



NETZSCH

Polymer Identification by Means of KIMW-Database and *Identify*

Dr. Alexander Schindler and Dr. Tobias Pflock, NETZSCH-Gerätebau GmbH, Selb
Martin Doedt, KIMW Prüf- und Analyse GmbH, Lüdenscheld

Introduction

Over the years, the Kunststoff-Institut Lüdenscheld [1] – an experienced contact for any question regarding plastics – has built up a materials database which currently contains DSC curves for more than 600 commercially available polymers. Thanks to collaboration between the Kunststoff-Institut and NETZSCH-Gerätebau GmbH, this extensive database has now been integrated into the *Identify* curve identification software within *Proteus*[®] analysis. In conjunction with *AutoEvaluation*'s automatic, user-independent evaluation of DSC measurements, this not only simplifies polymer analysis with regard to such issues as identification, failure analysis and quality control, but also makes the results more meaningful [2].

What Does *Identify* Offer?

The *Identify* database system was introduced for direct comparison and thus classification and interpretation of DSC curves, but can now also be employed for $\Delta L/L_0$ measurements stemming from DIL and TMA instruments), for c_p -data from DSC instruments and, most recently, also for TGA measurements [3]. Once *Identify* is available within *Proteus*[®], it can automatically be used for all signal types of any of the supported instruments. The user always has access to the entire database with all of its possibilities, such as overlaying of the current measurement curve with any database curves – including those of different data types.

The entire NETZSCH part of the database comprises more than 1,100 entries from the fields of polymers, organics, food and pharma, ceramics and inorganics, and metals and alloys as well as chemical elements (see figure 1). These entries are composed of measurements and literature data of different data types (DSC, TGA, DIL/TMA and c_p). Users can, of course, create or expand libraries with their own measurements and literature data, and these can simultaneously be shared with other users via the computer network.

Basically, *Identify* offers different search algorithms; the database search can be limited to certain temperature ranges and the results can be filtered according to various criteria, such as the measurement conditions.

Search Libraries:	
Library	Entries
<input checked="" type="checkbox"/> Alloys Poster NETZSCH	42
<input checked="" type="checkbox"/> Ceramics Poster NETZSCH	32
<input checked="" type="checkbox"/> Ceramics_Inorganics NETZSCH	255
<input checked="" type="checkbox"/> Elements Poster NETZSCH	104
<input checked="" type="checkbox"/> Metals_Alloys NETZSCH	135
<input checked="" type="checkbox"/> Organics_Food_Pharma NETZSCH	309
<input checked="" type="checkbox"/> Polymers DSC KIMW	600
<input checked="" type="checkbox"/> Polymers NETZSCH	176
<input checked="" type="checkbox"/> Polymers Poster NETZSCH	70

1 Libraries within *Identify* (Status: December 2016)

The Advantages of the KIMW Database

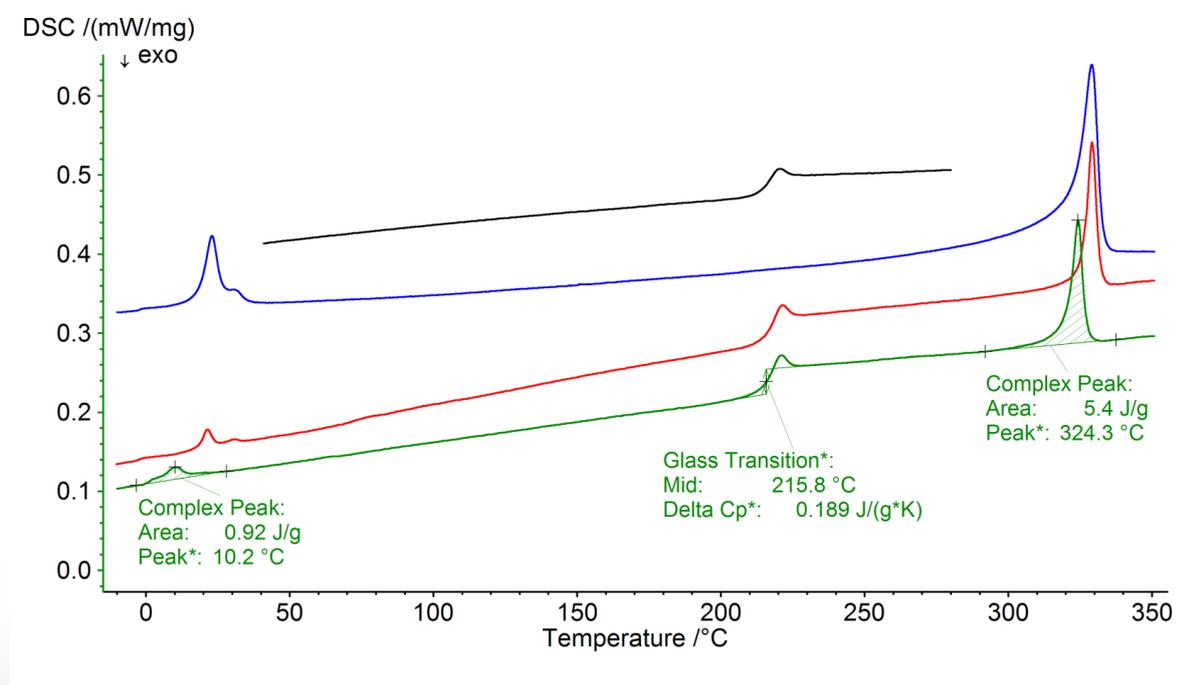
While the NETZSCH part of the *Identify* database forms a solid foundation due to its large variety of materials and methods, the optional KIMW part additionally features previously unachieved depth in the area of DSC on polymers: It includes 600 DSC measurements on different commercially available polymers and blends, reflecting about 130 different polymer types. This means that for many polymer types there are measurements on different products of the same type present which may exhibit significantly different DSC profiles. In addition to the multitude of DSC curves, there is the advantage that for each of the 600 polymers, the exact trade name and manufacturer are stored, along with color and filler content.

In summary, their integration into *Identify* allows the 600 DSC curves of the KIMW database to be used directly and intelligently – either via a purely visual comparison or for automatic identification of a polymer as shown with the following example.

Identification of a Polymer Blend

Figures 2a and 2b illustrate an exemplary database search where a measurement on the polymer blend “PEI-PTFE Ultem 4001”, which is already available in the KIMW database, serves as an input curve. The *AutoEvaluation* and *Identify* results appear with a single click: First, automatic detection and evaluation of the effects were carried out; in this case, an endothermic effect was found in the temperature range between approximately 0°C and 30°C, as well as a glass transition at approximately 216°C and another endothermic (melting) effect at a peak temperature of 324°C. The database search yielded the same curve as the most similar hit along with another PEI-PTFE blend, but also measurements on pure PTFE and PEI (see figure 2b).

In contrast, the DSC curves of most of the other polymer types had a much lower similarity so that they could be ruled out. For more details such as measurement conditions or interpretation of the effects, please see reference [2].



2 Comparison of the DSC curves for the “PEI-PTFE Ultem 4001” polymer blend (green) with the database curve for “PEI-PTFE Luvocom 11067223” (red) and with typical database curves for PTFE (blue) and PEI (black). For better illustration, the curves were offset in relation to each other in the y-direction.

Results:

Measurement/Literature Data	Similarity [%]	Class	Similarity [%]
PEI-PTFE_Ultem_4001_DSC	100,00	+ PEI-PTFE (2)	83,15
PEI-PTFE_Luvocom_1106-72...	66,31	+ PTFE (3)	50,90
PTFE_5-15G_DSC	54,09	+ PESU-PTFE (1)	48,40
PTFE_1-24G_DSC	53,74	+ PEBA (2)	37,98
PESU-PTFE_Ultrason_KR_41...	48,40	+ PPA-PTFE (1)	35,00
PTFE_Algoflon_L203_DSC	44,88	+ LCP-PTFE (1)	30,40
PEI_Ultem_1000_DSC	43,74	+ EVM (1)	29,95
PEI_Ultem_2312_GP30_DSC	43,68	+ PEEK-PTFE (1)	29,37
		+ PEI (14)	27,92

3 Results of the *Identify* database search with regard to the „PEI-PTFE Ultem 4001“ sample. The hit list on the left shows comparisons with individual measurements; the hit list on the right, with classes; i.e., defined groupings (the number in parentheses always indicates the number of measurements in the class).

Summary

The KIMW database integrated into *Identify* allows for direct comparison of a measurement with many hundred DSC curves on commercially available polymers. This makes polymer identification not only easier, but also more reliable!

Literature

- [1] <http://kunststoff-institut-luedenscheid.de/>
- [2] M. Doedt, A. Schindler, T. Pflock. DSC-Auswertung mit einem Klick – Datenbank-Integration und Evaluationssoftware vereinfachen Polymeridentifizierung. *Kunststoffe* 10/2016. S.189-191
- [3] A. Schindler, C. Strasser, S. Schmölder, M. Bodek, R. Seniuta, X. Wang. Database-Supported Thermal Analysis Involving Automatic Evaluation, Identification and Classification of Measurement Curves. *Journal of Thermal Analysis and Calorimetry*, DOI 10.1007/s10973-015-5026-x [to the Article](#)