Quantachrome INSTRUMENTS
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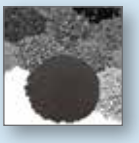
VersaWin™

Gas Sorption Data Reduction Software

Gas Sorption Software



VersaWin™ is a new stand-alone data reduction package that can open existing Quantachrome physisorption file types and import physisorption isotherm data from a user-generated "comma separated values" (csv) file containing data which could have originated from the literature, a competitor's instrument data set, or from a home built adsorption apparatus. VersaWin also imports "absolute adsorbed amount" isotherm data files generated by the specialized software (iSorbHP Suite) used with the iSorb-HP instruments. VersaWin does not communicate with any instrument; it opens or imports pre-existing data files from a location(s) specified by the user. VersaWin is only included with iSorbHP and VStar instruments or can be purchased separately. The basic VersaWin package comes with the software and manual on CD and a protection device (dongle). Additional licenses (dongles) can be purchased for use on multiple computers simultaneously.

Compatibility:

PC Operating System: Windows XP or newer (32 or 64bit).

OVERVIEW

VersaWin was developed to provide non-Quantachrome instrument users (third-party or home built instruments, even published literature) access to our comprehensive data reduction and reporting software, and to extend the data reduction capabilities to iSorb and VStar users.

VersaWin will appeal to sophisticated users that want a data reduction software that has the ability to:

A) Analyze data without having to utilize a physical instrument
B) Compare data between different instrument platforms
C) Compare data from different manufacturers

There are several reasons why a stand alone data reduction package might be of interest:

1. Sometimes research involves collaboration between many different researchers, often located in multiple geographic locations. Each of these researchers might have different instrument platforms, or might not have instrumentation at all.

2. A researcher active in these areas might want the ability to do data reduction analysis independent from a physical instrument. They might be working remotely, or might not have access to their instrumentation for a variety of reasons.

3. A researcher might want to utilize data taken from several different instruments, or from historical information that they previously tested. This software allows researchers to have one software package that can import data feeds from any instrument platform as long as they are in .csv format.

4. A researcher might want to be able to utilize some of the superior data reduction capabilities within the Quantachrome software unique to Quantachrome.

FEATURES

Non-native or obsolete file formats can be read via the "import" function; these are:

*.csv = comma separated value format isotherm data regardless of column order

*.txt = iSorbHP absolute adsorbed amount data document, and VStar data files

*.raw = older Autosorb instruments

*.drf = older Autosorb instruments supplemented data file (P, P_O, time)

*.dat = old NOVA instruments, Hydrosorb

*.qnv = older NOVA software (vintage between .dat and .qps)

VersaWin reads the following current standard Quantachrome file formats:

*.qps = physisorption data document
(i.e.Autosorb-iQ, Autosorb-6iSA and newer models of NOVA, Quadrasorb, AquaWin)

*.qpScan = scanmode data document (i.e. isotherm hysteresis scanning data file from iQ)

*.qcSuperCritical = supercritical gas sorption document (i.e. data file saved from within VersaWin)

*.qkn = gas sorption kinetics document (i.e. sorption kinetics data file from iQ)

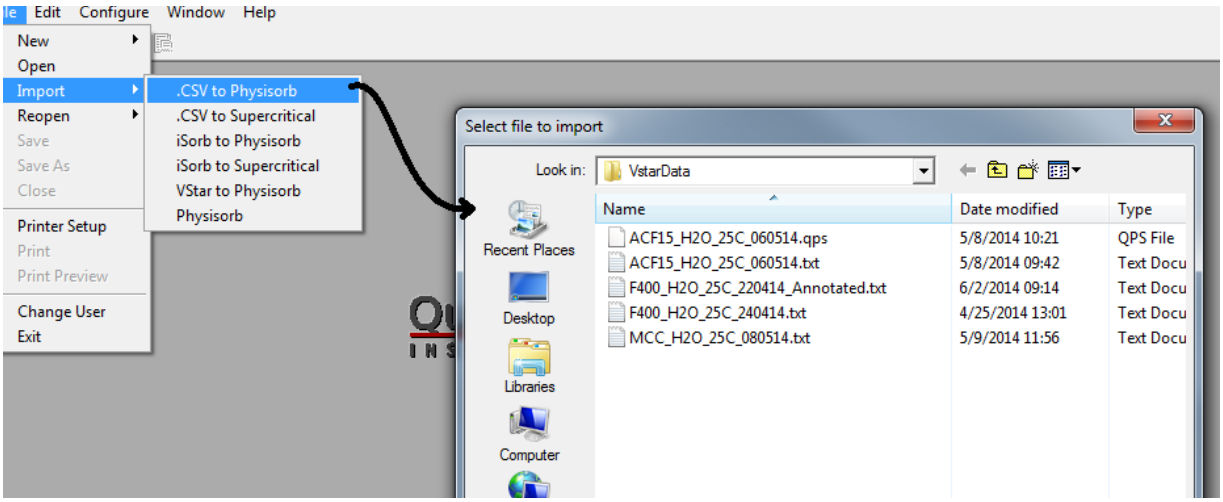
*.ovp = physisorption overlay document (i.e. overlay file from iQWin, QuadraWin and NovaWin)

*.hoa = heats of adsorption document (i.e. physisorption HOA file from iQWin, QuadraWin and NovaWin)

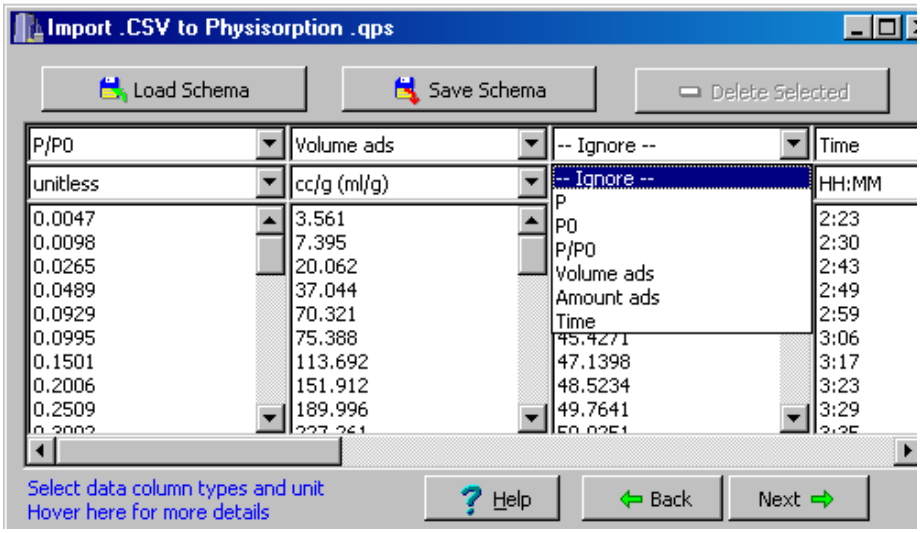
Contains all current data reduction methods, models, and reporting features found in iQWin software (but no new calculations).

FEATURE DETAILS:

Import csv data: If original data were already in csv format the file can be imported directly. Otherwise data can be typed into a text editor with commas separating data columns in each line and saved with csv extension. Alternatively an excel spreadsheet of tabular data can be saved as csv file before importing. VersaWin displays the imported file first in the data selection window in which the user identifies (by highlighting them) which rows contain data to be extracted:

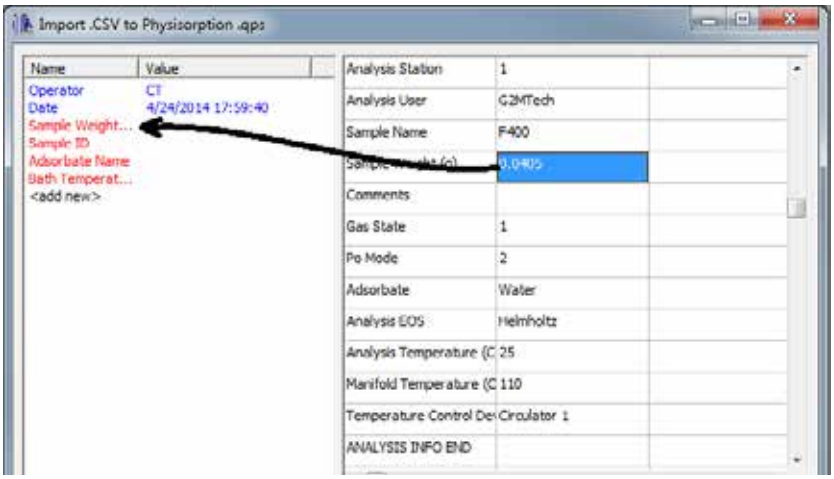


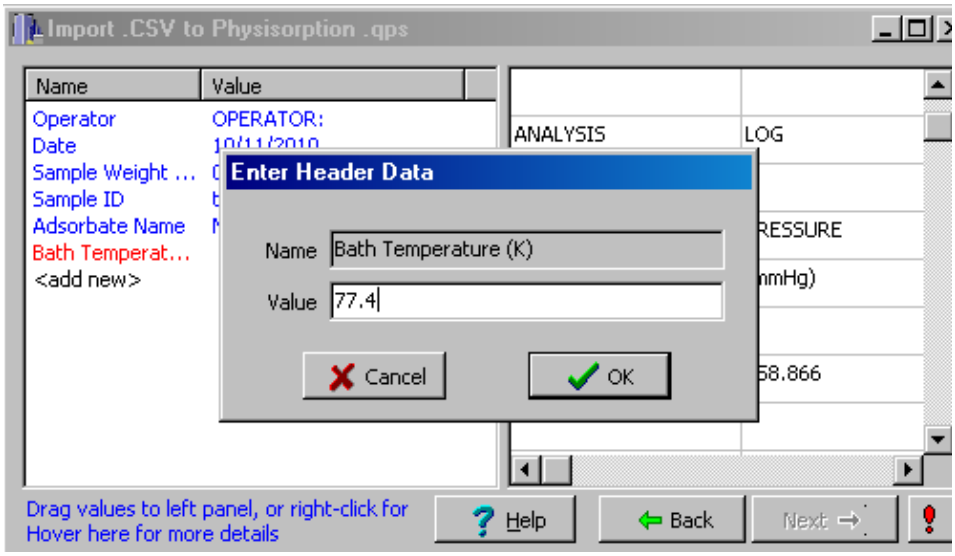
VersaWin sorts the rows into columns and the user identifies what each column of values represents, and its measurement units, using the drop down lists above each column (see figure below). These column identifiers can be saved as a "Schema" to be used in the future on a file whose formatting is the same, significantly streamlining the importation of data.



FEATURE DETAILS:

Next, the user provides the required header information either by dragging the values from the representation of the data as extracted from the original file or by entering directly in the left side panel.





Custom header fields can be added by clicking on <add new>.

VersaWin DATA REPORTING CAPABILITIES

NLDFT-Methods

- N_2 at 77K on carbon (slit pore, equilibrium model)
- N_2 at 77K on carbon (cylindrical pore, equilibrium model)
- N_2 at 77K on carbon (slit & cylindrical pores, equilibrium model)
- Ar at 77K on carbon (slit pore, equilibrium model)
- Ar at 87K on carbon (slit pore, equilibrium model)
- Ar at 87K on carbon (cylindrical pore, equilibrium model)
- CO_2 at 273K on carbon (slit pore, equilibrium model)
- N_2 at 77K on silica (cylindrical pore, equilibrium model)
- N_2 at 77K on silica (cylindrical pore, adsorption branch model)
- N_2 at 77K on silica (cylindrical and spherical pores, adsorption branch model)
- Ar at 87K on zeolites/silica (spherical/cylindrical pore equilibrium model)
- Ar at 87K on zeolites/silica (spherical/cylindrical pore adsorption branch model)
- Ar at 87K on zeolites/silica (cylindrical pore, equilibrium model)
- Ar at 87K on zeolites/silica (cylindrical pore, adsorption branch model)

GCMC-Methods

- CO_2- carbon at 273K based on a slit-pore model

Fractal Dimension

- Neimark-Kiselev (NK), Frenkel-Halsey-Hill (FHH)

QSDFT

- QSDFT – N_2 – carbon equilibrium transition kernel at 77 K based on a slit-pore model
- QSDFT – Ar – carbon equilibrium transition kernel at 87 K based on a slit-pore model
- QSDFT – N_2 – carbon adsorption branch kernel at 77 K based on a cylindrical pore model
- QSDFT, N_2, carbon equilibrium transition kernel at 77 K based on a slit-pore model (pore diameter < 2nm) and a cylindrical pore model (pore diameter > 2 nm)
- QSDFT, N_2, carbon adsorption branch kernel at 77 K based on a slitpore model (pore diameter < 2 nm) and cylindrical pore model (pore diameter > 2 nm)
- QSDFT, N_2, carbon adsorption branch kernel at 77 K based on a cylindrical pore model (pore diameter < 5 nm) and spherical pore model (pore diameter > 5 nm)
- QSDFT, N_2, carbon adsorption branch kernel at 77 K based on a slitpore model (pore diameter <2 nm) and a cylindrical pore model (pore diameter 2-5 nm) and a spherical pore model (pore diameter > 5 nm)

VersaWin CALCULATIONS

- B.E.T. surface area, multi-point (features automatic point selector for microporous solids)
- B.E.T. surface area, single point
- Langmuir surface area, multi-point
- t-plot micropore area/volume, deBoer (a.k.a. Harkins Jura)
- t-plot micropore area/volume, Halsey
- t-plot micropore area/volume, generalized Halsey
- t-plot micropore area/volume, STSA (carbon black)
- alpha-s method micropore volume (features selectable reference isotherm and adjustable normalization relative pressure value)

- MP method micropore volume/v-t surface area (features automatic starting value)
- DR (Dubinin Radushkevich) micropore area/ volume, adsorption energy, average pore width (features adjustable affinity coefficient: beta)
- DA (Dubinin Astakhov) micropore size distribution (features adjustable parameters, E, n, interaction constant)

- BJH (Barrett Joyner Halenda) pore size distribution (adsorption) with choice of statistical thickness models (see t-plot), pore volume/area
- BJH (Barrett Joyner Halenda) pore size distribution (desorption) with choice of statistical thickness models (see t-plot), pore volume/area
- DH (Dollimore Heal) pore size distribution (adsorption) with choice of statistical thickness models (see t-plot), pore volume/area
- DH (Dollimore Heal) pore size distribution (desorption) with choice of statistical thickness models (see t-plot), pore volume/area

- KTPS (Krypton Thin Film Pore Size) pore size distribution
- HK (Horvath Kawazoe) micropore size distribution
- SF (Saito Foley) micropore size distribution
- QSDT (Quenched Solid Density Functional Theory) pore size distribution.
- NLDFT (Non-Local Density Functional Theory) pore size distribution.
- MC (Monte Carlo) micropore size distribution

- Total pore volume (Gurvich type)
- Average pore size

- NK (Niemark Kiselev) Fractal Dimension (adsorption)
- NK (Niemark Kiselev) Fractal Dimension (desorption)
- FHH (Frenkel Halsey Hill) Fractal Dimension (adsorption)
- FHH (Frenkel Halsey Hill) Fractal Dimension (desorption)
- Heats of adsorption

User adjustable settings*:

- Pore size dimension: diameter or radius (thickness or half-thickness for slit shape pores)
- Pore size unit: angstrom, nm, micron (micrometer)
- Relative pressure: P/Po, RH%, Aw
- Absolute pressure: torr, kPa
- Volume: cc/g, g/g, mmoles/g, mg/g, % change

* available selection varies according to data type and calculation model.

Quantachrome
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Renowned innovator for today's porous materials community.

The quality of Quantachrome's after sales service support is the reason we are proud to maintain life time relationships with our customers.

Field Service

Our global service staff assure you that Quantachrome Instruments will continue to be the reliable engines of material characterization laboratories. We offer you the flexibility of choosing from service contracts tailored to provide you with the response time, service package, and spare parts discounts that best fit your needs.

Spare Parts

Quantachrome spare parts are certified to work with our instruments. We provide rapid response spare parts orders, and keep large inventories of replacement parts and hardware available.

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Our fully equipped, state-of-the-art powder characterization laboratory, email: application.qt@anton-paar.com, provides the option of contracting for expert testing services. Laboratory services are also available to validate the applicability of our products prior to your purchase using your actual samples.

Lifetime Application Support

We view the field support of our instruments as an essential component of our business strategy. Our expert scientists are always available to answer questions on applications, or the use of our instruments. We do this as a standard service regardless of whether you have a service contract with us or not.

Partners in Science

Quantachrome has a scientific research department consisting of world renowned experts in material characterization. Our staff, led by Dr. Matthias Thommes, conducts collaborative research projects with leading material research labs around the world. They regularly publish articles in leading peer reviewed journals, and speak at technical symposiums around the world.

For almost half a century Quantachrome's scientists and engineers have revolutionized measurement techniques and designed instrumentation to enable the accurate, precise, and reliable characterization of powdered and porous materials. We have an unwavering commitment to providing state of the art technology, along with superior and unparalleled customer service and support.

Our commitment to customers is to support you before, during, and after the sale throughout the lifetime of our instruments. This is a big commitment because our products are so robust and reliable that we regularly find many still in use for decades.

Corporate Headquarters-USA
Quantachrome Instruments
1900 Corporate Drive
Boynton Beach, FL 33426

www.quantachrome.com

Your Local Representative:

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