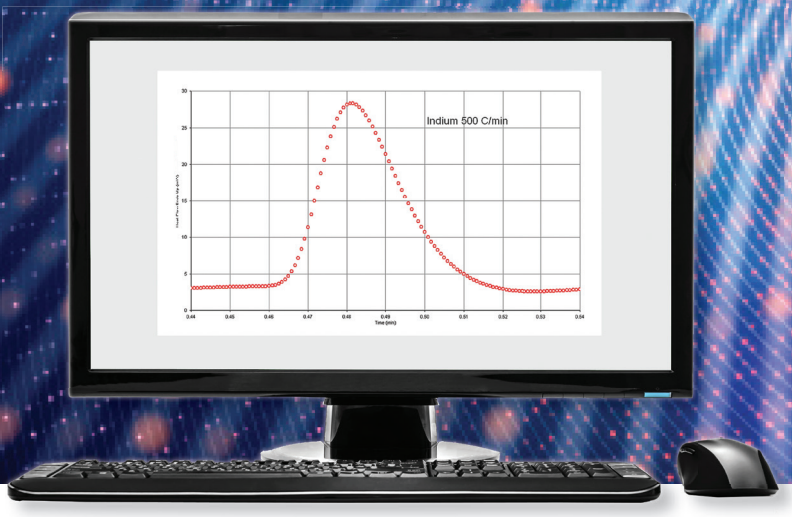
PRODUCT NOTE

Thermal Analysis



KEY FEATURES

- Minimizes risk of errors during calibration through Wizard approach
- Compares current measurement to reference curve during data collection
- Allows real-time calculation during sample run
- Provides fast method optimization during measurement
- Allows rapid document generation through Report Manager
- Technically compliant to 21 CFR Part 11 regulations
- Compatible with Windows® 10

Pyris™ Software Enabling High Sensitivity

Introduction

Your PerkinElmer thermal analysis instruments and data come to life on the Pyris™ software platform – the benchmark application for thermal analysis. Pyris is the preferred choice in thermal analysis because it is intuitive and user-friendly, and provides a wide-range of standard features and capabilities for maximum flexibility. PerkinElmer's family of highlysensitive thermal analysis instruments have been standardized on this powerful software platform. Add to this our superior customer service and support and you can be sure you are receiving a complete, robust system for accurate, reliable material characterization.

Whether you work in a research laboratory, an automated QA/QC lab, or on a stand-alone instrument, you can count on Pyris software to meet your thermal analysis needs.

Easy to Use

To ensure the highest user satisfaction, we designed and continuously enhance Pyris software based on customer feedback. A common platform for all instruments makes it easy to use and quick to learn.

Powerful

Pyris software is easy to use without losing capabilities. The software has been designed to allow you to conduct data acquisition and analysis in one window, and run multiple analyzers simultaneously. A wide range of analysis options, data import/export flexibility and customizable features are provided to meet a wide range of needs.

PerkinElmer®
For the Better

HyperDSC™ Support

Increased sensitivity at greater speeds

The fast data rates (up to 20 points per seconds) available on Pyris software make HyperDSC™ experiments routinely possible, even when scanning up to 500 °C/min. HyperDSC technology is a breakthrough method for materials characterization, providing sample information not normally obtained with traditional DSC. The technique is similar but with one exception: the HyperDSC method uses very fast controlled scanning rates, typically in the range of 200 °C/min to 500 °C/min. The greatest benefit is increased sensitivity, allowing you to run microgram samples and identify weak transitions such as the Glass transition (Tg) in low amorphous lactose material, highly filled polymers, and numerous other polymer and pharmaceutical materials. An additional advantage is improved laboratory productivity resulting from increased sample throughput by a factor of 10 or more.

The following is a quick snapshot of the extensive capabilities and standard features of Pyris software.

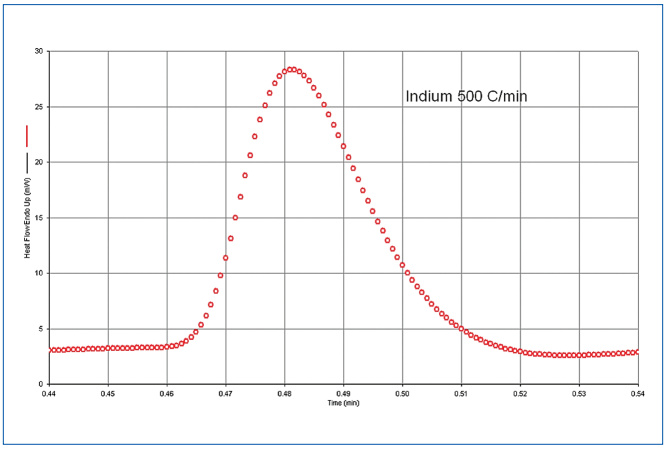


Figure 1: Pyris software makes your HyperDSC experiments possible.

Multitasking

Pyris software allows simultaneous operation of thermal analyzers from a single PC, providing productivity benefits for busy laboratories. Pyris software users can also benefit from the multitasking capability by performing data analysis, report generation and printing while running one or more measurements.

Remote Control

If you need to monitor your thermal analyzer from outside the laboratory, remote control allows you to see the instrument viewer over a network connection from another location within your facility.

Valet

The Valet feature allows creation of customized start-up and shut-down events. For example, Valet can be used to automatically condition and equilibrate your instrument prior to running experiments, or it can be used to automatically shut down the system after completion of runs. Valet runs outside of a method and can be used for any of the following tasks:

- Triggering events at a certain time of day
- Switching on/off power to instruments and accessories, such as chillers
- Triggering an external device using the X10 Relay switch

Calibration Wizard

The Calibration Wizard provides step-by-step guidance during the instrument calibration process (Figure 2). Easy to use, the Calibration Wizard assures the best procedure for instrument calibration.

Event Control using Methods Plus

This feature triggers events based on behavior of monitored signals (Figure 3). For example, this feature can be used to stop a run when an instrument signal reaches a certain threshold or it could be used to trigger an external event such as the control of a TG-MS coupling.

Fast Method Optimization

Being able to change a method during a sample run is important for laboratories that perform method development or are analyzing unknown samples. Pyris software allows you to adjust the end temperature, to add new method steps, such as an isothermal hold, extra cool or heat step while a measurement is running.

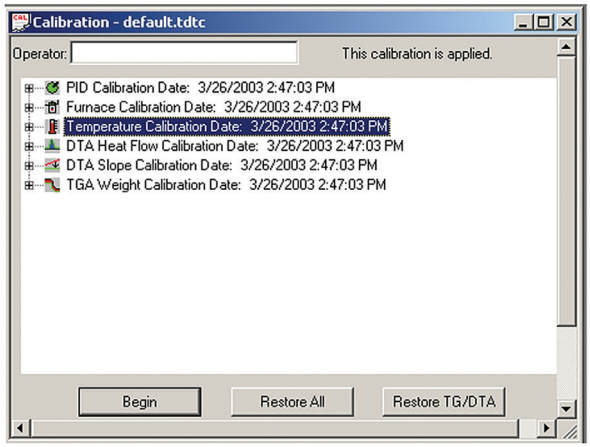


Figure 2: Calibration Wizard walks you through the calibration process.

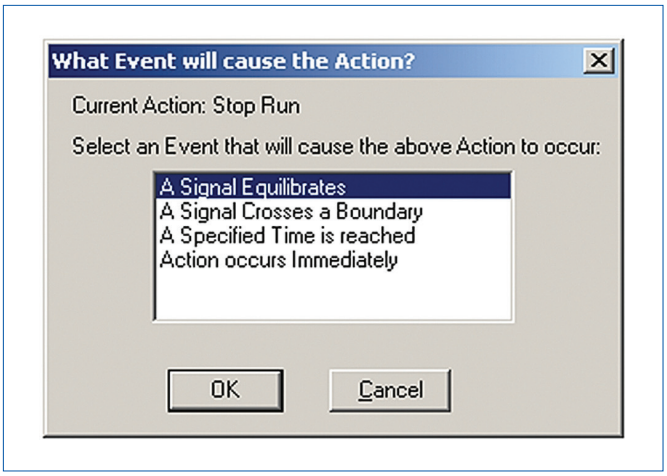


Figure 3: Methods Plus provides event control.

Pyris Player

Pyris Player, a standard feature in Pyris software, is the backbone of our automation software (Figure 4). It can group like analyses together to simplify setup, and can sequence analyses in any order you desire. This feature is of great support for all instruments under Pyris software control. Pyris Player not only controls our autosamplers for greater efficiency, but also allows automatic optimization and analysis of the data collected.

Pyris Player is of great use for laboratories that are running without an autosampler. In this mode of operation, the Play list stops after the single run and instructs the user to load the next sample. Automation of data analysis, report generation, and printing can be performed on user request. The following is a quick snapshot of the extensive capabilities and standard features of Pyris software.

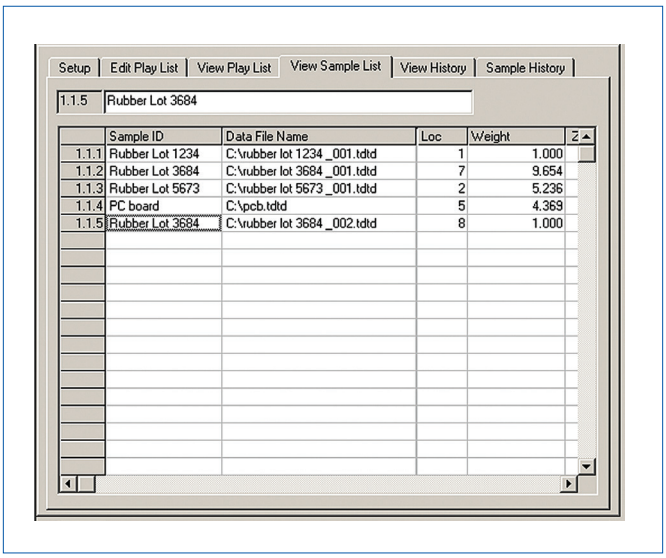


Figure 4: Pyris Player, the backbone of Pyris software.

Real-Time Reference Curve and Calculation

The real-time reference curve is ideal for a quick QA/QC analysis (Figure 5). It allows you to overlay a reference curve on a running measurement for direct comparison.

The real-time calculation allows you to perform basic data analysis on the current sample measurement.

Real-time reference curve and real-time calculation can support your efforts in increasing laboratory productivity.

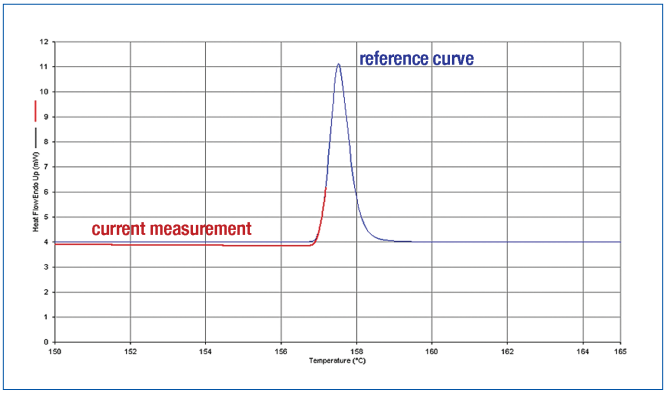


Figure 5: Real-time reference curve for quick QA/QC analysis.

Fully Integrated Data File

Pyris software allows you to see in a single data file all information from instrument calibration information and the measurement method to the raw data points and the calculated results. This feature allows you to look back at any data file and determine exactly how the experiment was performed.

Data File Import

Pyris software allows you to import any x-y data and display them in the same software platform as your thermal analysis data (Figure 6).

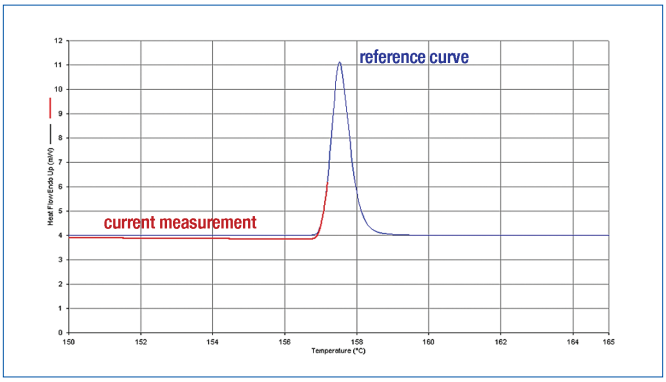


Figure 6: Data file import from an TG-MS coupling.

A Wide Range of Calculation Features

With Pyris software, you can choose to execute from a large variety of calculation options on a wide assortment of different curve types. Whether you are running a Differential Scanning Calorimeter (DSC), a Thermogravimetric Analyzer (TGA, TG/DTA , Thermomechanical Analysis (TMA), Dynamic Mechanical Analysis (DMA)) or a Mechanical instrument, data analysis is easy and reliable. (Please see specifications on Page 7 for a detailed list of calculations).

Define Result Properties

No matter what kind of thermal analysis laboratory you are part of, Pyris software has the flexibility to support your needs. The Define Result Properties feature allows you to select the best presentation of your results (Figure 7).

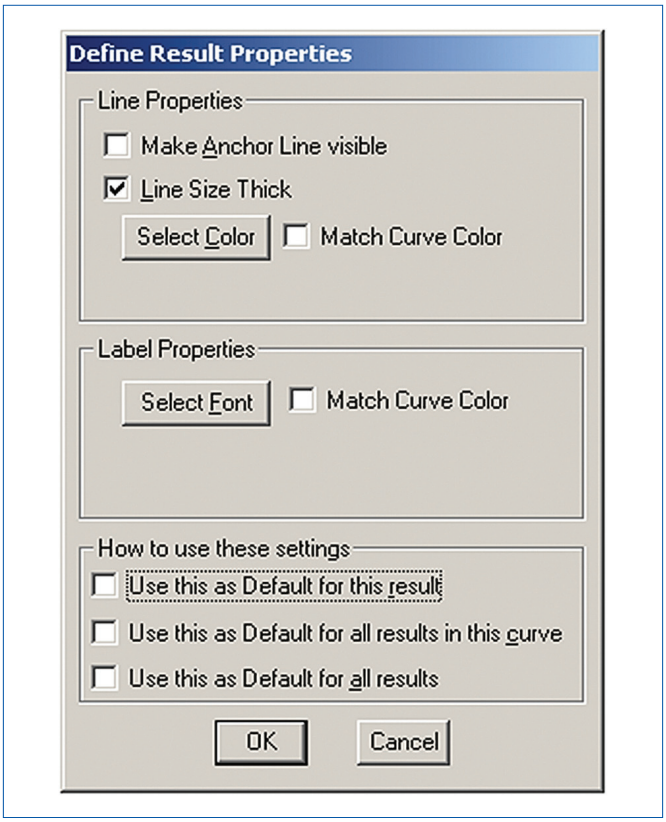


Figure 7: The Define Result Properties feature provides added flexibility.

Tolerance Test

A tolerance test can be used to determine at one glance if a material meets predefined requirements (Figure 8). Acceptability limits (pass/fail) of a thermal event can be entered. When a thermal event is not acceptable, the play list will automatically stop, pause, or continue with a notation in the history file to alert the analyst.

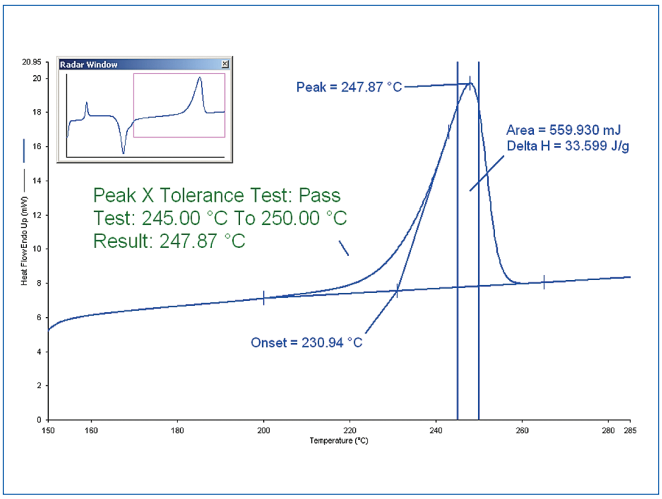


Figure 8: Tolerance test.

Post-Calculation Limit Adjustment

For added flexibility, a right mouse click option in the Data Analysis window offers easy access to data results and the possibility to conveniently change calculation limits.

Peak Area Calculation Also Available in kJ/mol

To increase the flexibility of your analysis, the peak calculation available in Pyris software provides an option to add the area result in kJ/mol.

MultiCurve

The MultiCurve™ feature allows you to save your view of several data files in a single file (Figure 9). This can include similar instrument files or an overlay of multiple thermal analysis instrument curves (such as DSC, TGA, TG/DTA or TMA). You can easily and quickly recall your MultiCurve data comparison at any time for review.

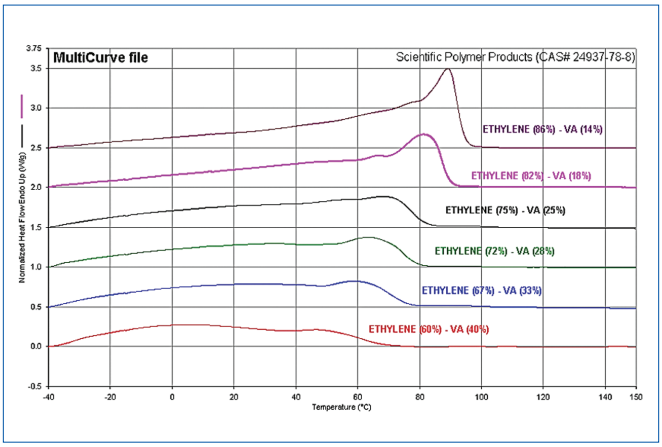


Figure 9: MultiCurve feature.

Report Manager

The Pyris Report Manager gives you the capability of exporting a Pyris data file (Figure 10) to a document in Microsoft Word® or HTML (Hypertext Markup Language) format including sample information, graphical images, results, text, data, tables, PDF formats – and more. The software provides user control of the design of the report and the information that the report contains. This report template can be re-used to conveniently facilitate the creation of new reports or to develop standard laboratory outputs.

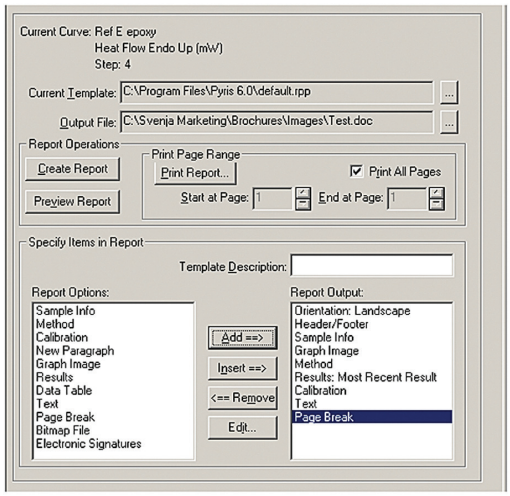


Figure 10: Report Manager.

Pyris Enhanced Security Software

In response to 21 CFR Part 11 and the increasing data security requirements in other industries, PerkinElmer's Pyris Enhanced Security™ (ES) option offers the technical compliance tools needed to meet these mandatory regulations. With Pyris Enhanced Security, the regulated industries will be confident in their ability to provide the whole story about the generation of the data. It provides all of the required 21 CFR Part 11 technical compliance features to ensure that data integrity is always maintained:

- User Level Management & Security
- File Protection
- Audit Trails
- Electronic Signature

PerkinElmer makes its higher level security functionality available to both existing and new customers. Pyris ES is fully compatible with all instruments running on the Pyris software platform. Users may be required to purchase an update of the applications software (Pyris TA Manager software Version 5.0 or above) to run the Pyris ES option.

Pyris Specific Heat (Cp) Software

When a material is subjected to a linear temperature program, the heat-flow rate into the sample is proportional to its instantaneous specific heat. Specific heat is most accurately, rapidly and easily determined with a power-compensation DSC which directly measures the heat flow as a function of temperature. Two calculation modes are available:

- 2-curve method allows you to run a baseline and sample to calculate the Cp and enthalpy change of the sample.
- 3-curve method, also included in the package, allows you to be compliant with ASTM method 1269E that requires sample, baseline and reference runs for analysis of Cp and enthalpy change of the sample.

Pyris StepScan DSC Software

StepScan DSC is a modulated temperature DSC technique that operates in conjunction with power-compensation DSC. The approach applies a series of short interval heating and isothermal hold steps to cover the temperature range of interest (Figure 11). This approach requires a DSC with very fast responsiveness to achieve short interval linear heating and isothermal steps.

Pyris StepScan DSC software for the DSC was conceived and developed to provide the ability to determine accurate specific heat capacity (Cp) under a variety of conditions. For example, moisture release by the sample or sample movement can produce changes in the baseline that produce errors in standard Cp determination. Using StepScan DSC minimizes these errors, and those caused by adverse experimental conditions. Moreover, StepScan DSC can provide information of both thermodynamic and kinetic processes of your sample. StepScan DSC is one of several techniques in the MTDSC family but is faster and easier to use than other MTDSC techniques.

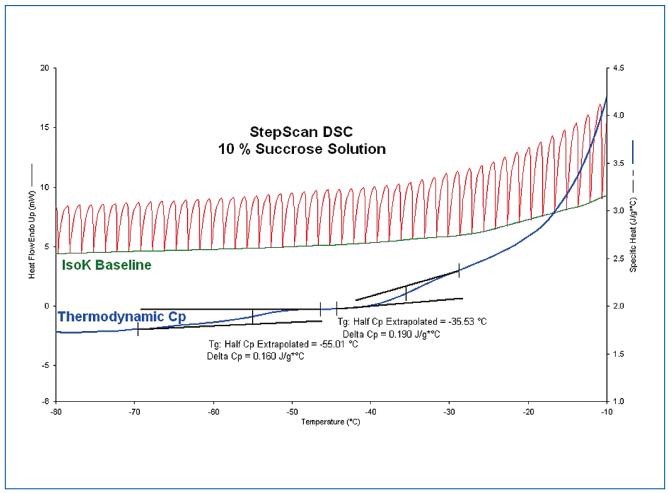


Figure 11: Pyris StepScan DSC software.

Pyris Purity Software

Pyris DSC Purity Software allows you to determine the absolute purity of an organic sample. Purity values are obtained from a single DSC scan and can even be obtained if the sample decomposes during melting. A Van't Hoff plot (Figure 12) is used to calculate the purity and other values such as the heat of fusion, the theoretical melting point of a pure sample and a correction factor for the melting part below the lower calculation limit.

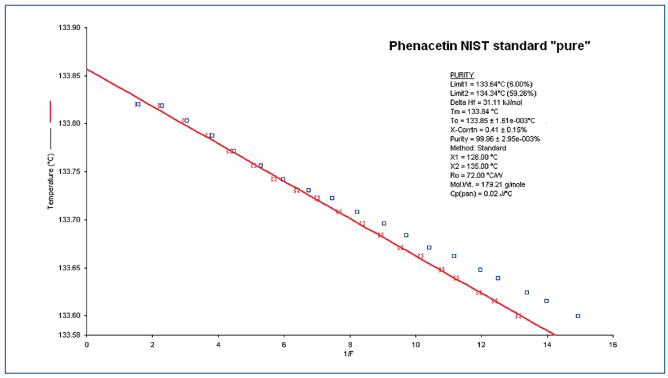


Figure 12: Purity software.

Pyris Temperature Dependent Crystallinity Software

In determining the enthalpy change for a first-order transition, you are often faced with the problem of where to draw the so-called "base-line" for a DSC peak. In polymers, crystallization usually gives rise to a semicrystalline morphology consisting of crystalline and amorphous phases. A characteristic quantity in such a two-phase morphology is the enthalpy-based mass crystallinity. This software package provides a procedure which leads to an analyst-independent determination of transition enthalpies within the two-phase model (Figure 13). Combining such transition enthalpies with data available (mainly from the ATHAS Databank) makes it possible to determine temperature dependent crystallinity on the basis of DSC curves.

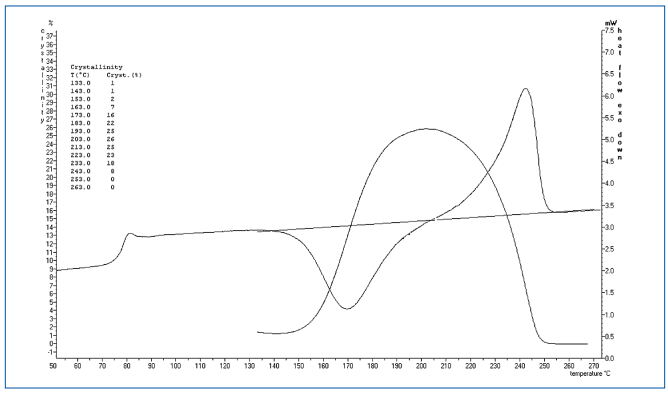


Figure 13: Temperature Dependent Crystalline software.

Pyris AutoStepwise TGA Software

Pyris AutoStepwise TGA software for the vertical bottom-loading thermogravimetric analyzer (TGA) can be used to easily and fully separate the various transitions associated with multi-component materials, such as polymer blends, elastomers and materials containing solvents. This approach is very easy to use and is flexible in terms of handling different samples and applications. With AutoStepwise TGA, the sample heats at a constant rate until a significant weight loss event is encountered. The instrument then automatically holds the sample under isothermal conditions until the rate of weight loss becomes negligible. The TGA then resumes heating until the next significant weight loss is detected (Figure 14). Pyris AutoStepwise TGA software allows the user to change the various experimental criteria to accommodatea wide range of sample types and applications.

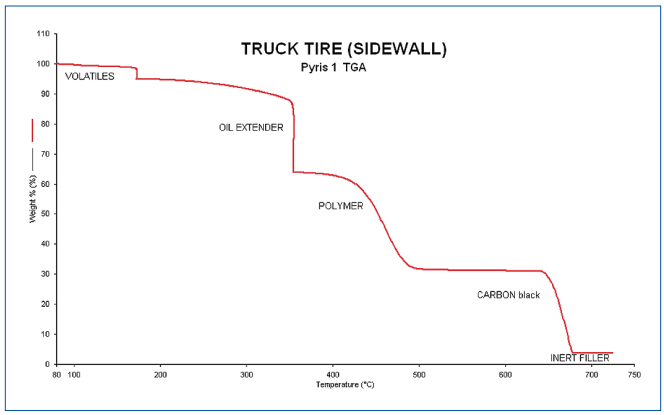


Figure 14: Pyris AutoStepwise software.

Pyris Kinetics Software

The Pyris Kinetics software package is comprised of three accessories that can be purchased in a kit or separately:

- DSC Scanning Kinetics
- DSC Isothermal Kinetics
- TGA Decomposition Kinetics

DSC Scanning Kinetics

This software uses a multilinear regression to fit a single data curve, which has been taken at constant heating rate, to the Arrhenius relationship and thereby determine the preexponential factor, activation energy and order of reaction. Various calculation inputs can be adjusted in order to make the data more meaningful. For each calculation the data fit is indicated by the confidence limits for the kinetic parameters and by the fit of the partial area data to the Arrhenius relationship (the plot of ln k vs. 1/T). If satisfactory, the parameters and four key inputs can be saved with a comment.

The reaction parameters can be used to predict the behavior of the tested material under either of two conditions – isothermal or adiabatic. With either calculation, the user can constrain one variable, such as temperature, time or percent reacted and look at a plot of the other two. Finally, a label-positioning routine allows the user to customize the screen displays and plots.

DSC Isothermal Kinetics

This software performs reaction kinetics calculations based on nth order and autocatalyzed reactions. By using the Avrami method, crystallization kinetics of a material can be evaluated. To perform the isothermal kinetics calculations, the software fits three to six data curves (Figure 15) that have been taken at a constant temperature, to the Arrhenius relationship and thereby determines the pre-exponential factor, activation energy and rder of reaction. Various calculation inputs can be adjusted in order to make the data more meaningful. For each calculation the statistical fit is indicated by the confidence limits for the kinetic parameters and by observing ln k vs. 1/T and Log – Log plots. The reaction parameters can be used to predict the behavior of the tested material under isothermal conditions. The user can constrain one variable, such as temperature, time or percent reacted, and look at a plot of the other two.

True isothermal measurements are unique to a powercompensation DSC because it holds the sample at constant temperature while other systems control only the furnace temperature, not the sample. Thus power-compensation DSC is the only system to truly and correctly measure isothermal kinetics.

TGA Decomposition Kinetics

This software uses the Flynn and Wall method or a multi-linear regression (MLR) method to fit three to six data curves that have been taken at constant heating rates, to the Arrhenius relationship and thereby determine the pre-exponential factor, activation energy and order of reaction. Various calculation inputs can be adjusted in order to make the data more meaningful. For each calculation the statistical fit is indicated by the confidence limits for the kinetic parameters and by observing the plot of ln Beta vs. 1/T. The reaction parameters can be used to predict the behavior of the tested material under isothermal conditions. The user can constrain one variable, such s temperature, time or percent reacted and look at a plot of the other two.

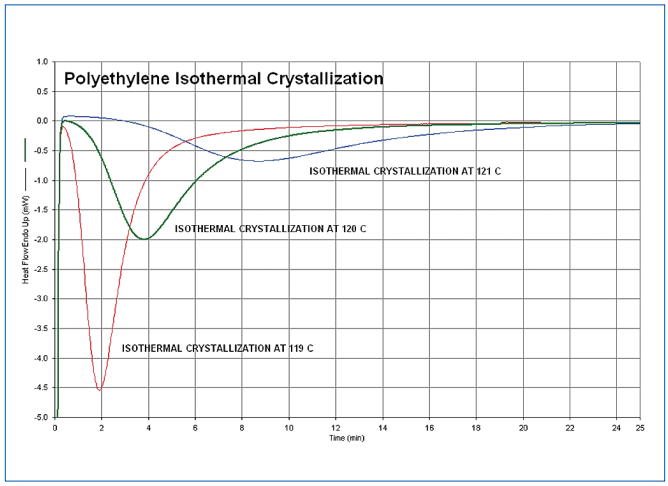


Figure 15: DSC Isothermal Kinetics.

Table 1: Specifications.

Standard			
Curve Types	Heat flow	Probe position	Phase angle
	Un-subtracted heat flow	Static force	Amplitude
	Baseline heat flow	Static stress	Tan delta
	Enthalpy	Static strain	Modulus
	Micro volt	Static modulus	Stress
	Baseline micro volt	Static compliance	% Strain
	Un-subtracted micro-volt	Expansion coefficient (CTE)	Viscosity
	Heat flow calibration	Sample/program temperatures	Compliance
	Weight	Height %	
	Un-subtracted weight	Height	
Mathematical Operations	Substraction	Smoothing	Derivative
	Addition	Average	

Table 1: Specifications. Continued ...

Standard			
Calculations	Peak area/partial	Delta Y	Peak search
	Step	Onset	Delta X
	OIT	Event mark	Response ratio
	Trigger	Glass transition (Tg) (several algorithms)	Slope
	Specific Heat (Cp)	Heat flow	
	Expansion coefficient (CTE)	Crystallinity	
Features	Calibration Wizard	Report Manager	Method change during a run
	Pyris Player	Real-time reference curve	MultiCurve
	Real-time calculation	Selectable result properties	Tolerance test
	Valet	Multitasking	HyperDSC
	Event control with Methods Plus	Raw data access	
Optional			
Software Packages	Pyris Enhanced Security	Pyris Kinetics	Temperature Dependent
	(21 CFR Part 11)	Pyris StepScan DSC	Crystallinity software
	Pyris DSC Purity	Pyris AutoStepwise TGA	
Requirements			
Operating System	Microsoft Windows* 10 (32 or 64 bit)		

For more information, visit www.perkinelmer.com

PerkinElmer, Inc.
940 Winter Street
Waltham, MA 02451 USA
P: (800) 762-4000 or
(+1) 203-925-4602
www.perkinelmer.com

PerkinElmer®

For a complete listing of our global offices, visit www.perkinelmer.com/ContactUs

835383 PKI