiple GC and Auto-Sampler platforms

- Ambiant +3°C-450°C temperature range
- Dead Volume minimized via variable length SS or glass columns
- High throughput: 2 columns + 2 parallel channel injections
- Interchangeable FID and TCD detectors for each channel

Fast and accurate surface energy determination

NeuronIC is able to run two samples simultaneously. Hence, the determination of the dispersive component of the surface energy becomes easy and very fast. As an example, the measurement, at 25°C of γ_s^d on two lactose monohydrate samples requires only 1200 seconds, i.e. 20 minutes (Fig. 1) to analyze two samples (packed in two columns) simultaneously, thus doubling the productivity of a single channel IGC.

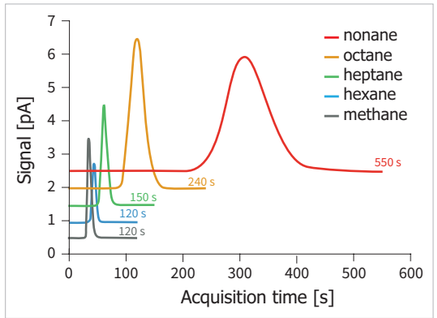


Fig 1

Results

- Nice gaussian symetric peaks are obtained
- The application of the Dorris and Gray method leads to two almost superimposed n-alkane straight lines.

Sample	Slope [kJ/mol]	γ_s^d [mJ/m²]	r²
Column A	3.021 ± 0.044	49.5 ± 1.5	0.9996
Column B	3.027 ± 0.016	49.7 ± 0.5	0.9999

Their slopes are very close and their correlation coefficients are close to 1.0000
The measured surface energy values are reproducible. Indeed on both columns, the measured γ_s^d values are respectively of 49.5 and 49.7 mJ/m².

Nanoroughness: a unique input

Surface energy is analogous to a symptom. It is important to detect it, but it is also more interesting to get insights into where it originated. The injection of branched and cyclic n-alkanes delivers such information and helps to determine if your surface is hard and nanorough, soft with some molecular mobility or a mix of both. In this example (Fig. 2), we applied the nanoroughness concept to the same API stored 1 and 6 months under different conditions (-20°C, RT and 40°C at 75%RH).

Results

- Intial state shows that the surface is partly soft. This explains why the surface energy value is low (38 mJ/m²).
- Storage at -20°C doesn't change anything.
- Storage at RT likewise has little effect after one month.
- Storage after 6 months at RT increases the γ_s^d value to 45 mJ/m² and reduces the molecular mobilty (shift to the blue domain).
- Storage at 40°C and 75% RH leads to the same effect after 1 month and remains stable after 6 months.

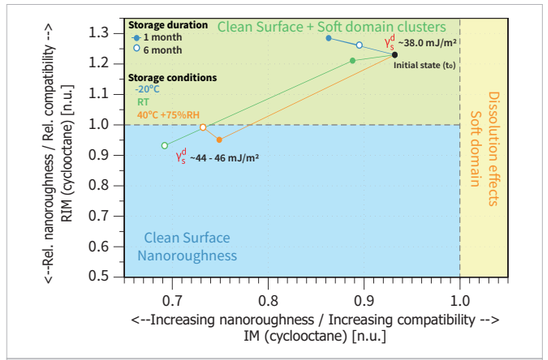


Fig 2

HSP determinations

The Hansen Solubility Parameters is a widely used method when developing new formulas of inks, paints, adhesives, cosmetics or pharmaceuticals. More than 20 solvents can be tested within a day (repeatability tests included) providing a complete covering of the HSP domain and an accurate determination of the three HSP components: δ_d, δ_p and δ_H.

Fig. 3 illustrates what is obtained when coupling neuronIC and HSPiP HSP data treatment software on a oily compound.

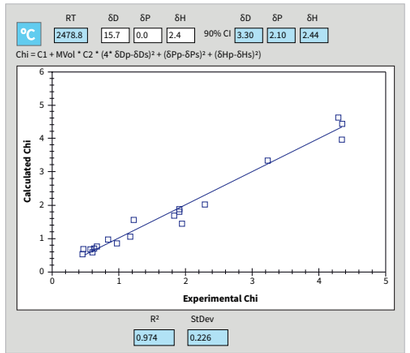


Fig 3

Hydrophilic surface area

Water is certainly the best molecular probe to assess surface hydrophilic character. neuronIC's proprietary IGC-FC method is able to use water (injected as a liquid) as a probe of hydrophilicity to deliver : desorption isotherms and a specific surface area value for the hydrophilic surface (S_{BET}) . This is shown here (Fig. 4) for two batches of the same API.

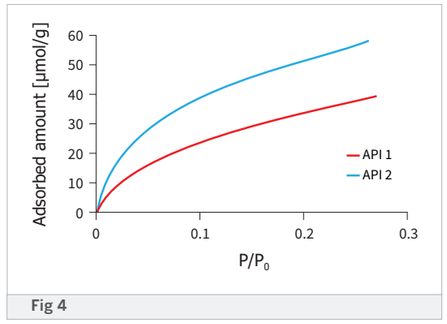


Fig 4

Sample	Q_0 [µmol/g] Q_0 is the monolayer capacity	S_{BET} [m²/g]	C_{BET} [n.u.]
API 1	25.1 ± 1.3	1.8 ± 0.1	19.8 ± 2.4
API 2	38.5 ± 3.4	2.8 ± 0.2	24.2 ± 1.7

- Recording of a water chomatogram is carried out within 1 hour
- The resulting isotherms are covering a P/P_0 range between 0 and 0.3
- These isotherms easily distinguish API 1 from API 2 API 2 is significantly more hydrophilic (2.8 m²/g) than API 1 (1.8 m²/g)

Surface heterogeneity

The IGC-FC chromatograms and isotherms are also used to compute Adsorption Energy Distribution Functions (AEDF) that describe the surface heterogeneity. This is illustrated on Fig. 5 keeping the same two API batches and water as molecular probe.

- Two components are dispayed on the water AEDF of API 1 and API 2.
  - A low adsorption energy (~ 20 kJ/mol)
  - A higher adsorption energy one (~25 kJ/mol)
- The high energy component is better defined for API 2. API 2 is more heterogeneous.

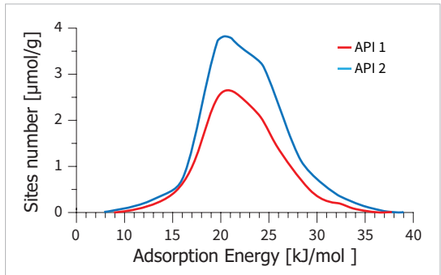


Fig 5

Diffusion coefficient: ZLC

Diffusion coefficients using a carefully selected molecular probe injected into a porous material (singular) are determined thanks to the Zero Length Column (ZLC) method. The filled column is by an union contain a small piece (~10 mg) of the material to investigate. In this example Fig. 6, the diffusion of toluene at 200°C in two zeolite samples is assessed.

D/R^2 (x 10^4) [s^{-1}]	Black	White
Toluene	3.73 ± 0.12	3.45 ± 0.02
Benzene	3.97 ± 0.21	3.39 ± 0.07
Methanol	2.48 ± 0.05	3.16 ± 0.12

The results are delivered in the form of a ratio (D/R^2) where R is the radius of the particle and D the diffusion coefficient. Concerning the D/R^2 ratios, the obtained values are higher for toluene and benzene on the black zeolite. For methanol the D/R^2 ratio is higher on the white zeolite. This suggests that the relative diffusion behaviour is different for the white and black zeolite depending on the type of molecular probe used.

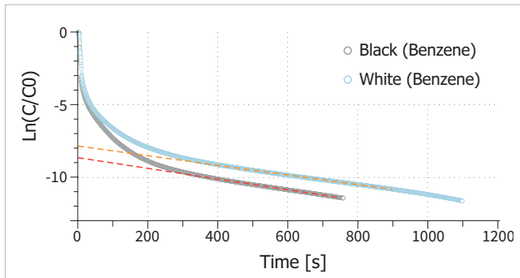


Fig 6

The behaviour of powders, fibres, plates, films and liquids in application are directly related to their interaction ability. Therefore, it is so important to measure it. NeuronIC is a unique solution to do it.

Measured properties

- Thermodynamic adsorption energies and entropy (ΔGa, ΔHa and ΔSa)
- Polar contribution to the adsorption energy (ΔGa^{sp}=ISP and ΔHa^{sp})
- Nanoroughness and soft matter detection (amorphous) and assessment
- Surface energy
- Acid-base character (Gutmann concept)
- Desorption isotherms and irreversible adsorbed probe amounts
- Specific surface area determination using any molecular probe including water
- Surface heterogeneity tuning thanks to Adsorption Energy Distribution Functions (AEDF)
- Hansen Solubility Parameter
- Probe's diffusion coefficient
- Tg and transition points

Featured capabilities

- Provide a direct measurement of the interaction ability of the samples at the molecular level.
- IGC is a unique technique that delivers numerous physicochemical parameters.
- Is molecular level sensitive.
- Varying and multiplying the molecular probe's structure and chemical functions leads to a fine characterization of several aspects involved in your sample interaction ability.

NeuronIC Solution Advantages

- Modular solution Based on reliable and renowned brand Instruments
- Configured to match your exact needs
- Evolutive to match your future expectation
- Automatized and easy to manage
- Simultaneous measurement of two samples
- Inject Up to 45 Probe Molecules via compatible PAL AutoSampler controlled by NUCLEUS

Adscientis added values

- Over 20 years of IGC expertise at your service and over 400 IGC measurements per year
- Specific measurement protocol development
- Free software up-dates
- Scientific support

The Adscientis team is always available to provide technical support for your instrument, and scientifiic expertise to assist with your most challenging applications.

References

NeuronIC

BASF The Chemical Company · SOLVAY asking more from chemistry® · KU LEUVEN

Services

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