Identify … the Next Stage
(from Proteus® 8.0)
1. Enlarged Database (> 2000 db entries available)
2. Combined and Simultaneous Signals
   (TGA+DSC, TGA+c-DTA®, STA)

Dr. A. Schindler, 10.09. 2018
Use, Applications and Benefits of *Identify*

- Curve-/Material Identification
- Quality Control (QC)
- Archiving/Searching „Data Mining“

*Identify* makes interpretations:
- easier
- faster
- more significant
01 Database Content (09/2018)
Identify: Database Status 2018 (Proteus® 8.0)
More than 2000 db entries available!

Database entries*: **1220 NETZSCH + 800 KIMW optional**

*Expandable without limits. Such libraries can be shared with several other users at the same time in the computer network.
**Identify**: NETZSCH Database Contents 2018 (~1220 entries)

Distribution regarding measurement types:

* Most of such entries contain several properties (\(T_g, T_m, \alpha, c_p\), mass changes) at once!
Identify: NETZSCH Database Contents 2018 (~1220 entries)

Distribution regarding materials:

- Ceramics/Inorganics: 27%
- Metals/Alloys: 15%
- Polymers: 21%
- Pharma/Food/Cosmetics: 14%
- Organics: 14%
- Chemical Elements: 9%
Proteus® 7.1 + higher:
The (optional) KIMW Database for DSC on Polymers

- DSC measurements on
  - 800 commercially available polymers
  - 151 polymer types.
- suppliers, trade names
- filler contents, colors
Combined and Simultaneous Signals
Problem: Multiple Interpretations of DSC Signals
Example: We can unfortunately not distinguish PS from PVC-U via DSC
Problem: Multiple Interpretations of TGA Signals

Example: And we can unfortunately also not distinguish PS from SAN via TGA
Solution: Combine (independent!) DSC and TGA signals
Select DSC+TGA with Ctr-button and left mouse and call Identify (right mouse button)
Solution: Combine (independent!) DSC and TGA

In *Identify*, search for TGA+DSC *in combination*, or consider either TGA or DSC

PS is the only material where DSC and TGA are similar to the unknown.

→ PS identified with high certainty!
Solution: Combine (independent!) DSC and TGA

In Identify, search for TGA+DSC \textit{in combination}, or consider either TGA or DSC.

PVC-U is not an option, because the TGA signal is totally different.
Solution: Combine (independent!) DSC and TGA

In Identify, search for TGA+DSC in combination, or consider either TGA or DSC.

SAN is also not an option, because the DSC signal is too different.
Let's have a look at further cases

Consideration of DSC and TGA will in many cases improve the situation of multiple interpretations!

Exemplary literature data [1].

STA measurement on “PA66-GF30_STA” (see ref. [1])

STA 449 F3 Jupiter®, steel furnace.
Identify on “PA66-GF30_STA” (see ref. [1])
Just considering the DSC signal → No definite identification!

<table>
<thead>
<tr>
<th>Measurement/Literature</th>
<th>Data</th>
<th>Similarity [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>PA66-PAGI-X_Grivory_GV-4H...</td>
<td>98,61</td>
<td></td>
</tr>
<tr>
<td>PA66_Grivory_GV-SH_GF50...</td>
<td>98,15</td>
<td></td>
</tr>
<tr>
<td>ETFE_Tefzel_200_DSC</td>
<td>97,73</td>
<td></td>
</tr>
<tr>
<td>PA66_Terez_PA66_7515_GF...</td>
<td>96,59</td>
<td></td>
</tr>
<tr>
<td>PA66_Altech_PA66_A_2030-...</td>
<td>96,08</td>
<td></td>
</tr>
<tr>
<td>FEP_Teflon_CJ_95_(CJ95)...</td>
<td>95,72</td>
<td></td>
</tr>
<tr>
<td>PA66_Terez_PA66_7400_GK...</td>
<td>95,56</td>
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</tr>
<tr>
<td>ETFE_lit</td>
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<tr>
<td>FEP_Neoflon_NP-101_DSC</td>
<td>95,30</td>
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<tr>
<td>PET_lit</td>
<td>95,02</td>
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</tr>
</tbody>
</table>

**Glass Transition**
- **Mid:** 74.4 °C
- **Delta Cp:** 0.039 J/(g K)

**Glass Transition**
- **Mid:** 81.1 °C
- **Delta Cp:** 0.128 J/(g K)

**Glass Transition**
- **Mid:** 79.1 °C
- **Delta Cp:** 0.036 J/(g K)

**PA66-GF30_STA**
- **Complex Peak:** Area: 45.24 J g⁻¹, Peak: 258.4 °C
- **Complex Peak:** Area: 36.38 J g⁻¹, Peak: 260.5 °C
- **Complex Peak:** Area: 50.31 J g⁻¹, Peak: 261.6 °C
Identify on “PA66-GF30_STA” (see ref. [1])

Just considering the TGA signal → Again no definite identification!
Identify on “PA66-GF30_STA” (see ref. [1])
Take both: DSC and TGA signal → Much better identification!

In this example, PA66 is the only material with a high similarity regarding, both, DSC and TGA.

This can most easily be seen when only the library „NETZSCH Polymer Poster“ is selected. These database entries contain DSC and TGA properties that are considered in combination!

→ PA66 is best hit, other materials are discriminated.
TGA measurement on “PB_TGA_new” (see ref. [1])

TG 209 F1 Libra®. Identify can consider TGA+c-DTA®

- PB is the only material where DSC and TGA are similar to the unknown.
- PB identified with high certainty!
TGA measurement on “PB_TGA_new” (see ref. [1])

TG 209 F1 Libra®. Identify can consider TGA+c-DTA®

Using library „NETZSCH Polymer Poster“, PB is clearly best hit; other materials are discriminated.

→ PB identified with high certainty!

<table>
<thead>
<tr>
<th>Measurement/Literature</th>
<th>Similarity [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>PB_lit</td>
<td>88.78</td>
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<tr>
<td>PE-LLD_lit</td>
<td>63.91</td>
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<tr>
<td>BR_12_lit</td>
<td>60.49</td>
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<tr>
<td>SBR_lit</td>
<td>59.16</td>
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<tr>
<td>PE-HD_lit</td>
<td>58.69</td>
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<tr>
<td>NBR_lit</td>
<td>55.88</td>
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<tr>
<td>PE-LD_lit</td>
<td>52.43</td>
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<tr>
<td>PE-UHMW_lit</td>
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<tr>
<td>TPS_lit</td>
<td>46.96</td>
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<tr>
<td>PP_isotactic_lit</td>
<td>46.16</td>
</tr>
</tbody>
</table>

Mass Change: -99.39 %
**c-DTA®** is the linkage between the TGA and DSC worlds

*Identify* features this linkage!

TGA-**c-DTA®** → TGA(-**c-DTA®**) but also DSC and STA are found by *Identify*

DSC → DSC but also TGA-**c-DTA®** and STA are found by *Identify*

STA → STA, DSC, TGA, TGA-**c-DTA®** are found by *Identify*
Overview
Which signals (A vs. B) can be found by Identify? Status 2018 (Proteus® 8.0):

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>DSC</th>
<th>TGA</th>
<th>STA</th>
<th>TGA-c-DTA®</th>
<th>DIL</th>
<th>TMA</th>
<th>C_p</th>
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<tbody>
<tr>
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<td>✓</td>
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<tr>
<td>TGA</td>
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<tr>
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<td></td>
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<td></td>
</tr>
<tr>
<td>TGA-c-DTA®</td>
<td>✓</td>
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<tr>
<td>C_p</td>
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<td></td>
<td></td>
<td></td>
<td>✓</td>
</tr>
</tbody>
</table>

Remarks:
- A, B: measurements or literature data ("unknown" is always a measurement).
- DSC can also be DTA.
- ✓✓: two signal types can be identified in combination - or just one of the signal types.
More than 2000 db entries are available!

*Identify* can now incorporate:
Combined signals (TGA+DSC indep. and TGA-c-\textit{DTA}®)
Simultaneous signals (TGA+DSC = STA)

This makes material identification more definite!

The contents of this presentation is published: