



The Total Sorption Solution



The Surface Energy Solution

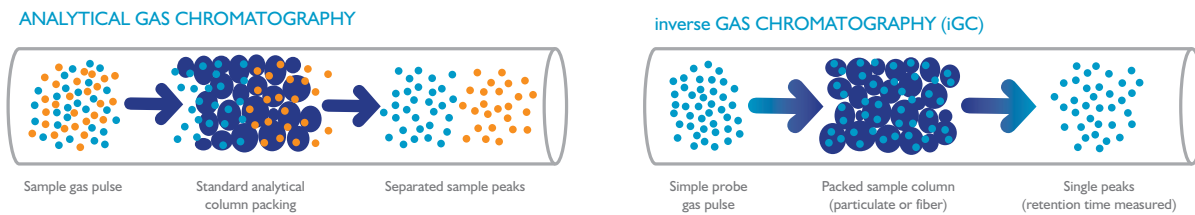
[www.TheSorptionSolution.com](http://www.TheSorptionSolution.com)



The iGC Surface Energy Analyzer continues SMS's pioneering history with inverse gas chromatography, which now spans more than fifteen years.

## iGC - inverse Gas Chromatography - the founding principle

iGC is a gas-phase technique for characterizing surface and bulk properties of powders, particulates, fibers, films and semi-solids. An experiment consists of a series of vapor pulses or frontal injections eluting through a column packed with the sample under examination.



The vapor's retention time is measured by a Flame Ionization Detector (FID). Varying the vapor probe molecule, flow rate, temperature, or column conditions elucidates a wide range of surface and bulk properties of the sample.

### SEA - the next generation

The Surface Energy Analyzer (SEA) represents a huge advance in iGC technology.

The heart of the SEA's innovation is its unique injection manifold system\*, which generates solvent pulse sizes of the greatest precision and range - accurately producing isotherms at unprecedentedly high and low sample surface coverages. This allows for the accurate determination of surface energy heterogeneity distributions. \*patent pending

Unique variable injection system with a 1:4000 injection volume ratio.

- 12 solvent reservoirs:**  
Easy access drawers.  
Temperature-controlled for vapor stability.
- Flame Ionization Detector (FID):**  
Adjustable gain.
- Fully integrated design:**  
Provides easy access to the sample column oven and solvent reservoirs.
- 2-sample column design:**  
Higher throughput.
- Sample column oven:**  
20°C to 150°C  
Fully integrated.



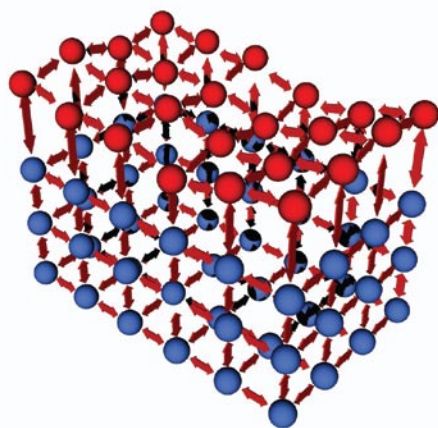
- Optional:**  
Film/monolithic sample holder.
- Optional:**  
Background humidity control.
- Optional:**  
Gas delivery manifold.
- Minimized bench requirements:**  
System Dimensions:  
W: ~490mm; H: ~650mm;  
D: ~564mm  
System Weight: 80kg
- Front panel LEDs:**  
Provides at-a-glance information including data saving, FID ignition, system status and leak detection.

# Surface Energy

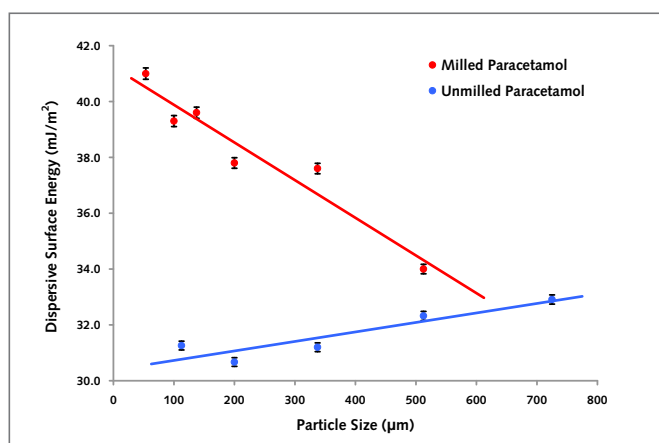
Surface energy  $\gamma$ , is the principle characteristic measured by the iGC SEA. For a solid to exist, it must be energetically favorable (of lower energy) for its molecules to form bonds with each other. It follows that the molecules at the solid's surface are in a less favorable state (ie; of higher energy), as they are not surrounded by other bulk molecules.

The surface energy of a solid is analogous to the surface tension of a liquid and quantifies the excess energy at the sample's surface relative to its bulk. If a solid sample has a high  $\gamma$  value, its surface molecules are in a high-energy state and it is energetically favorable for them to form intermolecular bonds.

Molecules at the surface are in a higher-energy state as they form fewer bonds with molecules in the bulk. These surface molecules have regions of different energy levels, giving rise to surface energy heterogeneity.



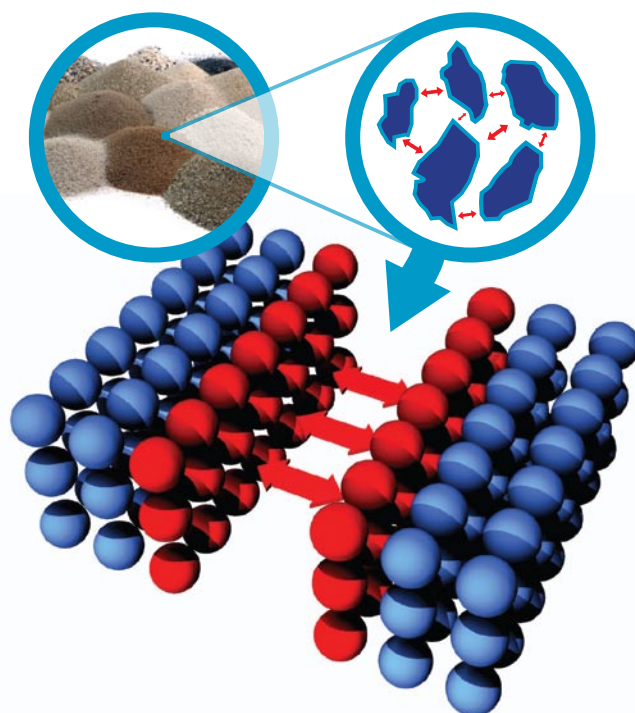
Molecules in the bulk bond with each other in three dimensions and are energetically more stable.



It is these intermolecular forces which are responsible for the attraction between powder particles and other solid surfaces. Thus, surface energy values (dispersive and polar) correlate to several key solids properties including powder flowability, agglomeration, process-induced disorder, adhesion, static charge and surface chemistry.

The SEA simulates the interface between a solid surface and other molecules by exposing the solid sample to vapor probes of known properties. The intermolecular forces that result from this interaction can be analyzed to quantify the total surface energy of the sample.

Intermolecular forces between the surfaces of powder granules contribute greatly to the powder's physical properties.



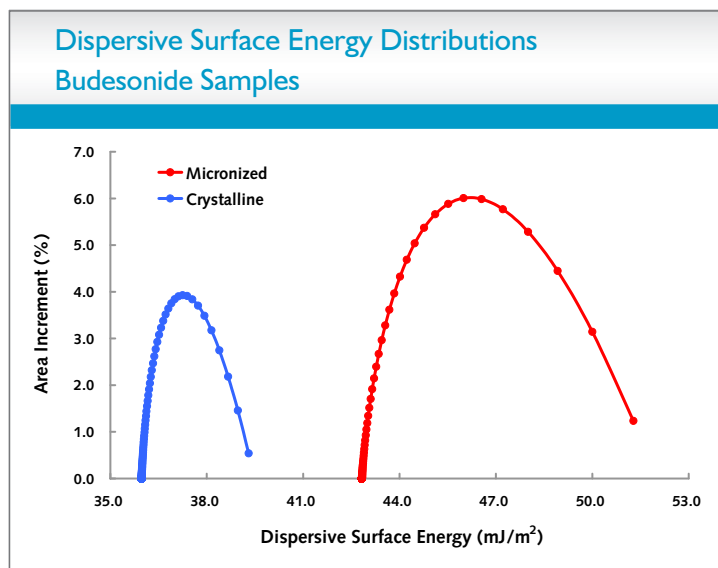
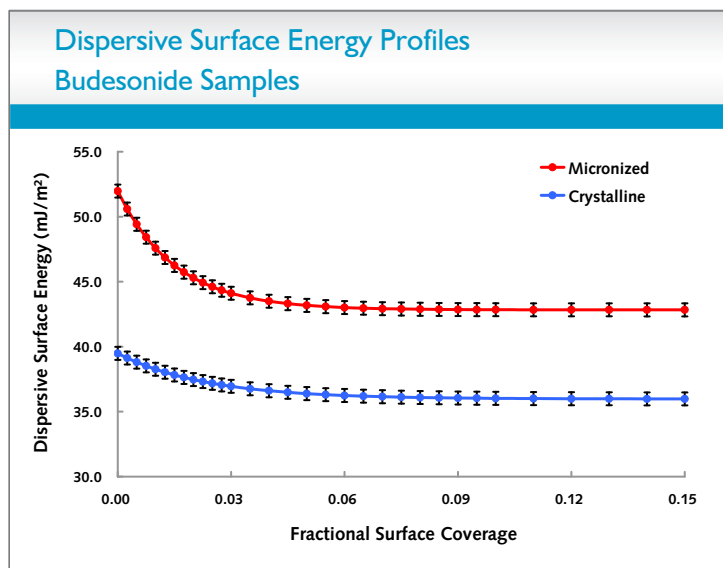
Dispersive surface energy values for milled and unmilled paracetamol vs. particle size. The data shows a strong dependence of surface energy on particle size for the milled sample. Unmilled paracetamol shows a much weaker correlation.

# Heterogeneity Mapping



Most materials are energetically anisotropic ie; they have regions of different surface energy. Therefore it is important to characterize the entire sample surface and not simply calculate average  $\gamma$  values, as liquid-based techniques do.

The SEA is the only commercial iGC system that provides detailed dispersive and polar (acid-base) component energetic heterogeneity analysis, with the ability to produce 'mapping' graphs, as shown below:



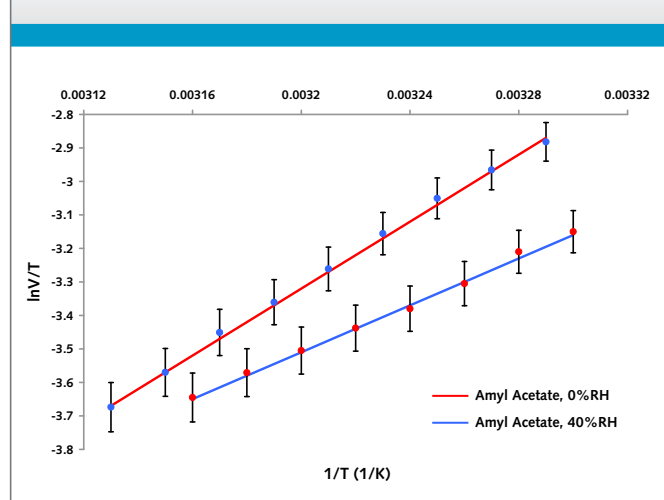
Surface energy heterogeneity profiles (left) and distributions (right) for micronized and crystalline budesonide powders. Micronized samples show broader surface energy distributions and higher average surface energies.

## Additional Surface Properties measured by the iGC SEA

Work of adhesion and work of cohesion values for different nanofiller-polyurethane composites correlate directly with composite mechanical strength.

Sample	$W_{ad} / W_{coh}$	Tensile Strength at Break (MPa)
Polyurethane Alone	----	$61 \pm 4$
As Received Multi-walled Nanotube	0.55	$60 \pm 7$
Oxidized Multi-walled Nanotube	0.49	$56 \pm 6$
As Received Nanoclay	0.47	$54 \pm 11$
Functionalized Nanoclay	0.86	$71 \pm 7$

Heats of sorption ( $\Delta H$ ) plots for Amyl Acetate on cotton fabric at 0%RH ( $\Delta H = 56.54\text{kJ/Mol}$ ) and 40%RH ( $\Delta H = 50.20\text{kJ/Mol}$ ). Background humidity has a larger effect on  $\Delta H$  for hydrophilic probe molecules.

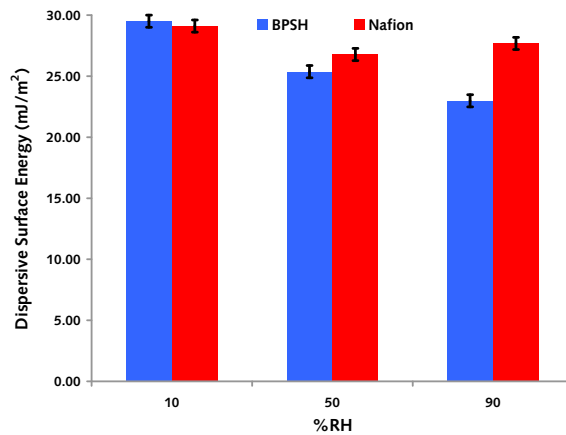




Gutmann acid ( $K_a$ ) and base ( $K_b$ ) values for different polymers along with their relative ranking on the triboelectric series.

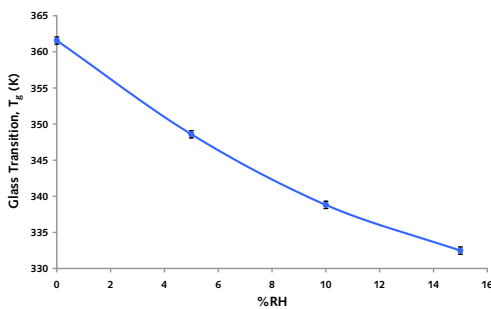
Triboelectric Series Order	$K_b / K_a$
Polymethyl methacrylate	1.33
Polycarbonate	1.10
Acrylonitrile	1.09
Butadiene Styrene	
Polypropylene	0.63
Polyvinylchloride	0.02

Competitive sorption: Dispersive surface energy values for different proton exchange membranes as a function of background relative humidity conditions.

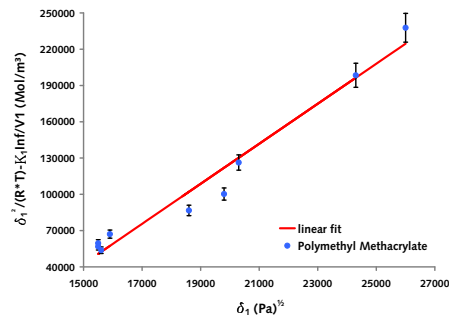


## Bulk Properties measured by the iGC SEA using optional Analysis Software Modules

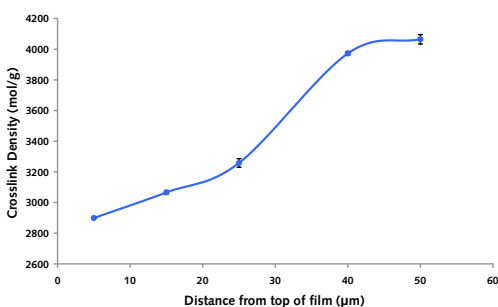
Glass transition temperatures for maltose as a function of relative humidity. The plasticizing effect of water vapor is clearly observed by the drop in  $T_g$ .



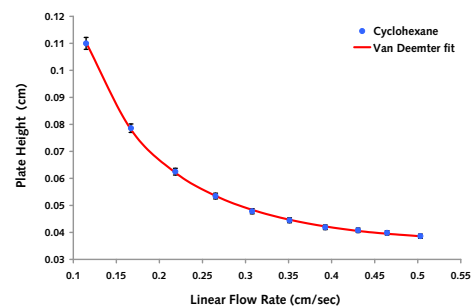
Hildebrandt solubility parameter for polymethyl methacrylate. Value of 19.08  $\text{MPa}^{1/2}$  agrees with literature values (17.4-21.3  $\text{MPa}^{1/2}$ ).



Degree of crosslinking as a function of film depth for a UV-cured automobile top coat. Crosslinking decreases at the surface as oxygen inhibits curing.



Van Deemter Plot: Diffusion coefficient (0.0034  $\text{cm}^2/\text{sec}$ ) for cyclohexane on a catalyst sample at 250°C.





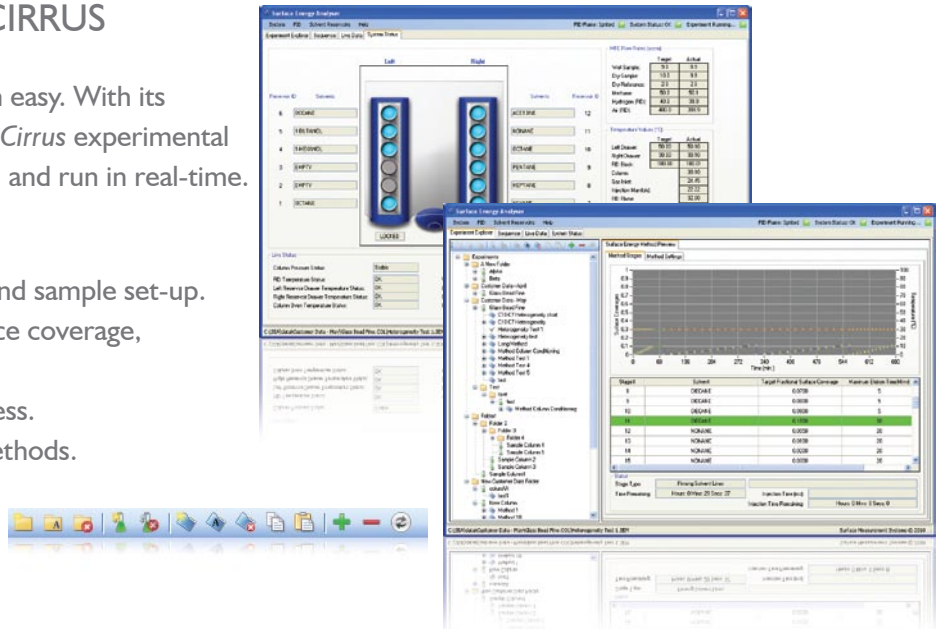
SMS continues to be the world leader in stable, flexible and intuitive system software. Designed entirely in-house with extensive customer participation and feedback, SMS software provides stable, flexible and easy-to-use sorption solutions.

## SEA Control Software: CIRRUS

*Cirrus* makes experimental sophistication easy. With its intuitive, windows-based user interface, *Cirrus* experimental methods can be flexibly designed, edited and run in real-time.

### Special features include:

- Intelligent, wizard-based experiment and sample set-up.
- Wide range of Method variables: surface coverage, solvents, temperatures and flow rates.
- Real-time display of experiment progress.
- Easy set-up, saving and restoring of Methods.
- Batch running of up to 10 Methods.
- Advanced system status diagnostics.



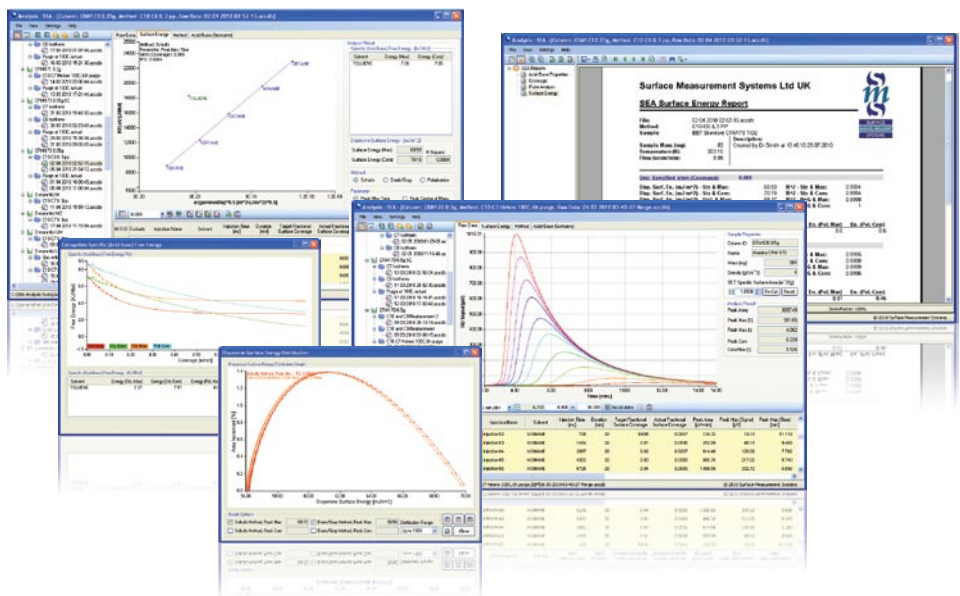
## SEA Data Analysis Software: CIRRUS PLUS

*Cirrus Plus* harnesses the experimental flexibility of the iGC SEA. Delivering extensive and user-friendly data analysis alongside one-click report generation, *Cirrus Plus* helps you make the most of your iGC data.

**Optional Bulk Analysis...** The SEA's capabilities can be extended even further by adding extra analysis modules for the calculation of bulk properties such as solubility parameters, diffusion coefficients and  $T_g$ .

### Standard features:

- Isotherm determination/BET/ Henry Constant.
- Surface Energy analysis.
- Surface Heterogeneity mapping.
- Work of Adhesion/ Cohesion determination.
- Competitive sorption measurement.
- Heats of Adsorption/ Sorption measurement.
- Acid-Base Chemistry analysis.



Head Office [smsinfo@smsuk.co.uk](mailto:smsinfo@smsuk.co.uk) • [www.TheSorptionSolution.com](http://www.TheSorptionSolution.com)