Analyzing & Testing

NETZSCH

Leading Thermal Analysis

Polymer Crystallization Behavior – Easy to Understand by Means of the Kinetics Neo Software

NETZSCH Webinar
Elena Moukhina
02/23/2022

Agenda

1. Target of kinetic crystallization analysis

   Brief overview of the problems solving by crystallization kinetics

2. Isothermal crystallization

   Measurements, Analysis methods, selection of analysis method

3. Non-isothermal crystallization (cooling over melting range)

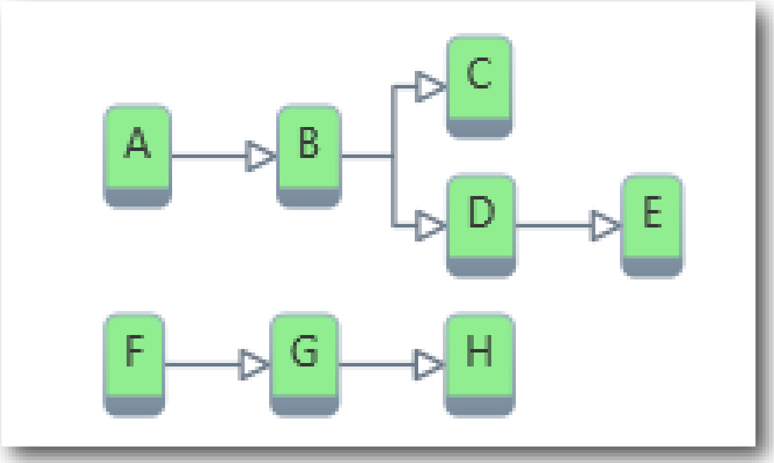
   Measurements, Analysis methods, selection of analysis method

4. Advantages and Limitation of different models for simulations

1. Target of thermokinetic crystallization analysis

Brief overview of the problems solving
by crystallization kinetics

Purposes of kinetic analysis



$$\mathbf{A} \rightarrow \mathbf{B}$$

reactant (melt) product (crystal)

Academic

*Crystallization mechanism is the **subject** of study*

- **Find** and describe the kinetic **mechanism of crystallization**

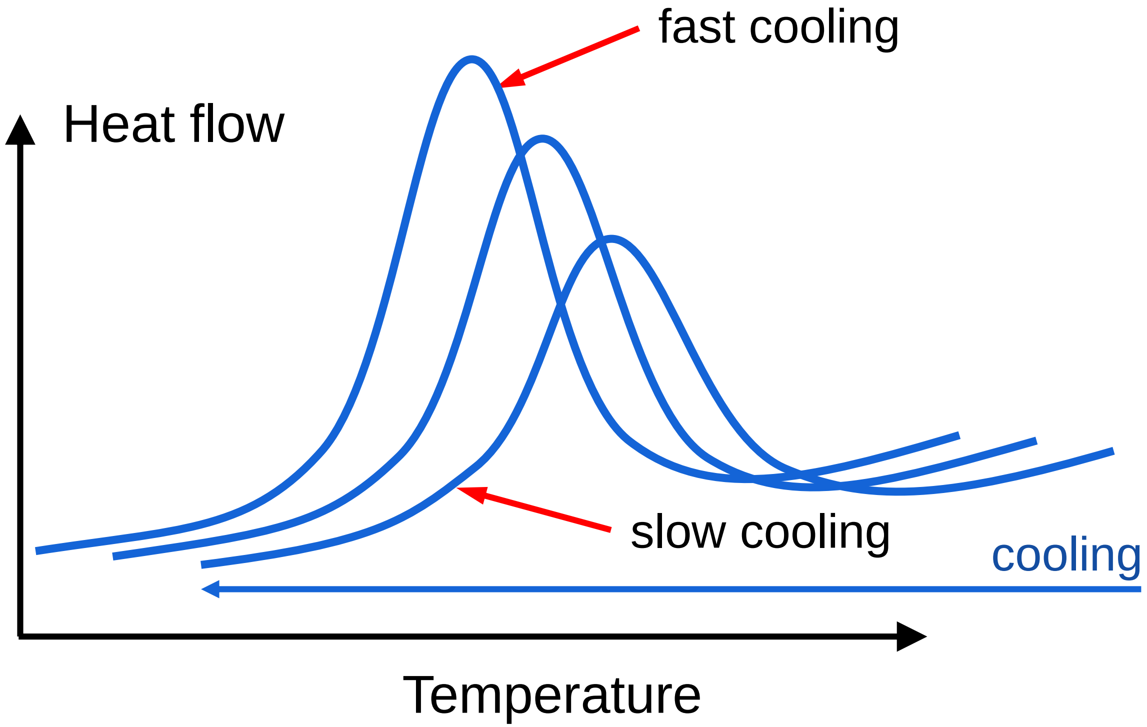
Industrial

*Crystallization mechanism is **unknown** or **not important***

- **Predict** crystallization rate and degree of crystallization for given temperature program

- **Optimize** industrial processes: decrease production time and costs and improve the quality of product

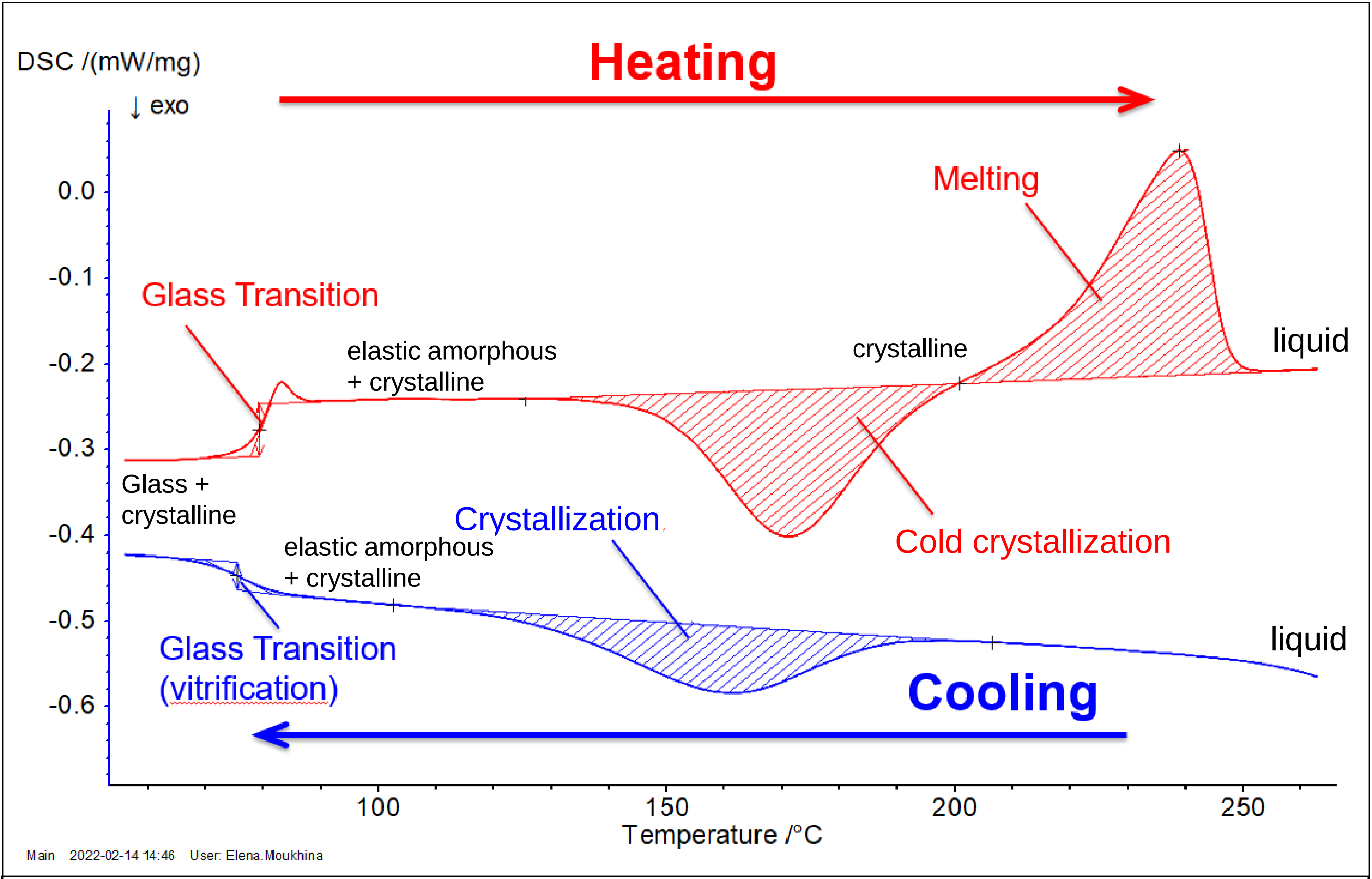
Measurements for kinetic analysis:
Differential scanning calorimetry



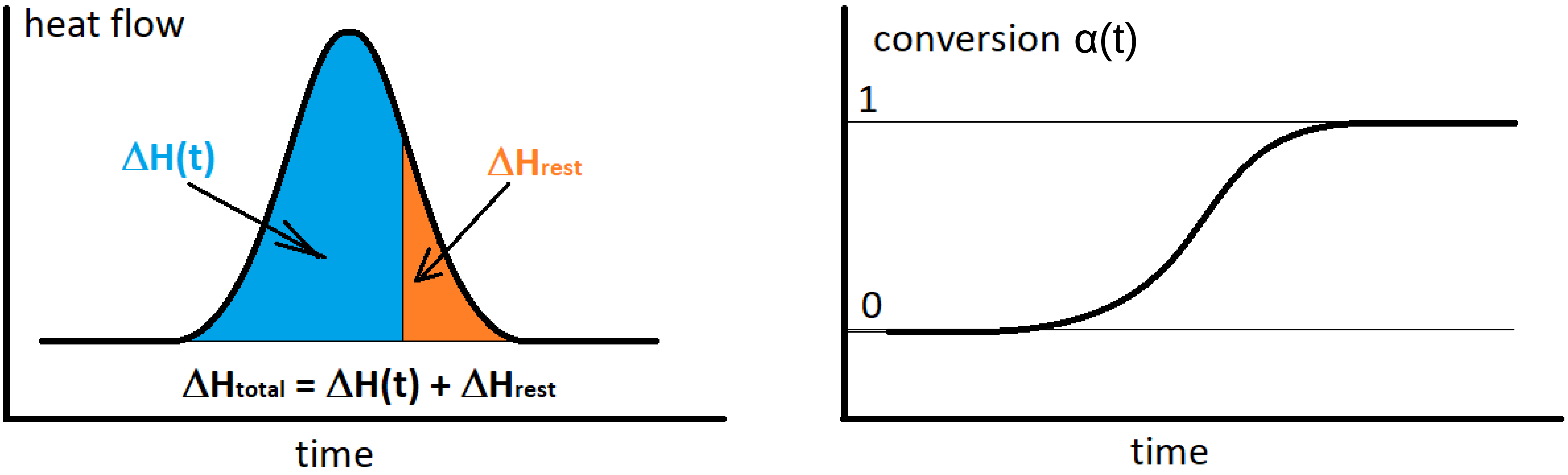
Differential scanning calorimetry: heat flow is measured during temperature change

Polymer for Heating and Cooling

NETZSCH



Conversion α(t) for DSC data is apparent degree of crystallization

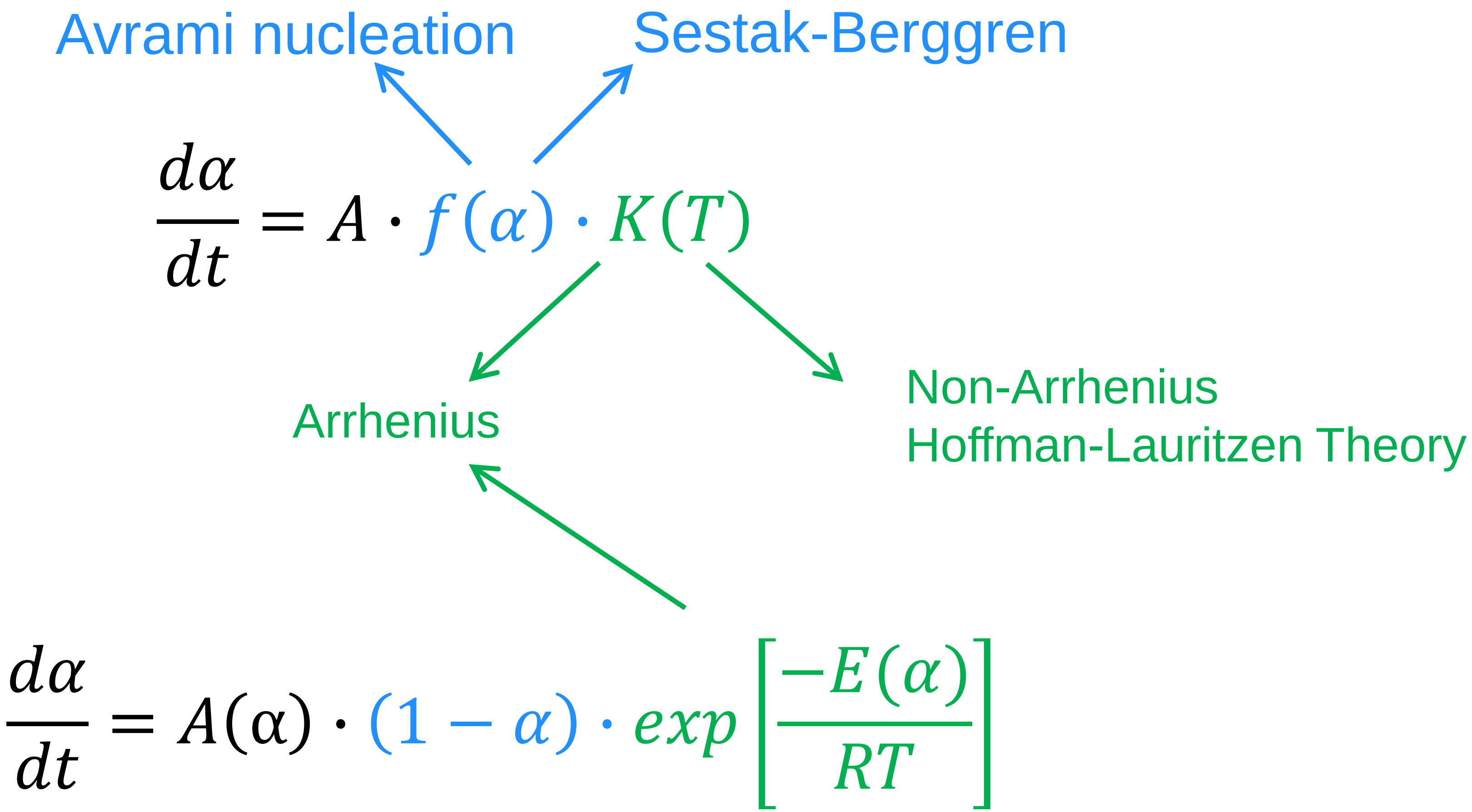


$$\alpha(t) = \frac{\Delta H(t)}{\Delta H_{total}}$$

DSC: Conversion is the ratio of the partial enthalpy change at given time point **to the total enthalpy change** at the final time point

Crystallization kinetics in Kinetics Neo

Crystallization rate



Avrami nucleation

Sestak-Berggren

Model based

$$\frac{d\alpha}{dt} = A \cdot f(\alpha) \cdot K(T)$$

Arrhenius

Non-Arrhenius
Hoffman-Lauritzen Theory

Model free

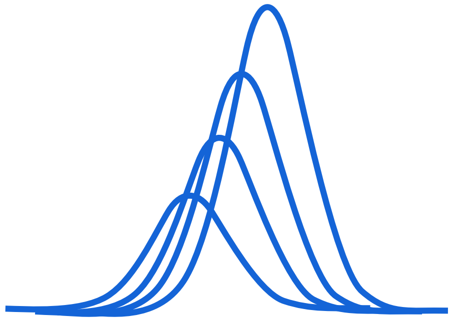
$$\frac{d\alpha}{dt} = A(\alpha) \cdot (1 - \alpha) \cdot exp\left[\frac{-E(\alpha)}{RT}\right]$$

Steps to solve Kinetic Tasks in Kinetics Neo

Measured
DSC data

- File 1
- File 2
- File 3
- File 4

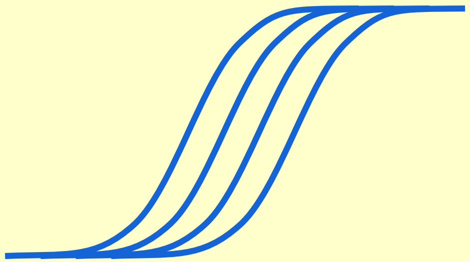
. . .



Data Import
and Processing

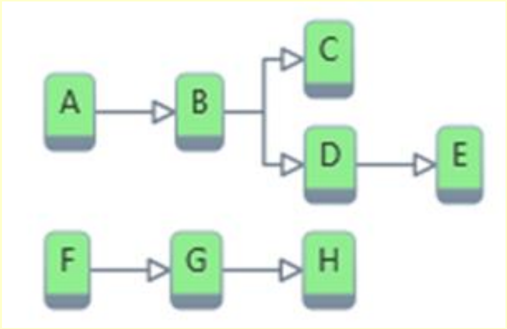
- Processed File 1
- Processed File 2
- Processed File 3
- Processed File 4

. . .



Kinetic Model / Method

- Avrami
- Nakamura
- Hoffman-Lauritzen
- . . .
- model free
- . . .



Simulations

Predictions:
isothermal / dynamic / arbitrary

Predictions:
degree of crystallization /
crystalization rate

. . .

Optimization:
crystallization rate

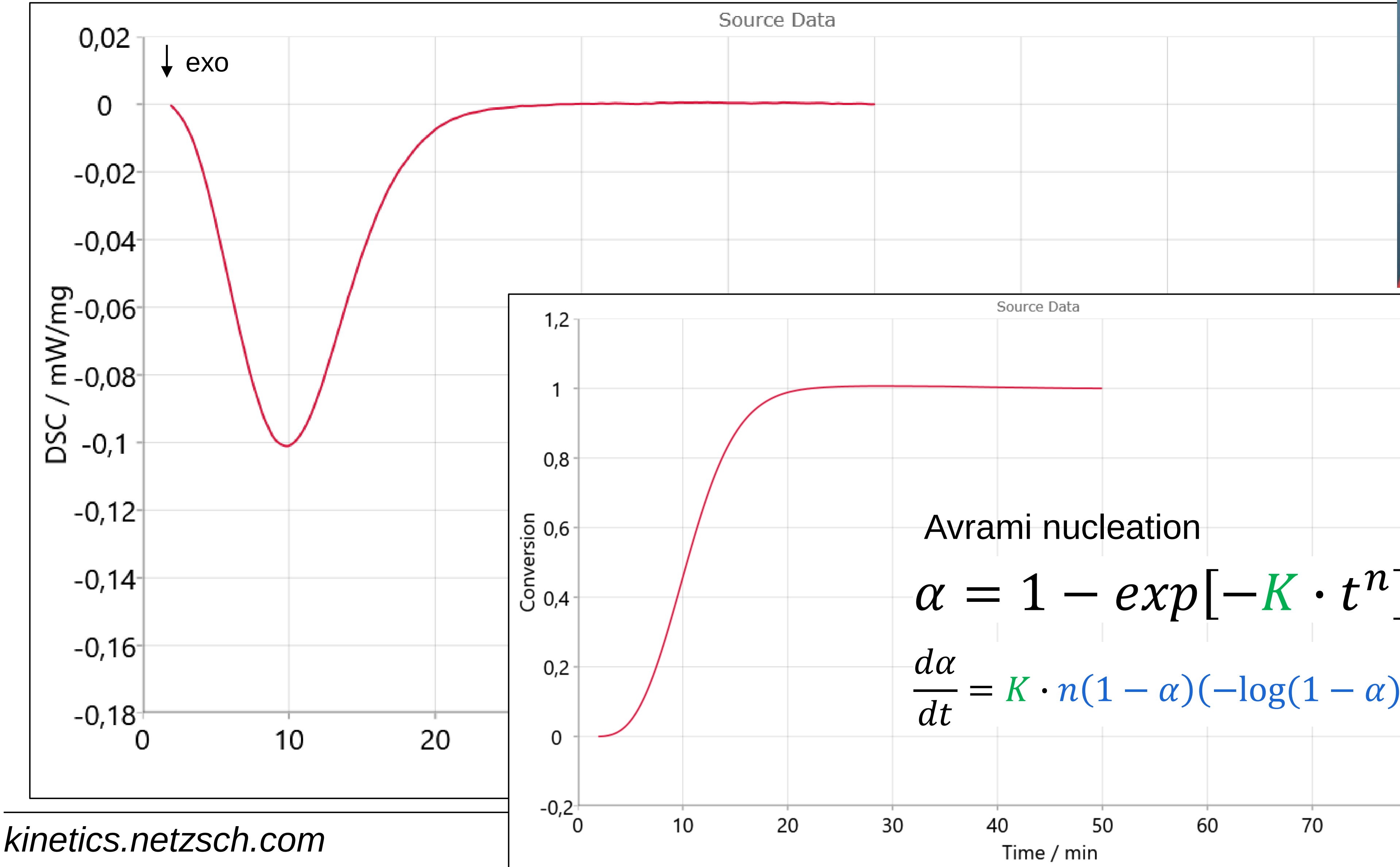
Optimization:
crystallization profile

. . .

2. Isothermal crystallization

Measurements, Analysis methods

Isothermal crystallization PA12 at 164°C



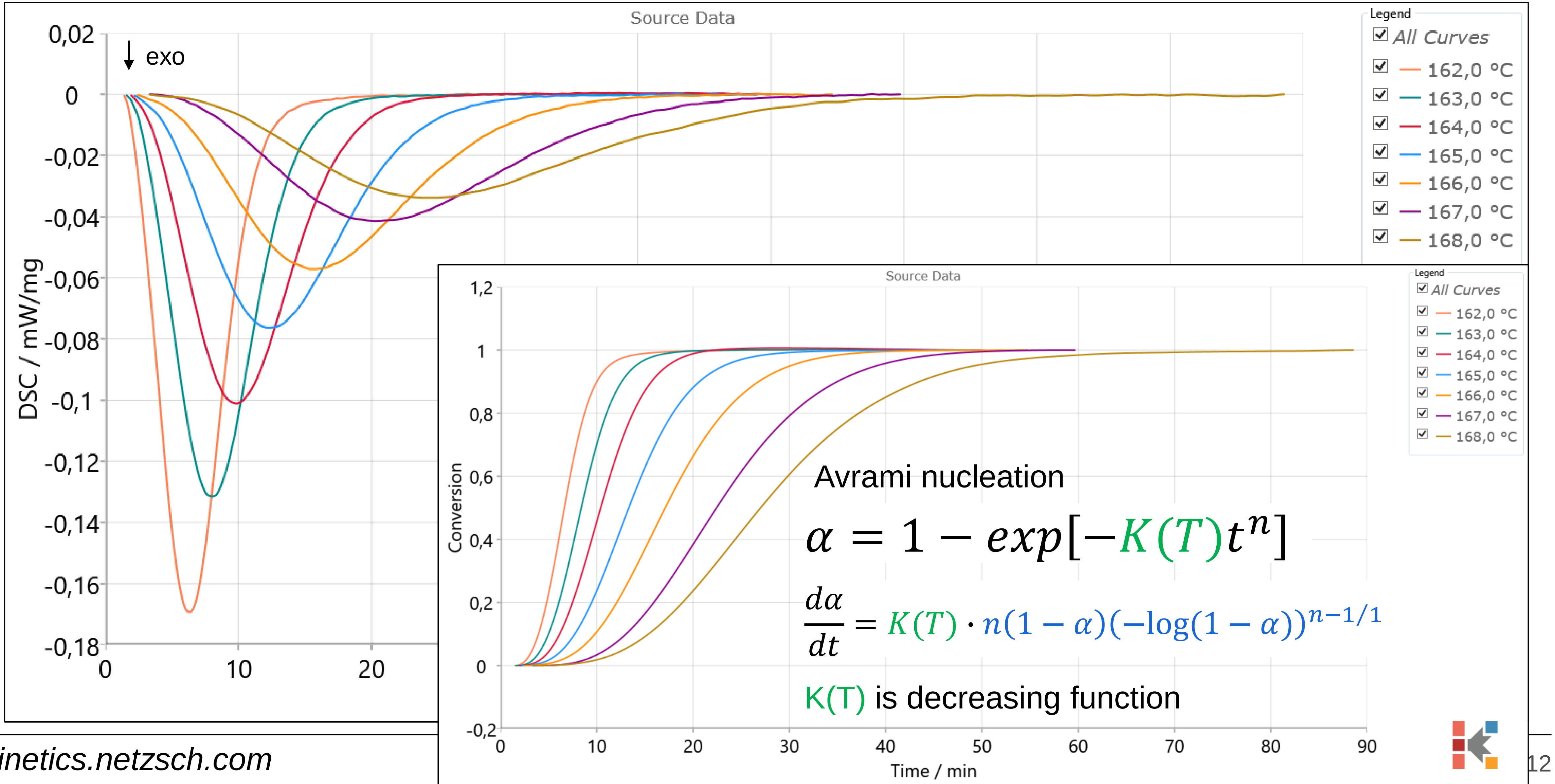
Avrami nucleation

$$\alpha = 1 - exp[-K \cdot t^{n}]$$

$$\frac{d\alpha}{dt} = K \cdot n(1-\alpha)(-\log(1-\alpha))^{n-1/1}$$

kinetics.netzsch.com

Isothermal crystallization PA12



Avrami nucleation

$$\alpha = 1 - exp[-K(T)t^n]$$

$$\frac{d\alpha}{dt} = K(T) \cdot n(1-\alpha)(-\log(1-\alpha))^{n-1/1}$$

K(T) is decreasing function

Crystallization kinetics: Arrhenius approach

Crystallization rate

Avrami nucleation

$f(\alpha)=n\cdot(1-\alpha)\cdot[-\ln((1-\alpha))]^{(n-1)/n}$

Sestak-Berggren

$f(\alpha)=(1-\alpha)^{n}\cdot\alpha^{m}\cdot[-\ln((1-\alpha))]^{q}$

Model based

$$\frac{d\alpha}{dt}=A\cdot f(\alpha)\cdot K(T)$$

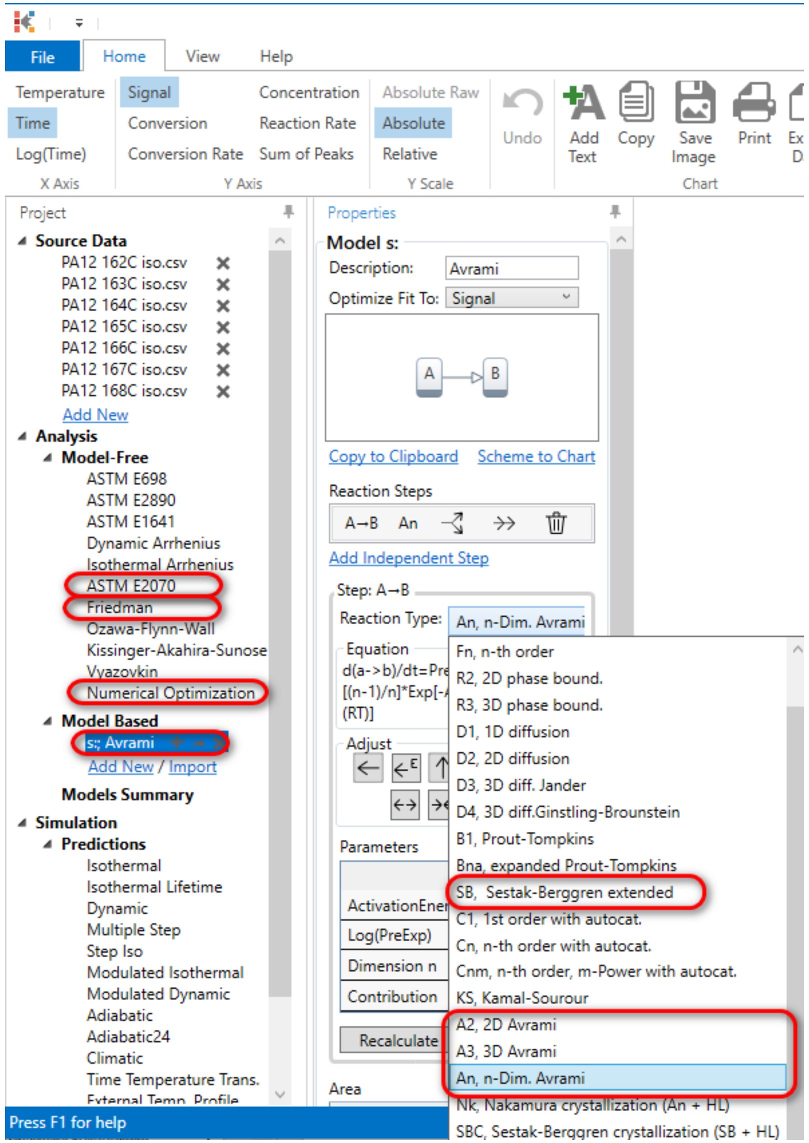
Arrhenius: $K(T)=exp\left[\frac{-E}{RT}\right]$

Non-Arrhenius
Hoffman-Lauritzen Theory

Model free

$$\frac{d\alpha}{dt}=A(\alpha)\cdot(1-\alpha)\cdot exp\left[\frac{-E(\alpha)}{RT}\right]$$

Kinetics Neo: kinetic methods for isothermal crystallization (Arrhenius approach)



Model s:

Description: Avrami

Optimize Fit To: Signal

Reaction Type: An, n-Dim. Avrami

Equation
d(a->b)/dt=Pre
[(n-1)/n]*Exp[-
(RT)]

Arrhenius approach
Like for chemical reactions

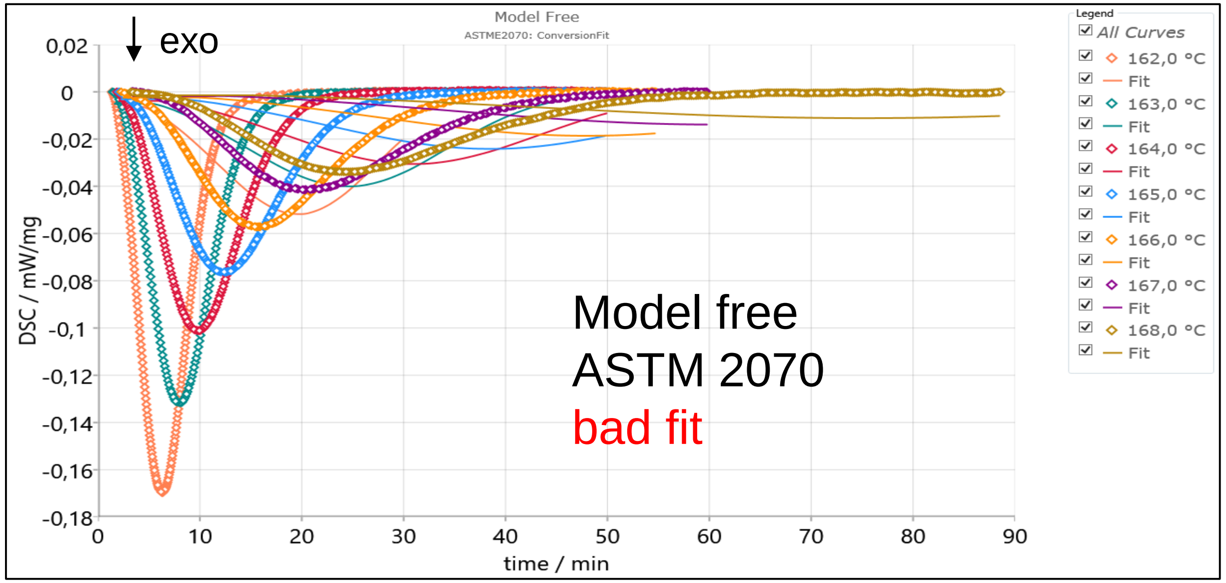
Arrhenius: $K(T) = exp\left[\frac{-E}{RT}\right]$

Positive activation energy: chemical reactions **go faster** with increasing of the temperature

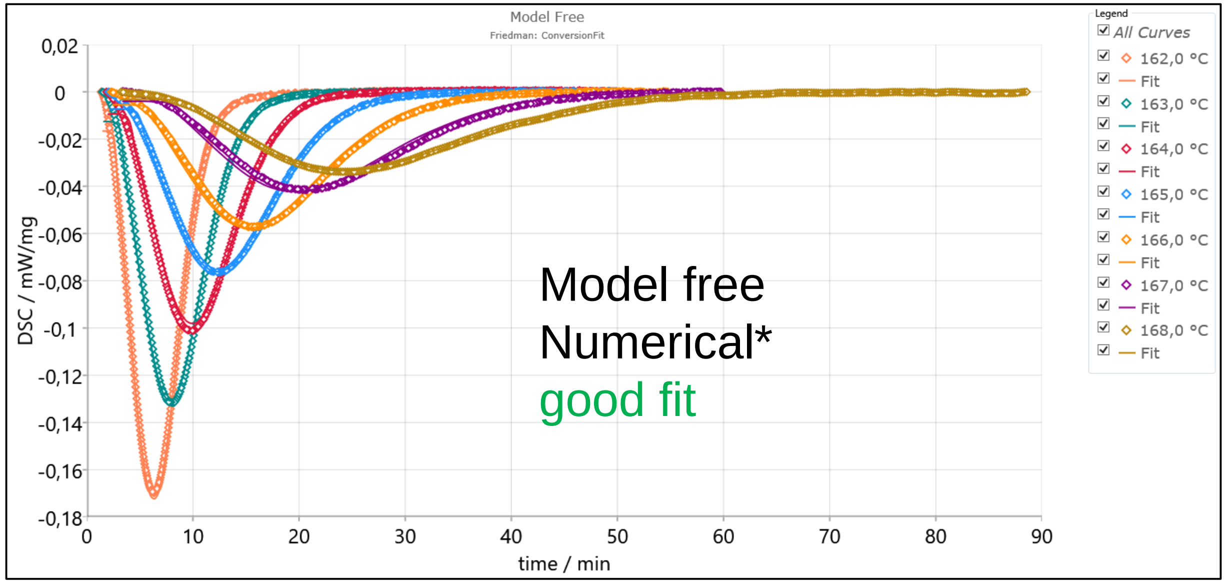
Negative activation energy (apparent value): crystallization **goes slower** with temperature increase

This approach may be applied only at the temperatures close to melting temperature Tm and below it

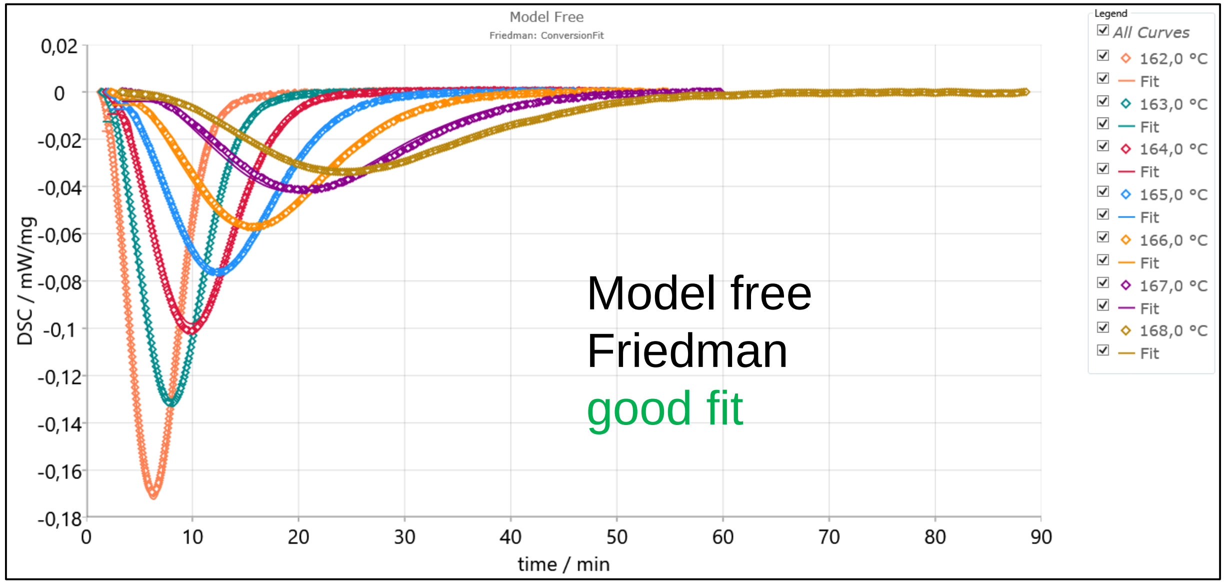
Isothermal crystallization: Arrhenius approach



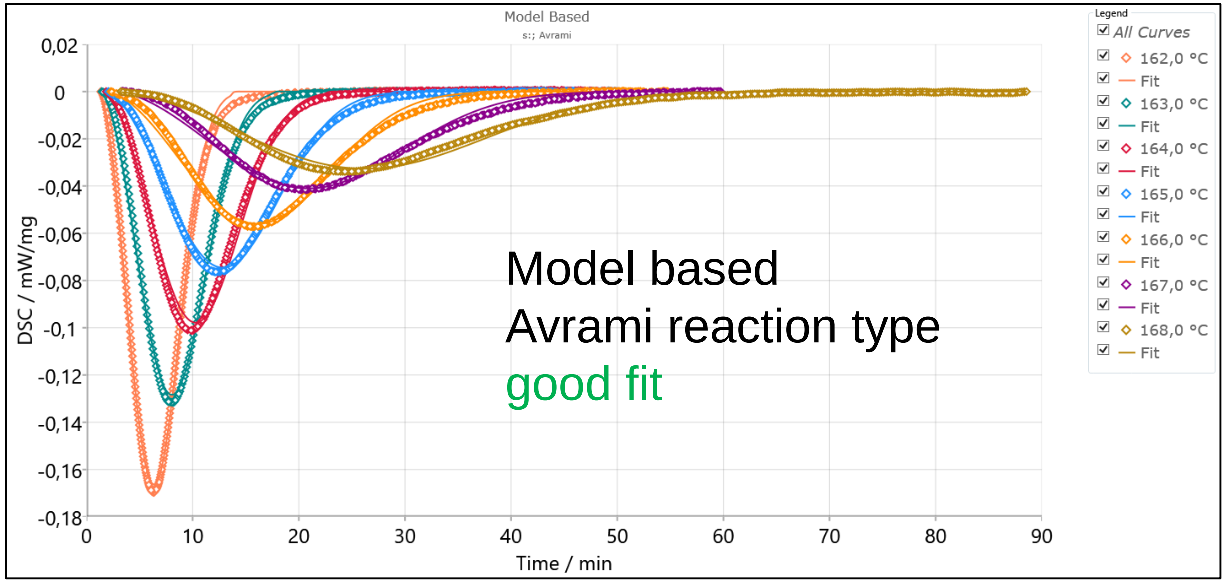
Model free
ASTM 2070
bad fit



Model free
Numerical*
good fit



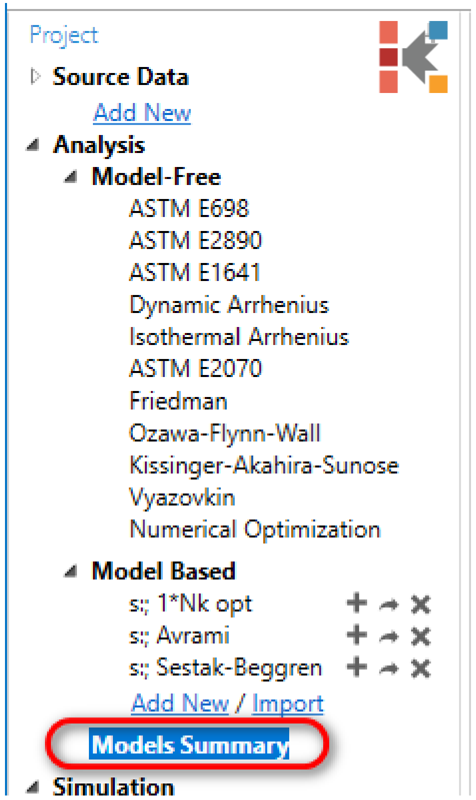
Model free
Friedman
good fit



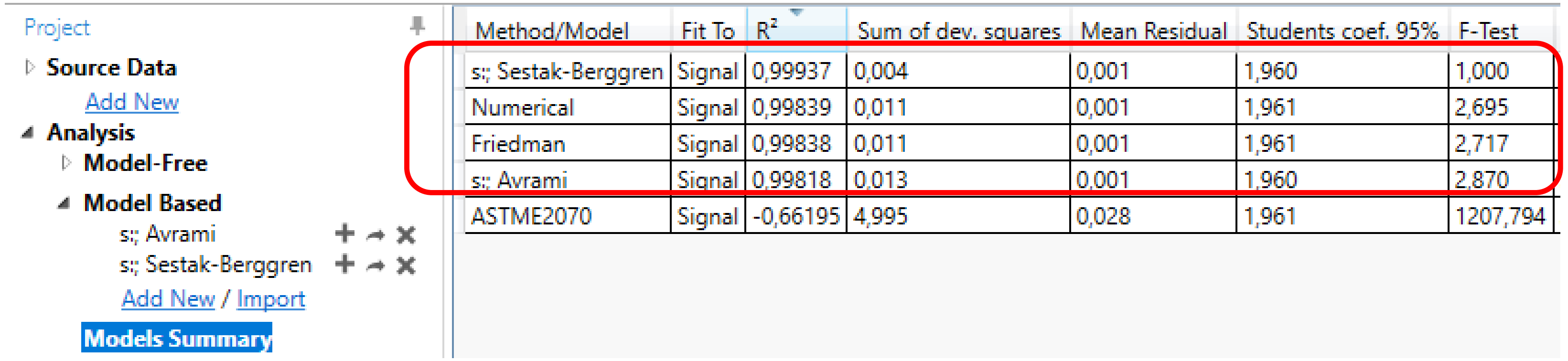
Model based
Avrami reaction type
good fit

Apparent activation energy is negative. Here E ≈ -400kJ/mol

Comparison of different results and selection the appropriate one



Project
- Source Data
  - Add New
- Analysis
  - Model-Free
    - ASTM E698
    - ASTM E2890
    - ASTM E1641
    - Dynamic Arrhenius
    - Isothermal Arrhenius
    - ASTM E2070
    - Friedman
    - Ozawa-Flynn-Wall
    - Kissinger-Akahira-Sunose
    - Vyazovkin
    - Numerical Optimization
  - Model Based
    - s;; 1*Nk opt
    - s;; Avrami
    - s;; Sestak-Beggren
    - Add New / Import
  - Models Summary
- Simulation



Project
- Source Data
  - Add New
- Analysis
  - Model-Free
  - Model Based
    - s;; Avrami
    - s;; Sestak-Berggren
    - Add New / Import
  - Models Summary

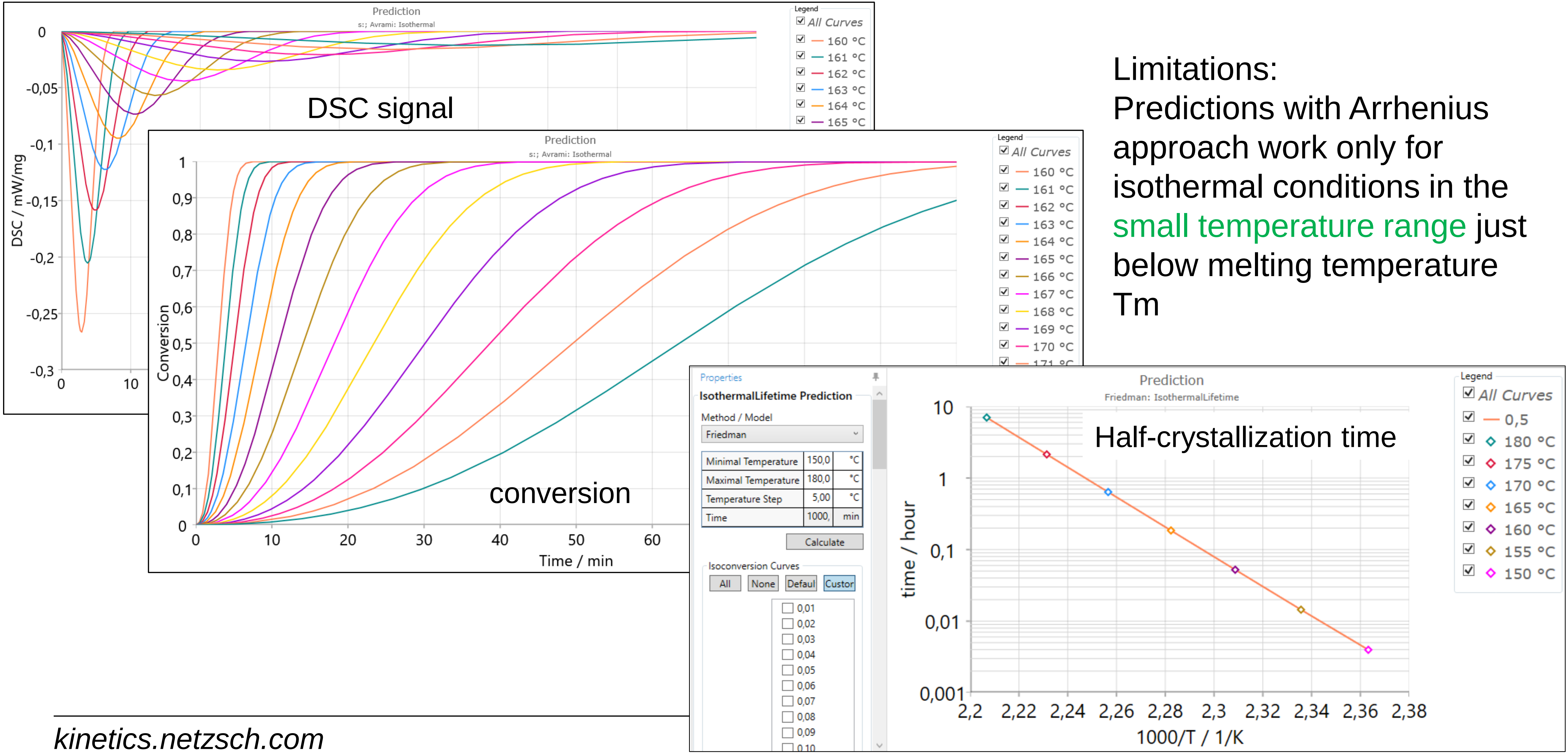
Method/Model	Fit To	R^2	Sum of dev. squares	Mean Residual	Students coef. 95%	F-Test
s;; Sestak-Berggren	Signal	0,99937	0,004	0,001	1,960	1,000
Numerical	Signal	0,99839	0,011	0,001	1,961	2,695
Friedman	Signal	0,99838	0,011	0,001	1,961	2,717
s;; Avrami	Signal	0,99818	0,013	0,001	1,960	2,870
ASTME2070	Signal	-0,66195	4,995	0,028	1,961	1207,794

Arrhenius approach
Like for chemical reactions

Works well by using of model free (Friedman and Numerical)
And for model based (Avrami and Sestak-Berggren)

We recommend to use model based Avrami mehod

Predictions with Avrami model



DSC signal

conversion

Half-crystallization time

IsothermalLifetime Prediction

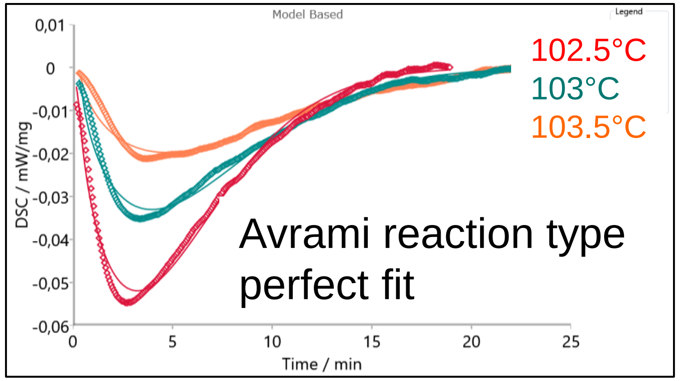
Method / Model: Friedman

Minimal Temperature	150,0	°C
Maximal Temperature	180,0	°C
Temperature Step	5,00	°C
Time	1000,	min

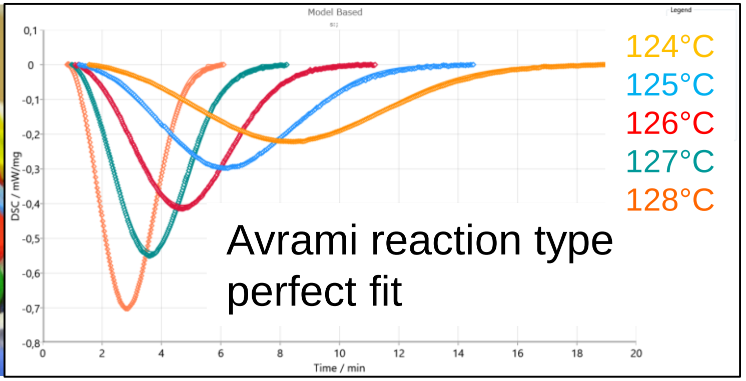
☐ 0,01
☐ 0,02
☐ 0,03
☐ 0,04
☐ 0,05
☐ 0,06
☐ 0,07
☐ 0,08
☐ 0,09
☐ 0,10

Limitations:
Predictions with Arrhenius approach work only for isothermal conditions in the small temperature range just below melting temperature Tm

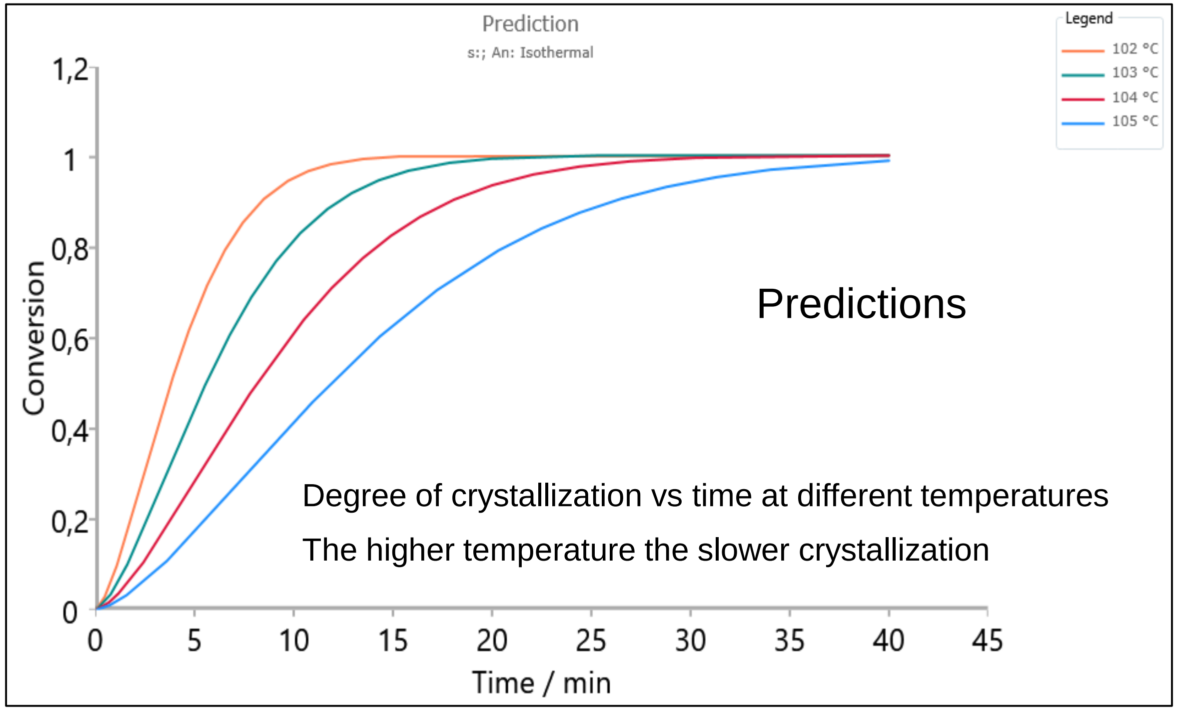
Isothermal crystallization: LDPE and PP



Avrami reaction type perfect fit



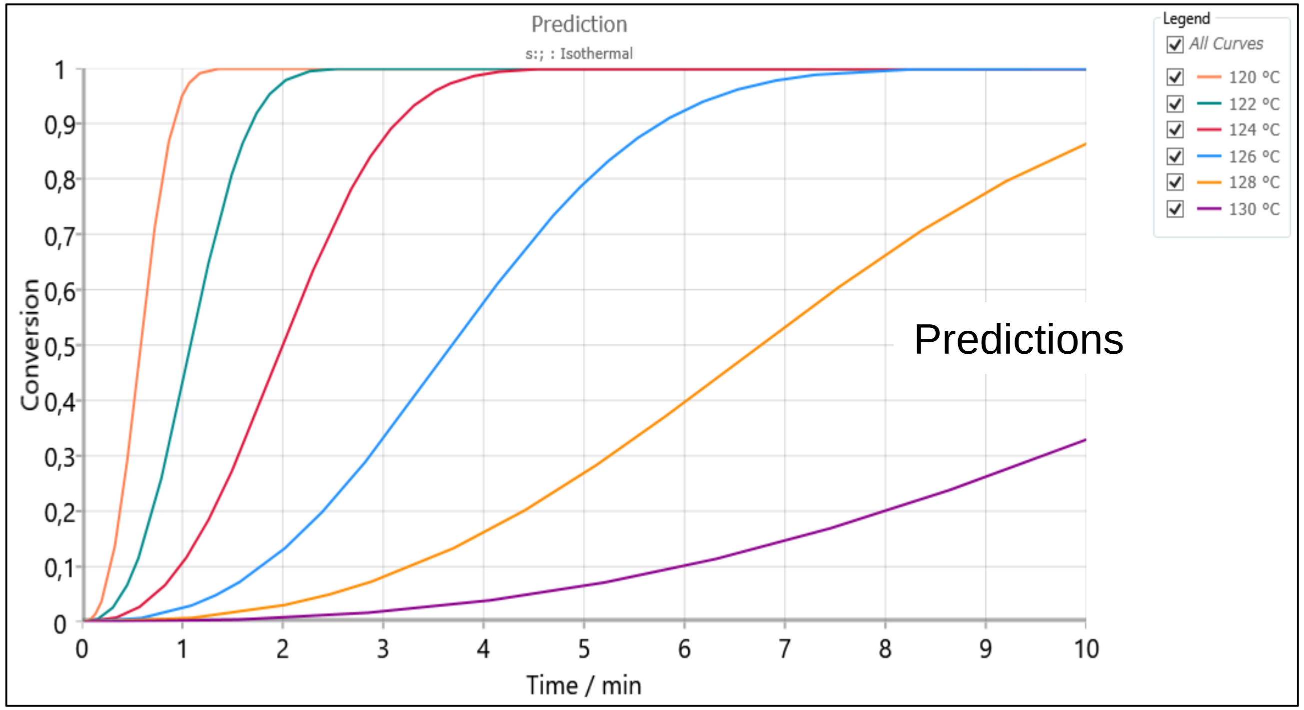
Avrami reaction type perfect fit



Predictions

Degree of crystallization vs time at different temperatures

The higher temperature the slower crystallization



Predictions

Isothermal Crystallization: Arrhenius approach

Advantage:
very simple and fast, mathematics of chemical kinetics can be used.

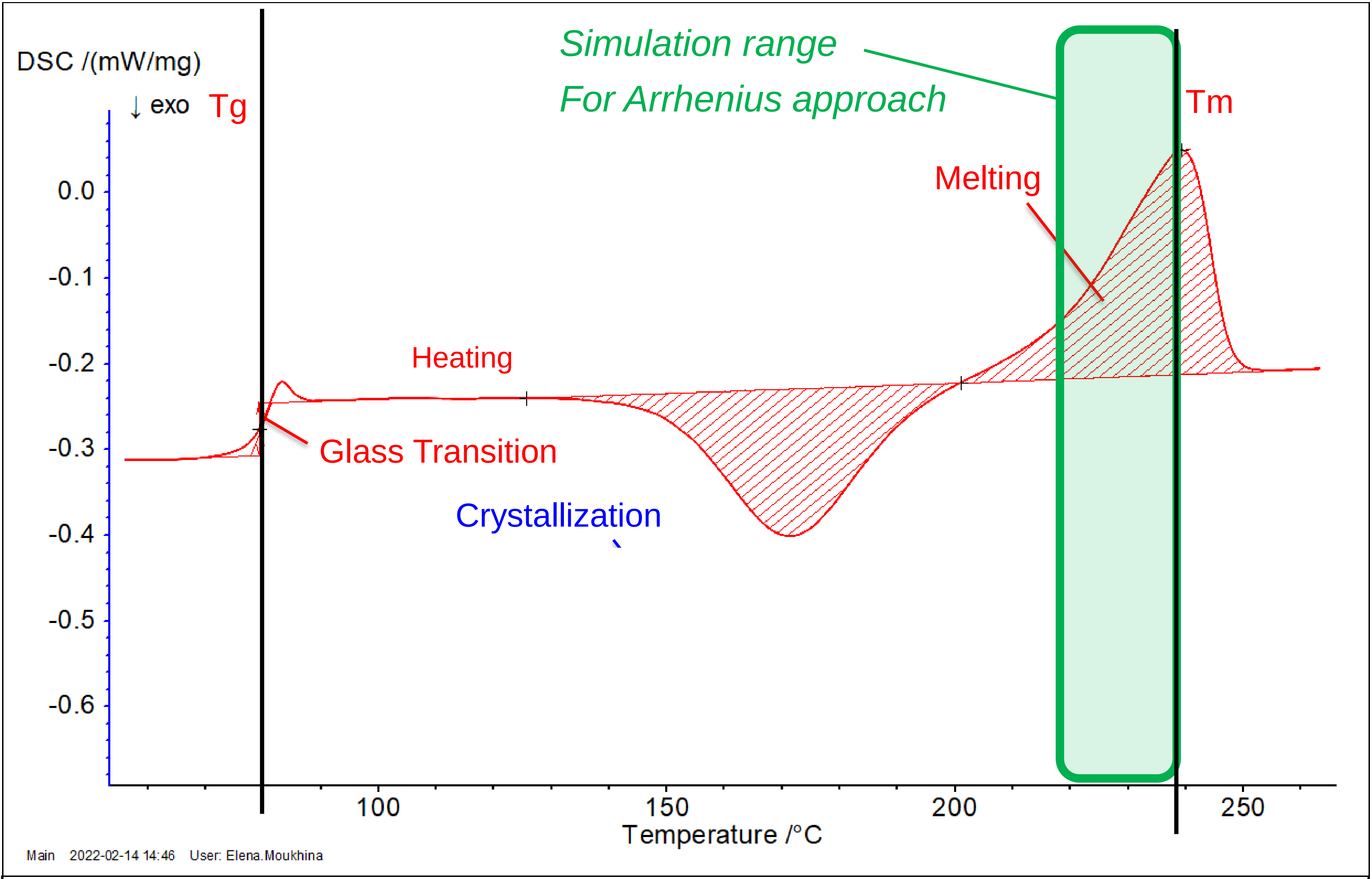
Disadvantages:

1. Arrhenius approach has no physical background. Activation energy is just the apparent value.
2. Does not take into account diffusion near glass transition temperature
3. Enables only for very small temperature range near melting point. Produces incorrect predictions outside of this range.

Conclusion: this approach is very simplified, and has very limited working temperature range

Isothermal Crystallization: Arrhenius approach

NETZSCH



3. Non-Isothermal crystallization (cooling over melting range)

Measurements; Analysis methods
Nakamura equation,
Hoffman-Lauritzen theory
Sestak-Berggren crystallization

Crystallization for Polyethylene Terephthalate (PET)

PET

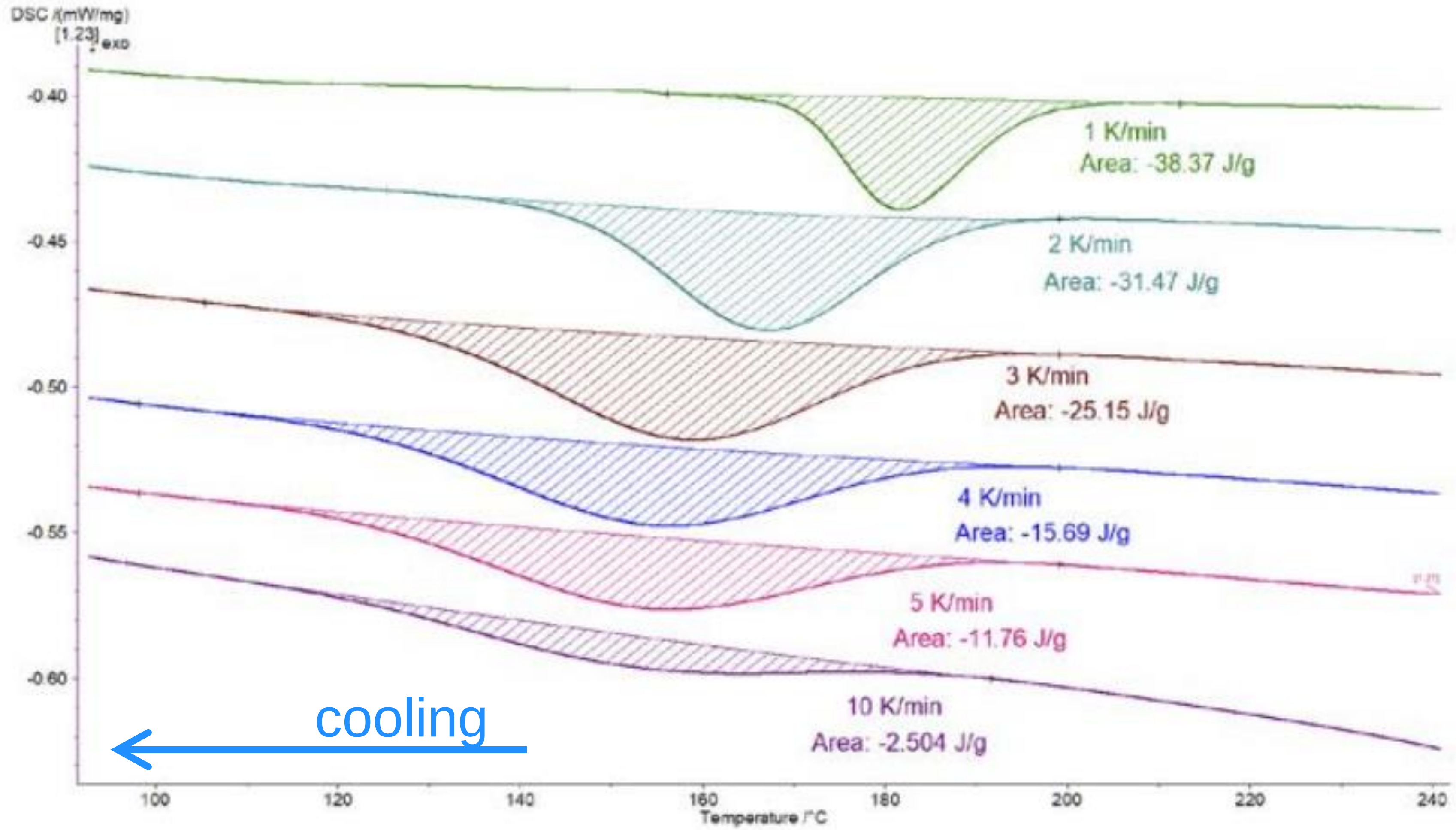
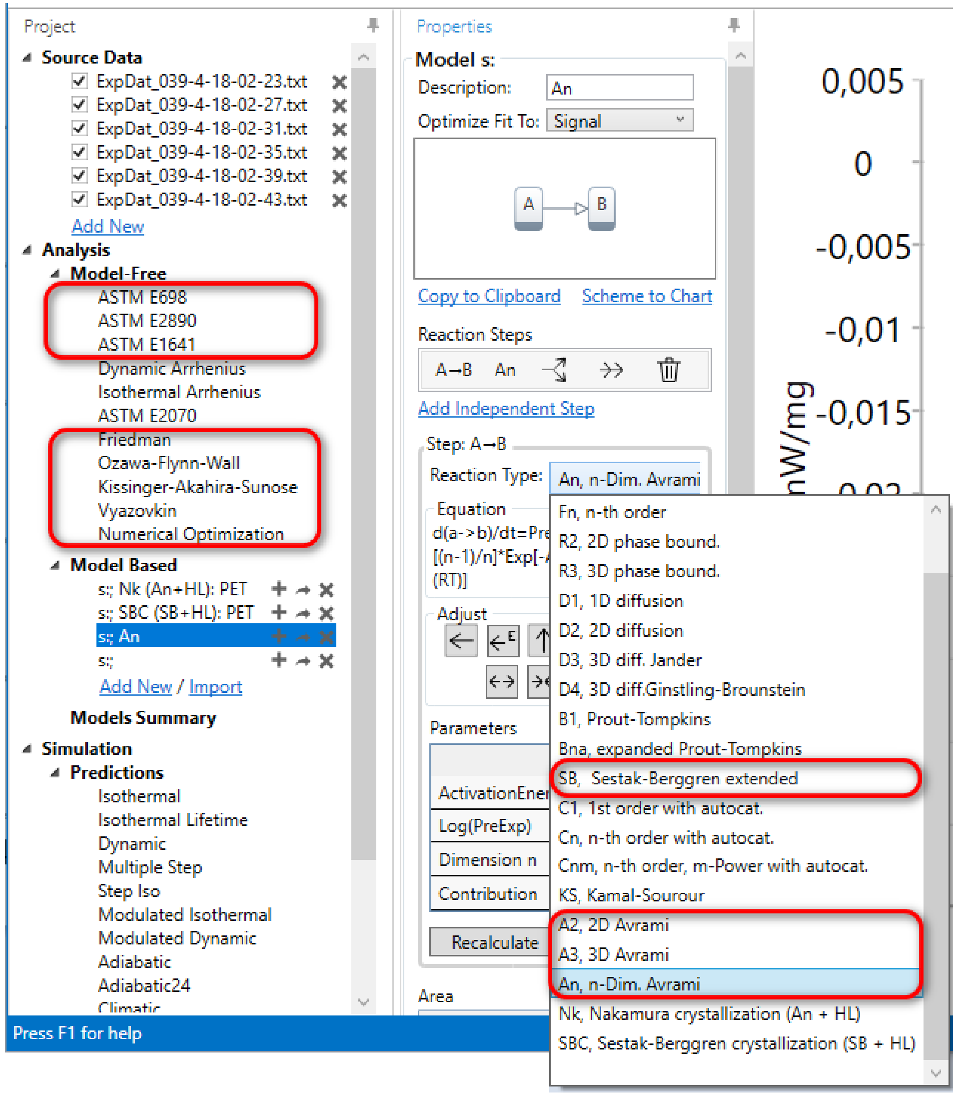


Fig. 1. Crystallization curves for polyethylene terephthalate (PET) measured at cooling rates from 1 to 10 K/min

Kinetics Neo: kinetic methods for non-isothermal crystallization
Arrhenius approach does not work

NETZSCH



Project

Source Data
- ☑ ExpDat_039-4-18-02-23.txt
- ☑ ExpDat_039-4-18-02-27.txt
- ☑ ExpDat_039-4-18-02-31.txt
- ☑ ExpDat_039-4-18-02-35.txt
- ☑ ExpDat_039-4-18-02-39.txt
- ☑ ExpDat_039-4-18-02-43.txt

Add New

Analysis
- **Model-Free**
  - ASTM E698
  - ASTM E2890
  - ASTM E1641
  - Dynamic Arrhenius
  - Isothermal Arrhenius
  - ASTM E2070
  - Friedman
  - Ozawa-Flynn-Wall
  - Kissinger-Akahira-Sunose
  - Vyazovkin
  - Numerical Optimization
- **Model Based**
  - s:; Nk (An+HL): PET
  - s:; SBC (SB+HL): PET
  - s:; An
  - s:;

Add New / Import

Models Summary

Simulation
- **Predictions**
  - Isothermal
  - Isothermal Lifetime
  - Dynamic
  - Multiple Step
  - Step Iso
  - Modulated Isothermal
  - Modulated Dynamic
  - Adiabatic
  - Adiabatic24
  - Climatic

Press F1 for help

Properties

Model s:

Description: An

Optimize Fit To: Signal

Copy to Clipboard Scheme to Chart

Reaction Steps

Add Independent Step

Step: A→B

Reaction Type: An, n-Dim. Avrami

Equation
d(a->b)/dt=Pre
[(n-1)/n]*Exp[-
(RT)]

Adjust

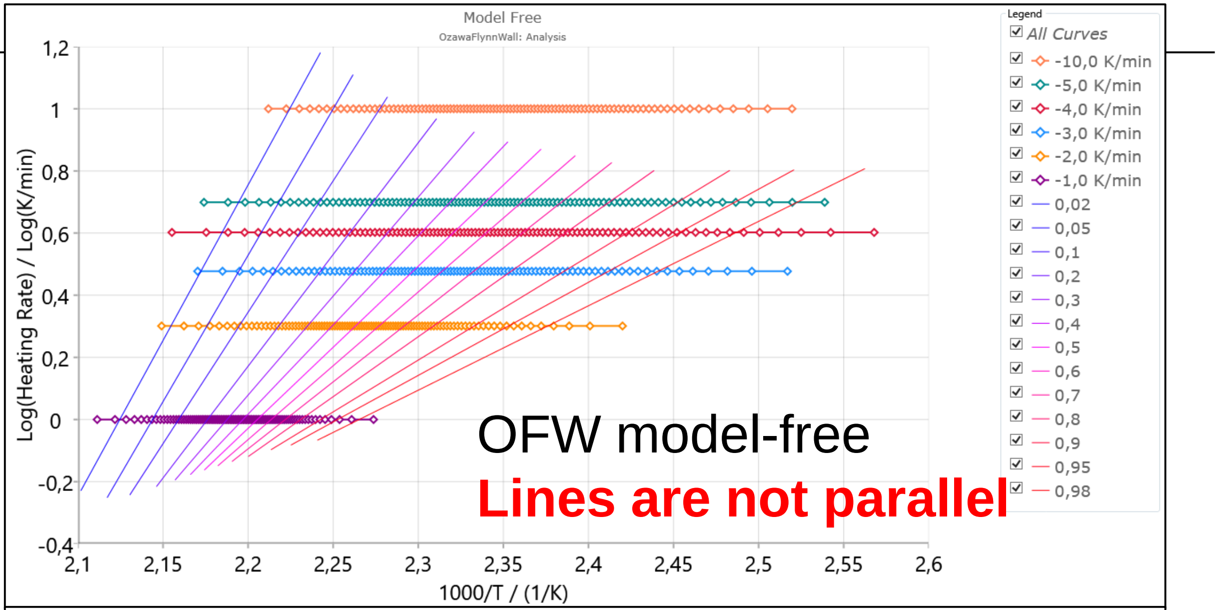
Parameters

ActivationEner
Log(PreExp)
Dimension n
Contribution

Recalculate

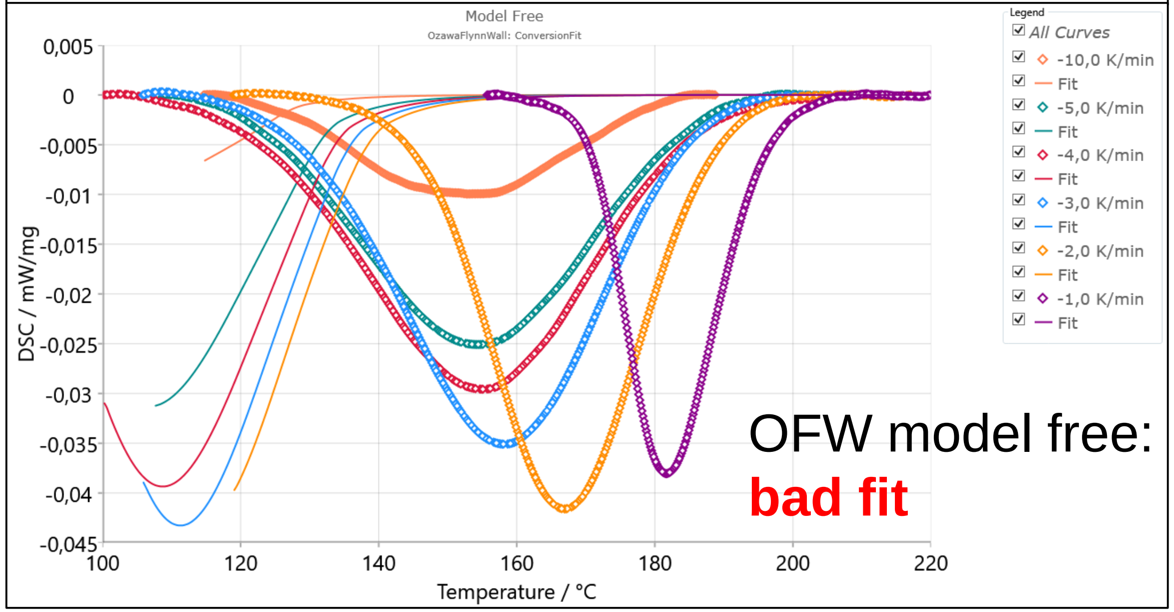
Area

- Fn, n-th order
- R2, 2D phase bound.
- R3, 3D phase bound.
- D1, 1D diffusion
- D2, 2D diffusion
- D3, 3D diff. Jander
- D4, 3D diff.Ginstling-Brounstein
- B1, Prout-Tompkins
- Bna, expanded Prout-Tompkins
- SB, Sestak-Berggren extended
- C1, 1st order with autocat.
- Cn, n-th order with autocat.
- Cnm, n-th order, m-Power with autocat.
- KS, Kamal-Sourour
- A2, 2D Avrami
- A3, 3D Avrami
- An, n-Dim. Avrami
- Nk, Nakamura crystallization (An + HL)
- SBC, Sestak-Berggren crystallization (SB + HL)



OFW model-free

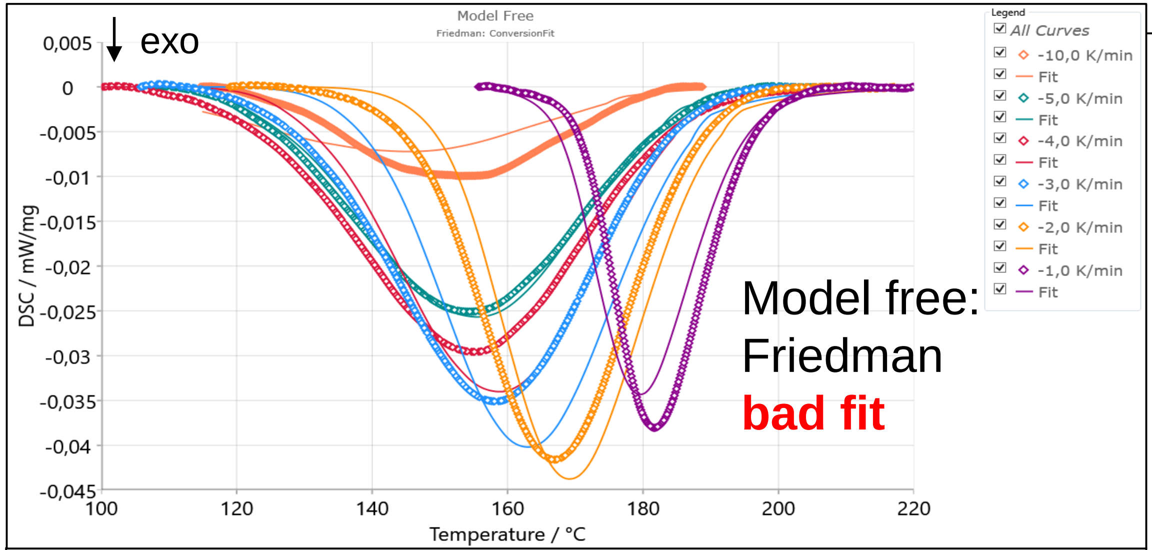
Lines are not parallel



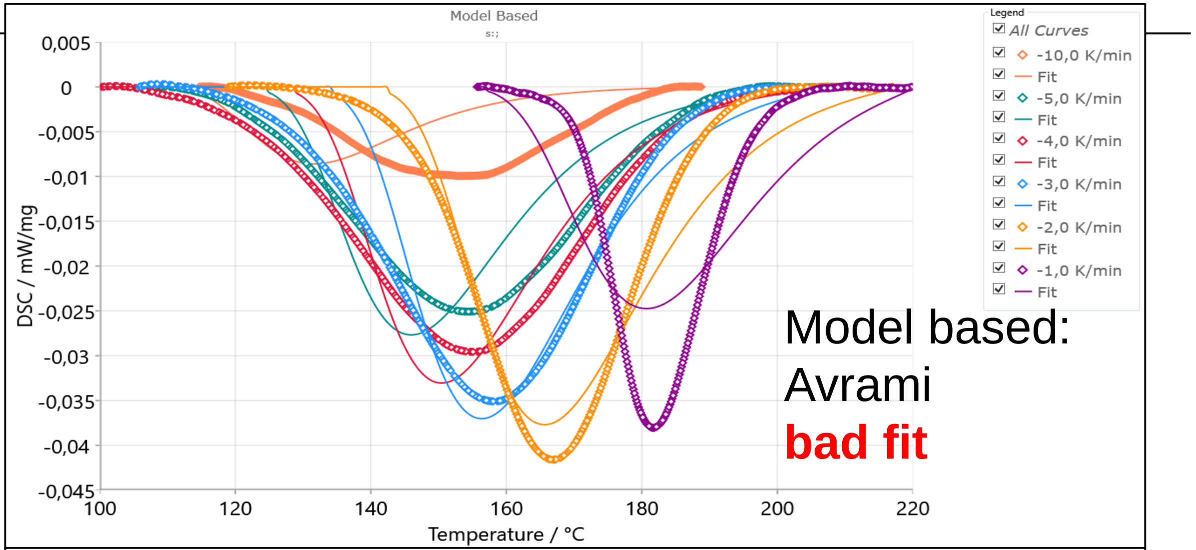
OFW model free:

bad fit

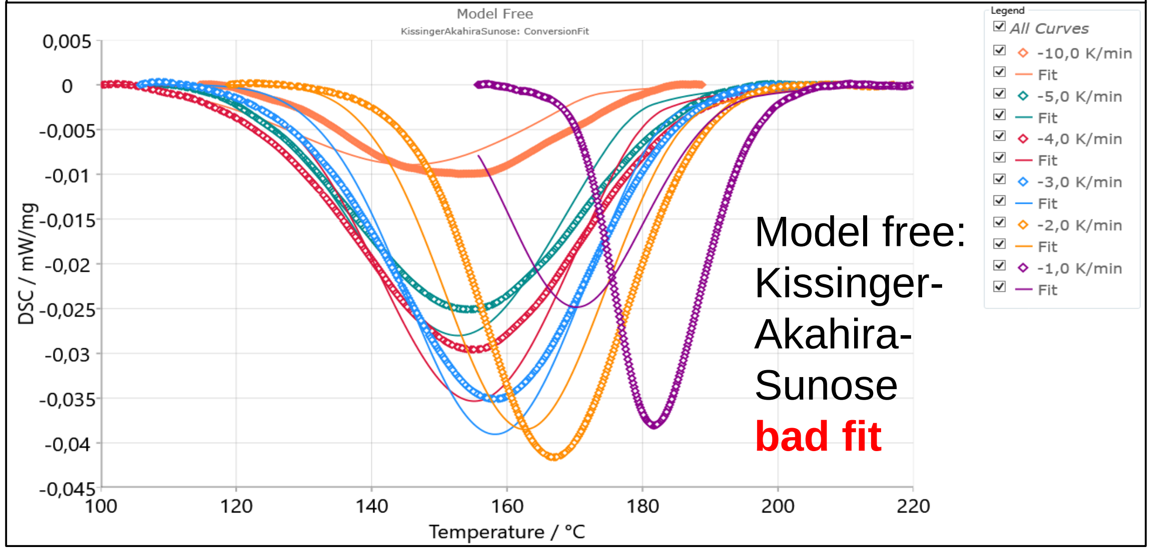
Arrhenius approach: bad fit for both model free and model based



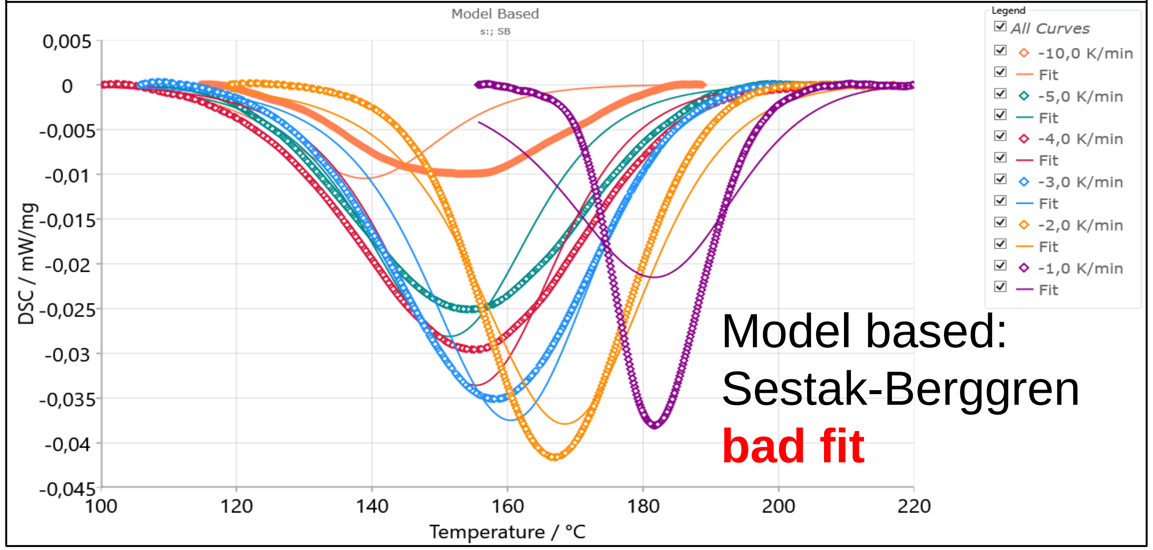
Model free:
Friedman
bad fit



Model based:
Avrami
bad fit



Model free:
Kissinger-
Akahira-
Sunose
bad fit



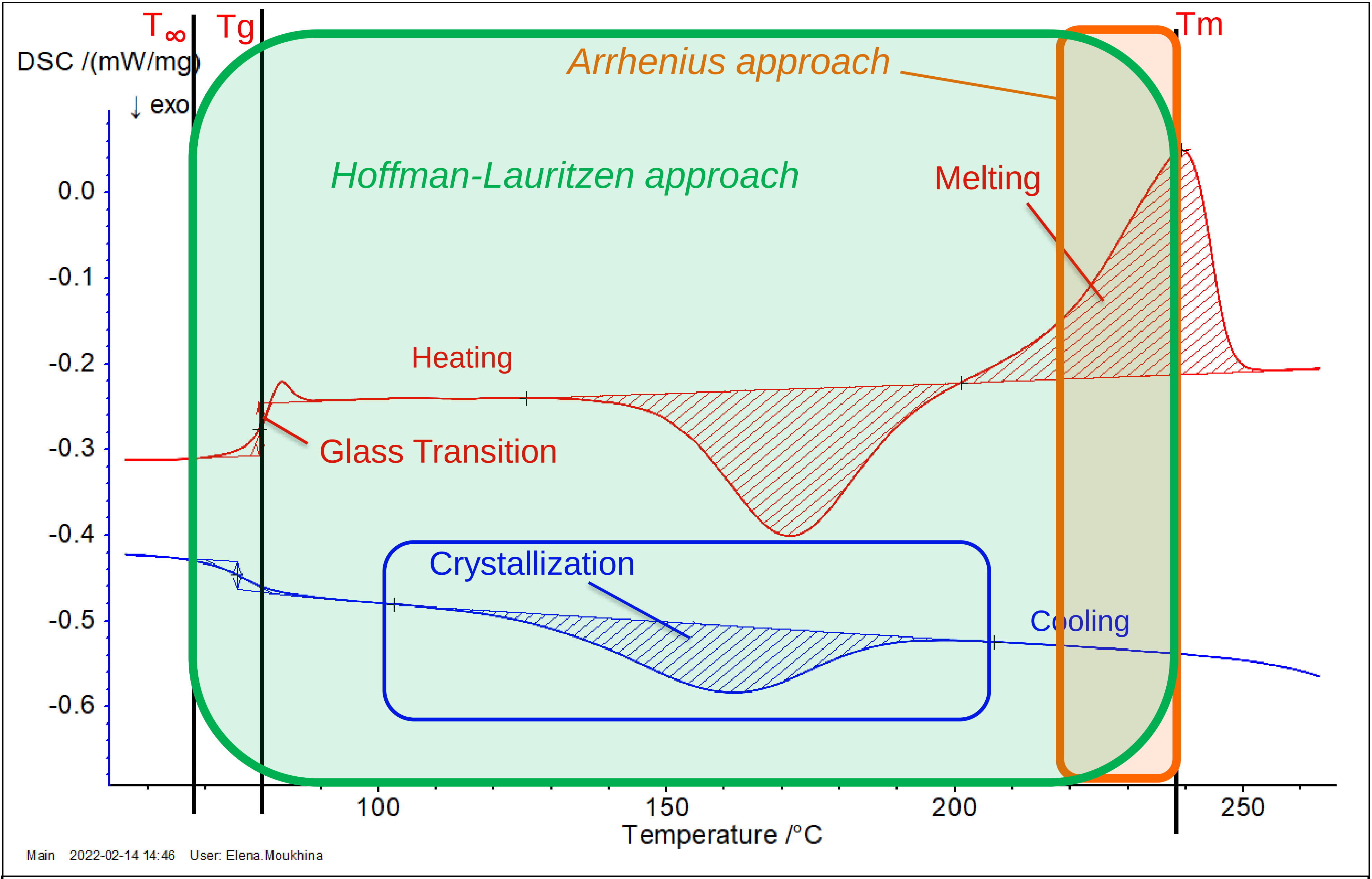
Model based:
Sestak-Berggren
bad fit

Methods working well for isothermal conditions, can not work for cooling conditions for wide temperature range

Reason: K(T) has non- Arrhenius dependence

Polymer: Heating and Cooling

NETZSCH



Crystallization kinetics: non-Arrhenius approach: Nakamura und Hoffman-Lauritzen

Avrami nucleation

$$\frac{d\alpha}{dt} = A \cdot f(\alpha) \cdot K(T)$$

Diffusion term

Nucleation term

$$K(T) = exp\left(\frac{-U^*}{R(T-\boxed{T_\infty})}\right) \cdot exp\left(\frac{-K_G}{T \cdot \boxed{\Delta T \cdot} f}\right)$$

No viscose flow below Tg

Supercooling

U*	activation energy of segmental jump in polymers, this parameter has universal value 6.3kJ/mol
K_G	kinetic parameter for nucleation
$\Delta T = Tm - T$	undercooling from the equilibrium ***melting point Tm***
$T_\infty = Tg - 30$	temperature at which crystallization transport is finished, this temperature is 30K below the ***glass transition temperature Tg***.
f=2T/(T+Tm)	correction factor

This method defined for total temperature range between T_∞ and $T_{melting}$

Hoffman-Lauritzen Theory

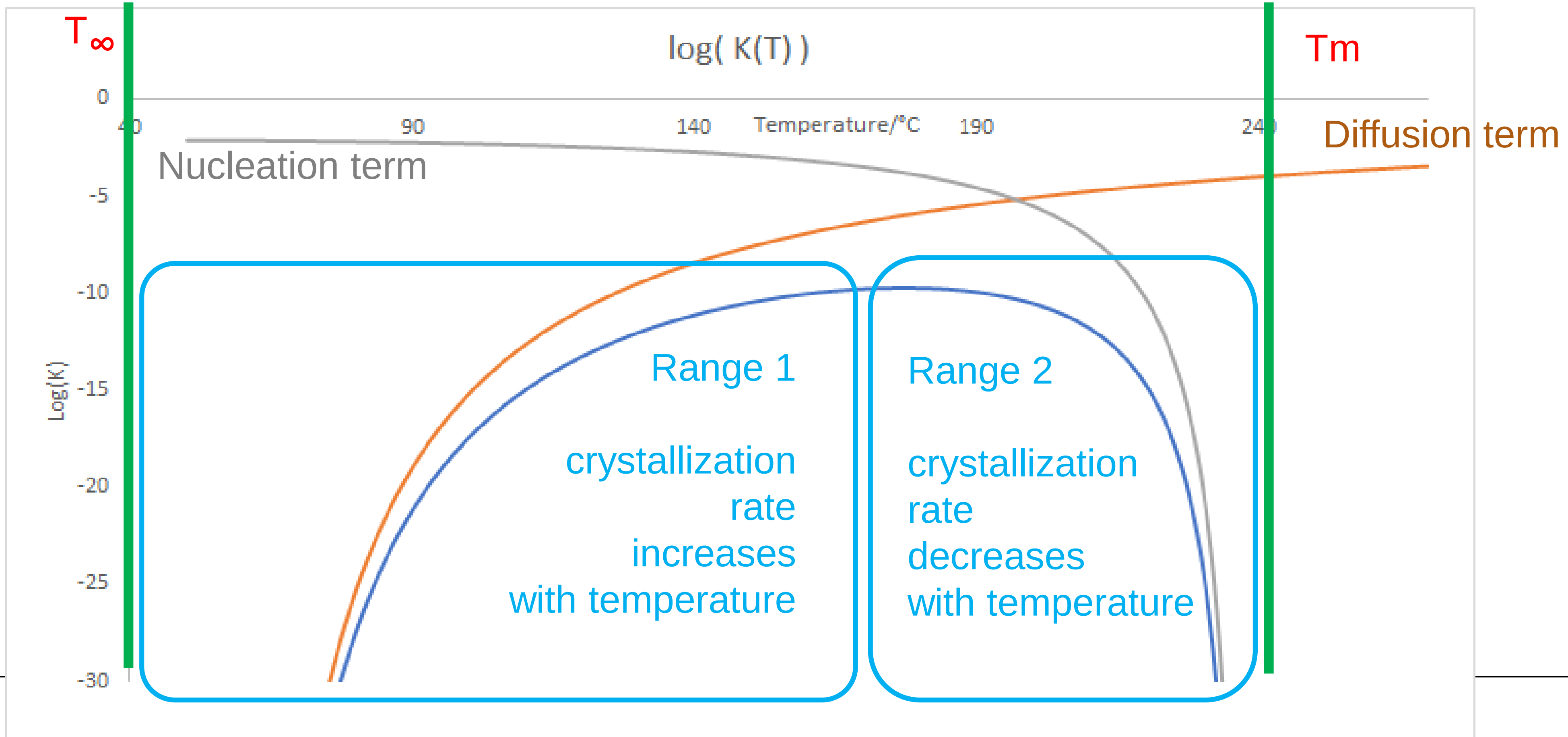
NETZSCH

$$\frac{d\alpha}{dt} = A \cdot f(\alpha) \cdot K(T)$$

$$\boxed{K(T)} = \boxed{exp\left(\frac{U^*}{R(T - T_\infty)}\right)} \cdot \boxed{exp\left(\frac{-K_G}{T(T - T_m)f}\right)}$$

Diffusion term

Nucleation term



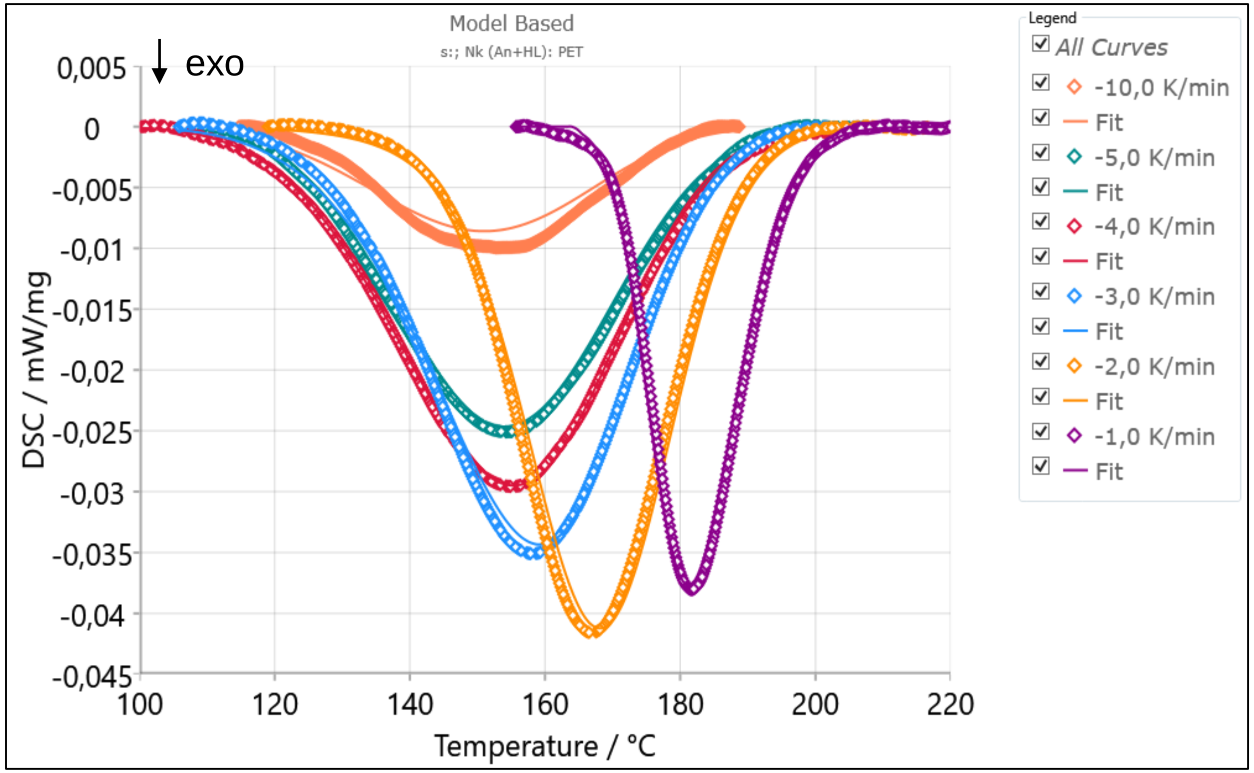
Range 1

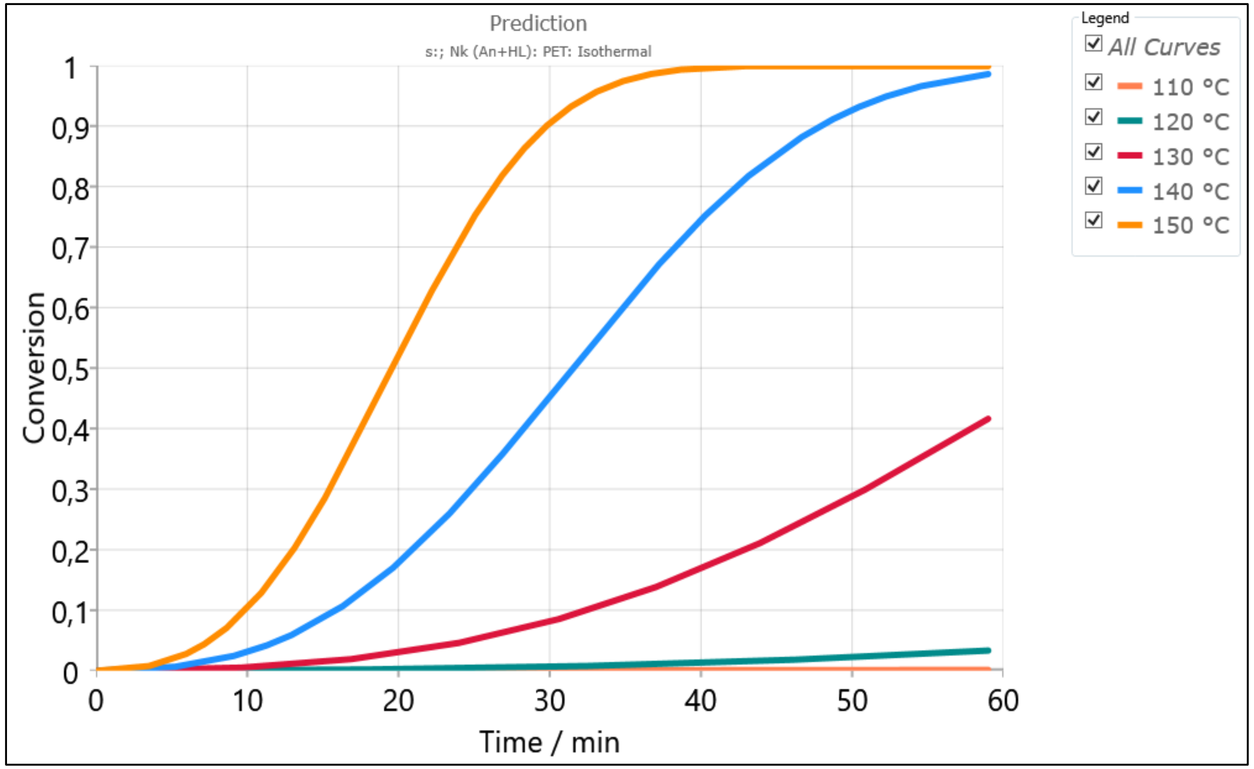
crystallization rate increases with temperature

Range 2

crystallization rate decreases with temperature

Crystallization Prediction for Polyethylene Terephthalate (PET)

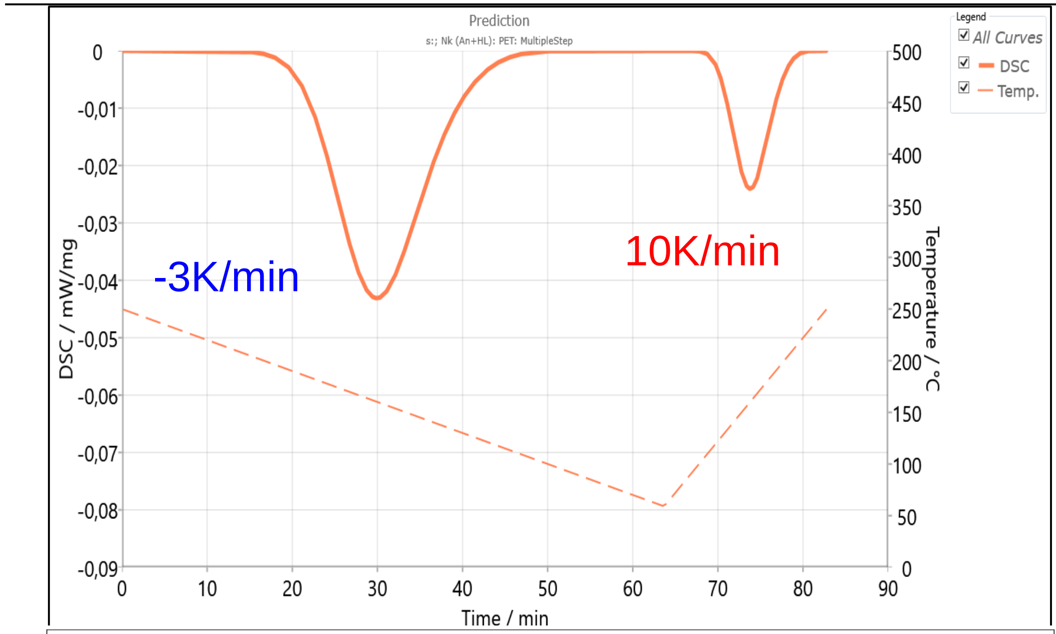


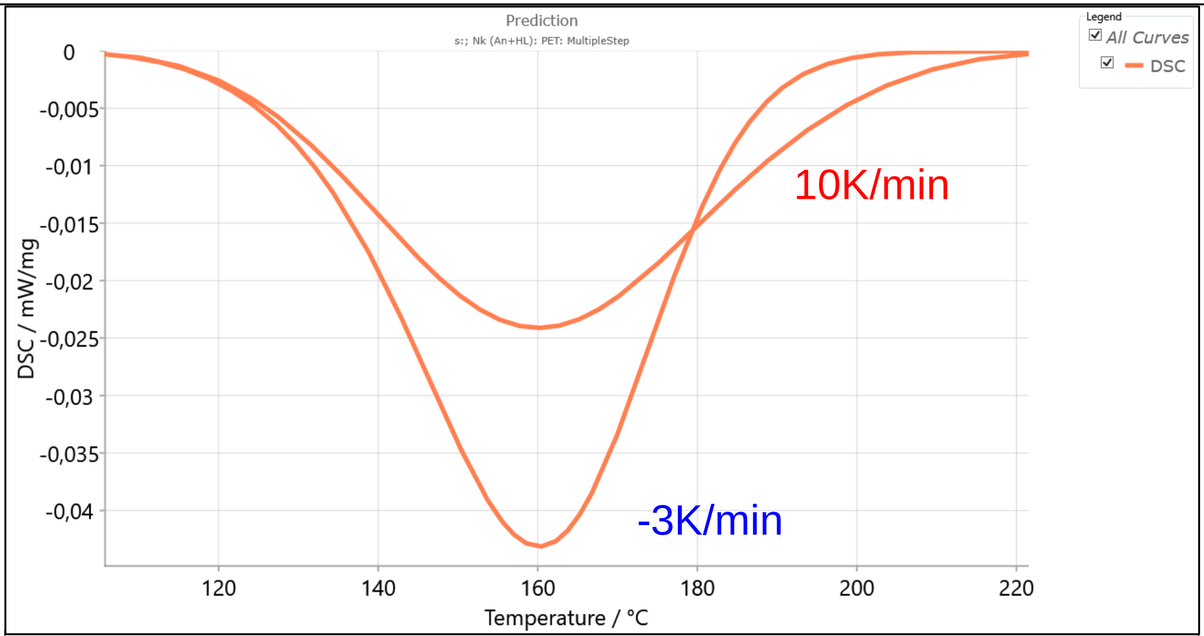


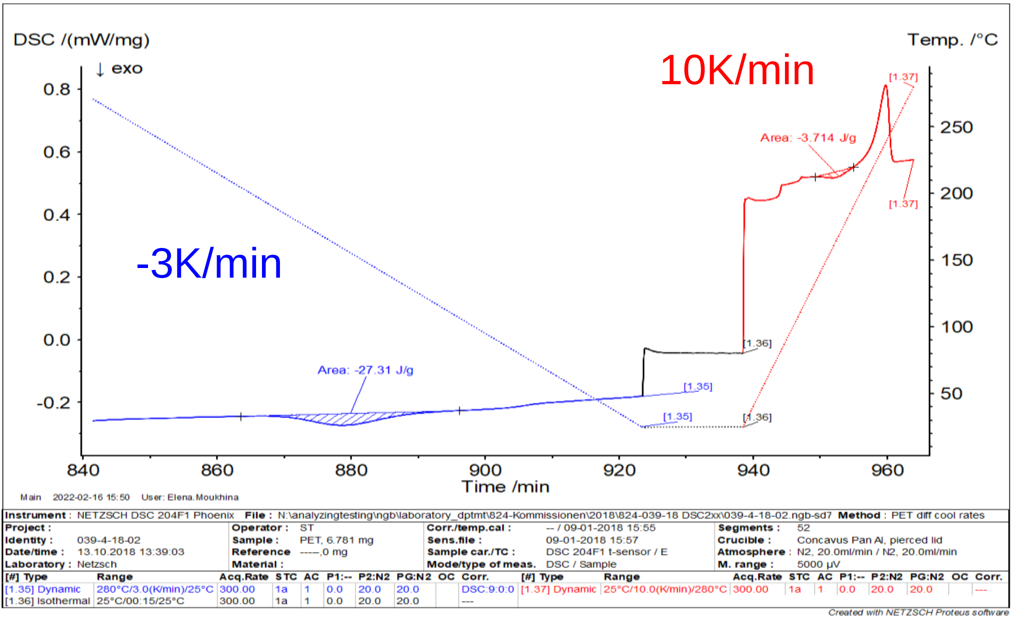
One can observe that at temperatures of 110°C to 120°C, no crystallization occurs and the bottles remain in the glassy state and transparent. If the production temperature is too high – e.g., 140°C – then crystallization starts earlier, and the bottles get turbid.

PET:
stretch
blow
molding

PET: Comparison with experiment for complex temperature program







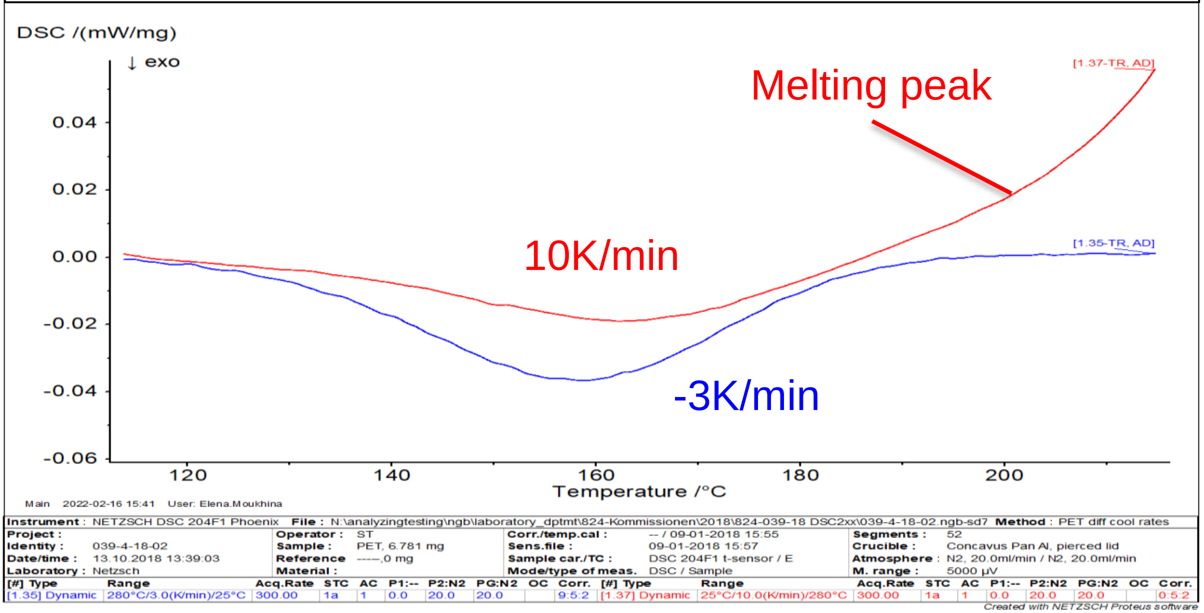
Main 2022-02-16 15:50 User: Elena.Moukhina

Instrument : NETZSCH DSC 204F1 Phoenix **File :** N:\analyzingtesting\ngb\laboratory_dptmt\824-Kommissionen\2018\824-039-18 DSC2xx\039-4-18-02.ngb-sd7 **Method :** PET diff cool rates

Project :
Identity : 039-4-18-02
Date/time : 13.10.2018 13:39:03
Laboratory : Netzsch
Operator : ST
Sample : PET, 6.781 mg
Reference ----,0 mg
Material :
Corr./temp.cal : -- / 09-01-2018 15:55
Sens.file : 09-01-2018 15:57
Sample car./TC : DSC 204F1 t-sensor / E
Mode/type of meas. DSC / Sample
Segments : 52
Crucible : Concavus Pan Al, pierced lid
Atmosphere : N2, 20.0ml/min / N2, 20.0ml/min
M. range : 5000 µV

[#] Type	Range	Acq.Rate	STC	AC	P1:--	P2:N2	PG:N2	OC	Corr.
[1.35] Dynamic	280°C/3.0(K/min)/25°C	300.00	1a	1	0.0	20.0	20.0		DSC:9:0:0
[1.36] Isothermal	25°C/00:15/25°C	300.00	1a	1	0.0	20.0	20.0		---
[1.37] Dynamic	25°C/10.0(K/min)/280°C	300.00	1a	1	0.0	20.0	20.0		---

Created with NETZSCH Proteus software



Main 2022-02-16 15:41 User: Elena.Moukhina

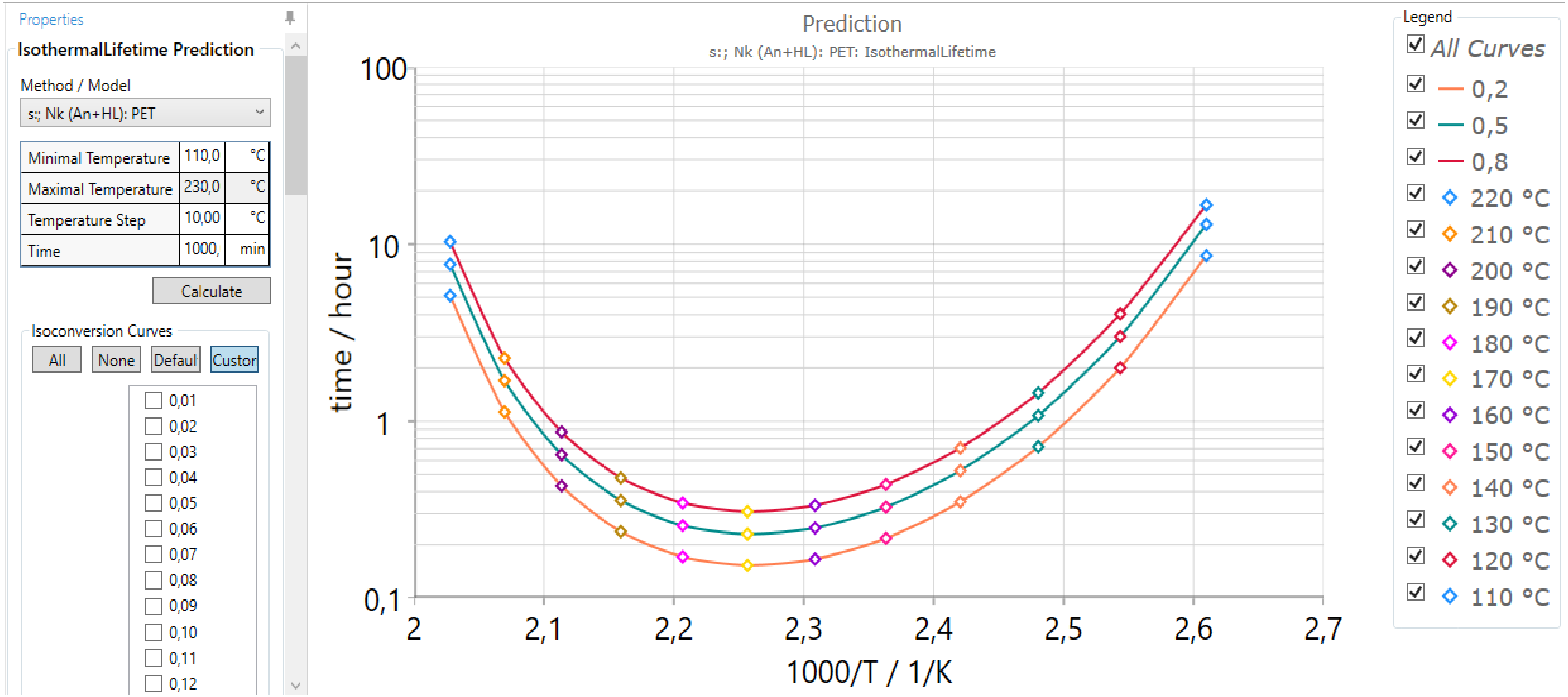
Instrument : NETZSCH DSC 204F1 Phoenix **File :** N:\analyzingtesting\ngb\laboratory_dptmt\824-Kommissionen\2018\824-039-18 DSC2xx\039-4-18-02.ngb-sd7 **Method :** PET diff cool rates

Project :
Identity : 039-4-18-02
Date/time : 13.10.2018 13:39:03
Laboratory : Netzsch
Operator : ST
Sample : PET, 6.781 mg
Reference ----,0 mg
Material :
Corr./temp.cal : -- / 09-01-2018 15:55
Sens.file : 09-01-2018 15:57
Sample car./TC : DSC 204F1 t-sensor / E
Mode/type of meas. DSC / Sample
Segments : 52
Crucible : Concavus Pan Al, pierced lid
Atmosphere : N2, 20.0ml/min / N2, 20.0ml/min
M. range : 5000 µV

[#] Type	Range	Acq.Rate	STC	AC	P1:--	P2:N2	PG:N2	OC	Corr.
[1.35] Dynamic	280°C/3.0(K/min)/25°C	300.00	1a	1	0.0	20.0	20.0		9:5:2
[1.37] Dynamic	25°C/10.0(K/min)/280°C	300.00	1a	1	0.0	20.0	20.0		0:5:2

Created with NETZSCH Proteus software

Isothermal Lifetime: predictions for 20%, 50% and 80% crystallization



Properties

IsothermalLifetime Prediction

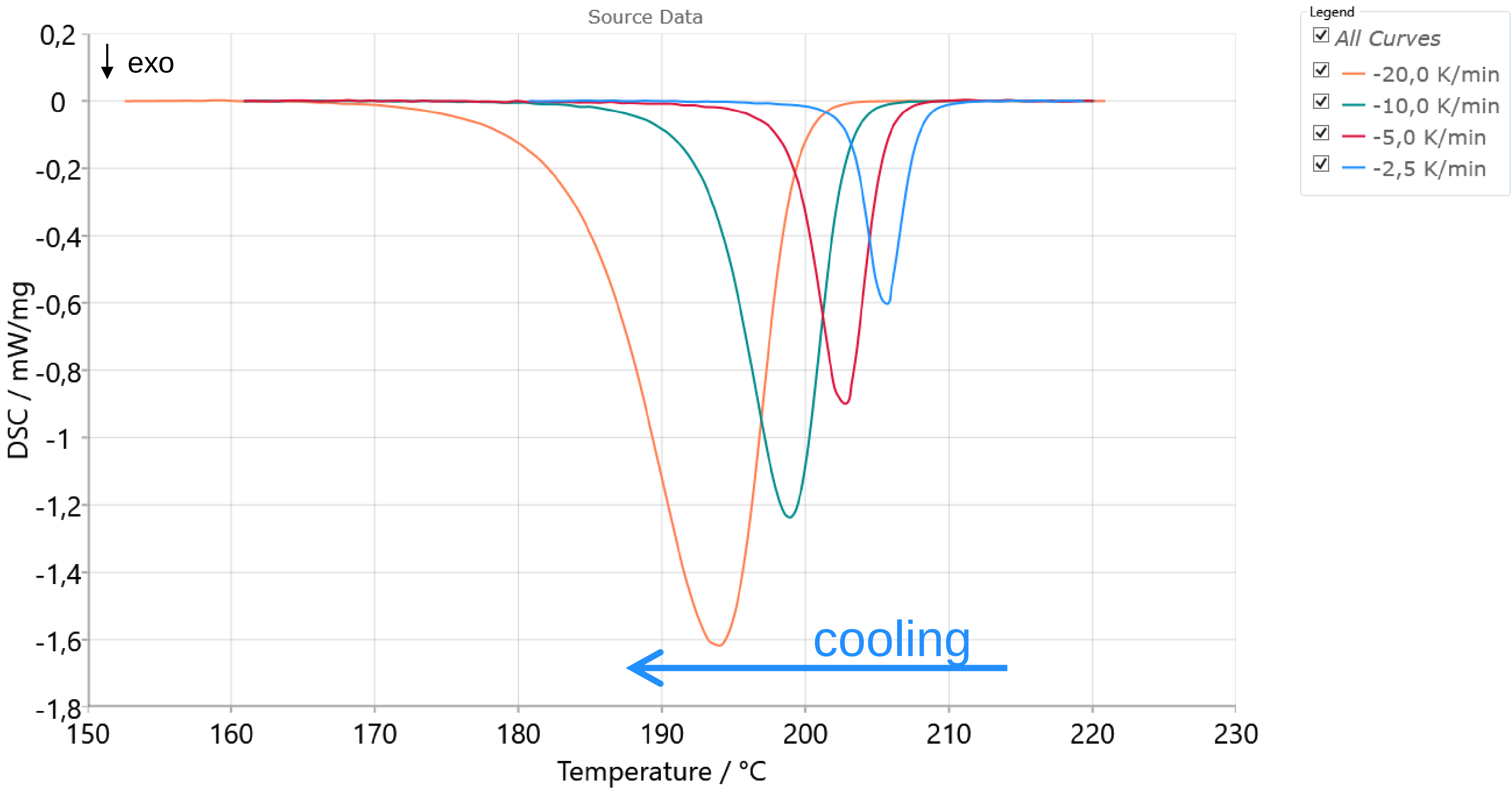
Method / Model: s:; Nk (An+HL): PET

Minimal Temperature	110,0	°C
Maximal Temperature	230,0	°C
Temperature Step	10,00	°C
Time	1000,	min

Crystallisation of PBT during cooling

PBT

Tg= 40-60°C, Tm=220-230°C



Crystallization model SBC with Sestak-Berggren reaction type

Crystallization rate

$$\frac{d\alpha}{dt} = A \cdot f(\alpha) \cdot K(T)$$

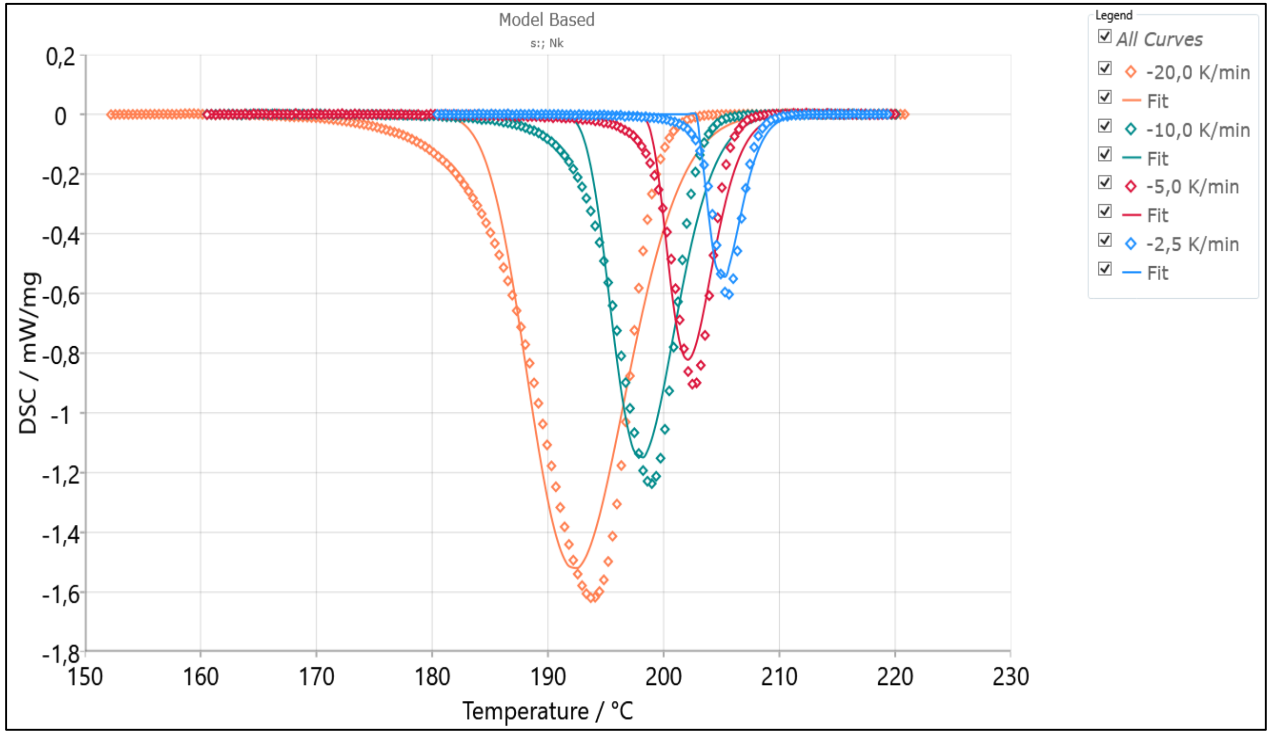
Hoffman-Lauritzen Theory

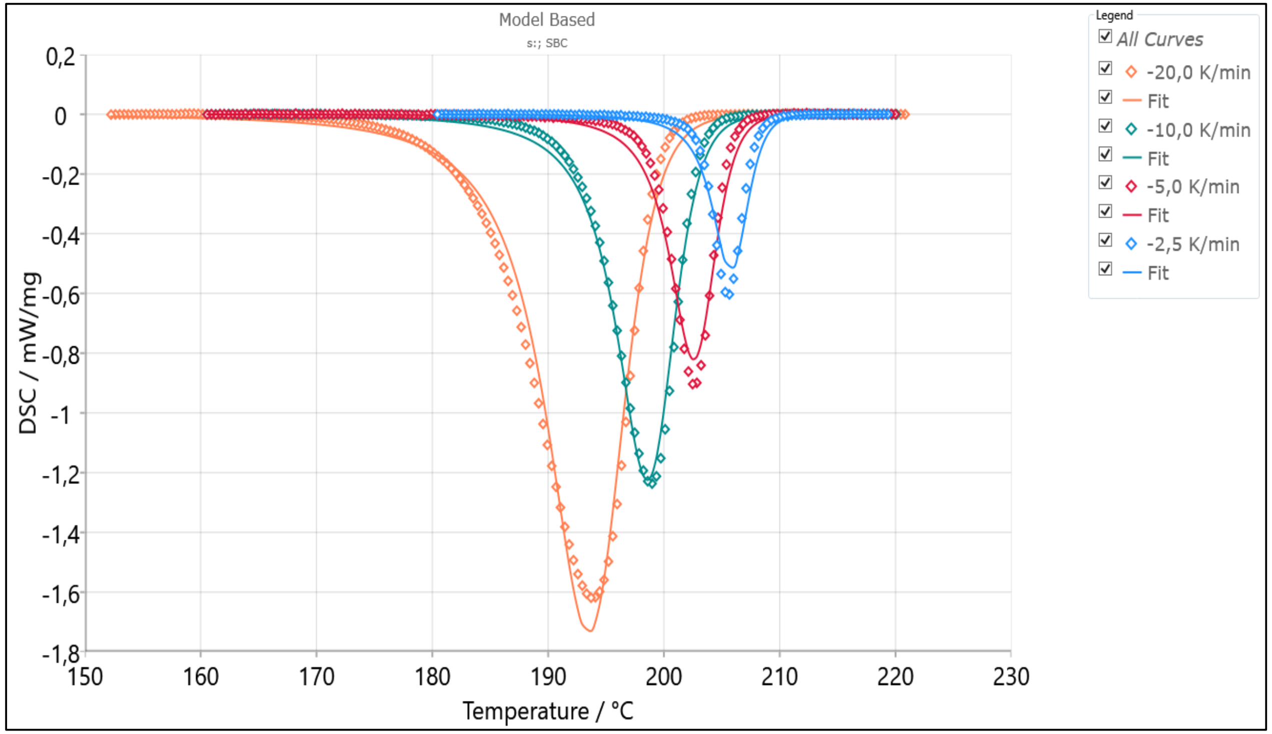
Avrami nucleation

$f(\alpha)=n \cdot (1-\alpha) \cdot [-\ln((1-\alpha))]^{(n-1)/n}$

Sestak-Berggren Crystallization

$f(\alpha)=(1-\alpha)^{n} \cdot \alpha^{m} \cdot [-\ln((1-\alpha))]^{q}$



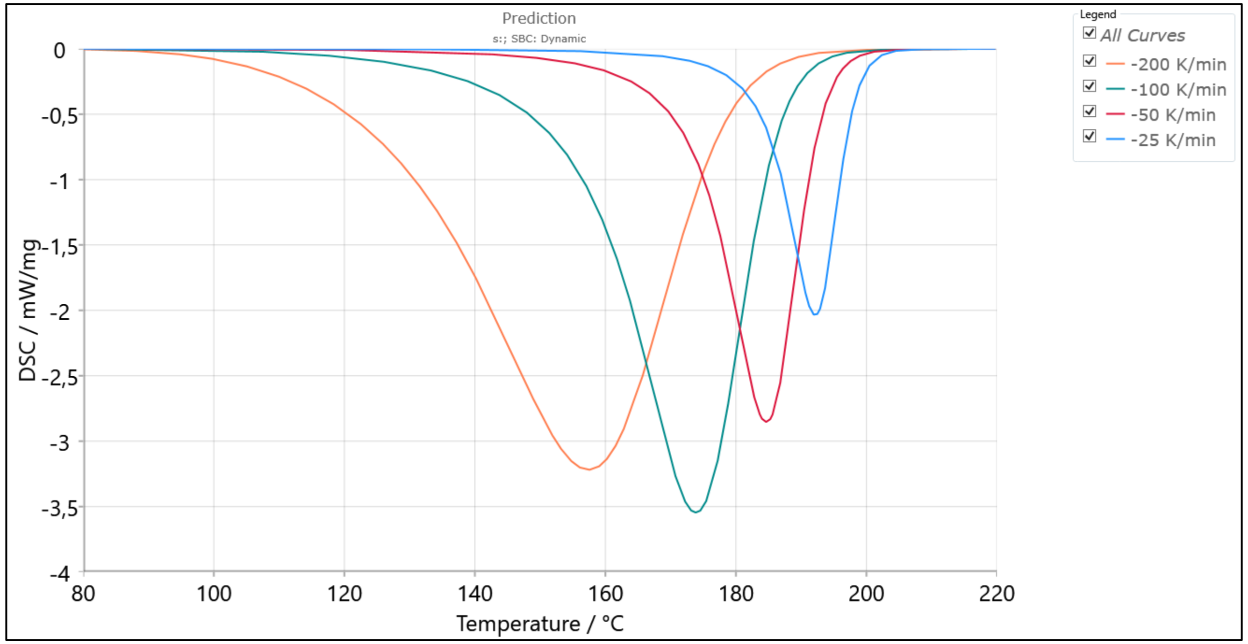


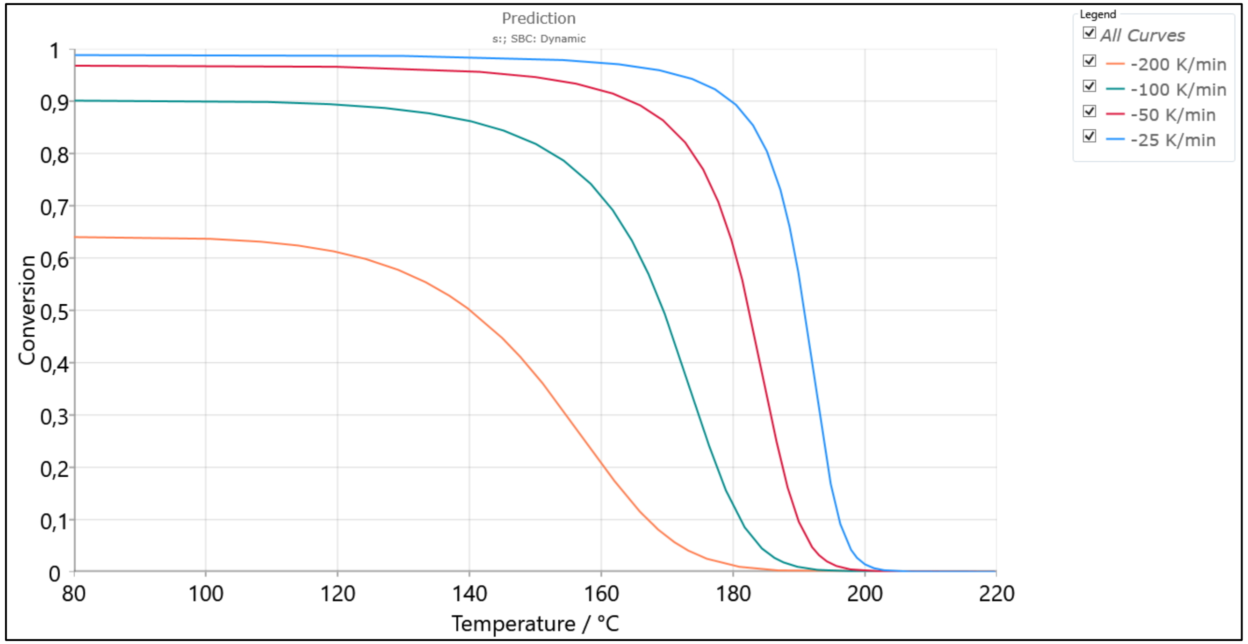
Nathanael Guigo, Jesper van Berkel, Ed de Jong , Nicolas Sbirrazzuoli, Thermochimica Acta 650 (2017) 66-75

PBT: Predictions for cooling with SBC model

Predictions: Signal

Predictions: Conversion





← cooling

Crystallization is **not complete** for fast cooling
because of diffusion near **glass transition**
Polymer is partially **amorphous**

4. Predictions, Simulations,

Advantages and Limitation of different models for simulations

Crystallization kinetics

Avrami nucleation

Sestak-Berggren Crystallization

Crystallization rate $$\frac{d\alpha}{dt} = A \cdot f(\alpha) \cdot K(T)$$

1. Arrhenius approach

(model free and model based)

$$K(T) = exp\left(\frac{-E_a}{RT}\right)$$

$E_a<0$

Partial solution only for isothermal crystallization
Works in small range below melting temperature

2. Non-Arrhenius approach

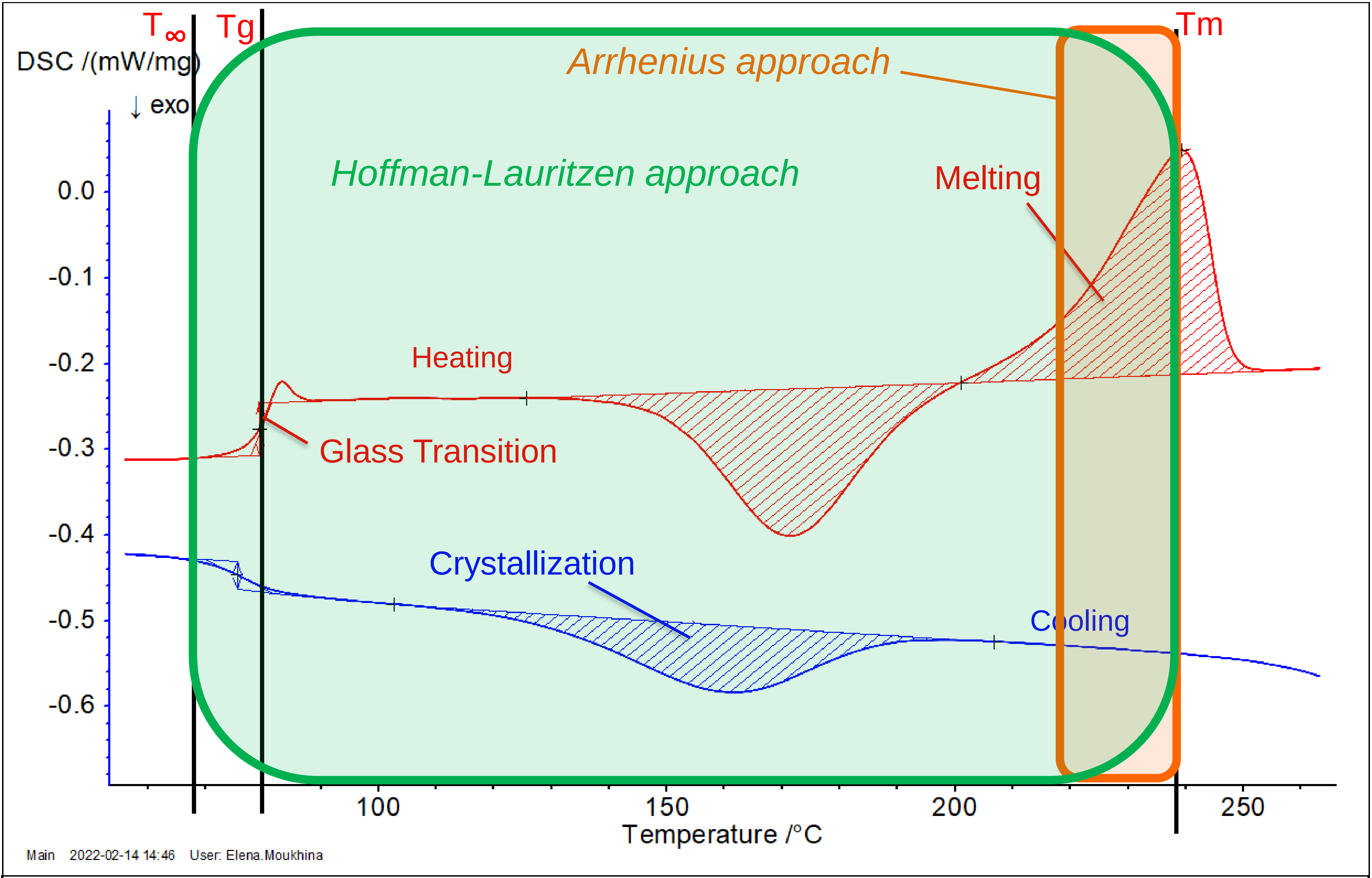
(model based only)

- Hoffman-Lauritzen Theory

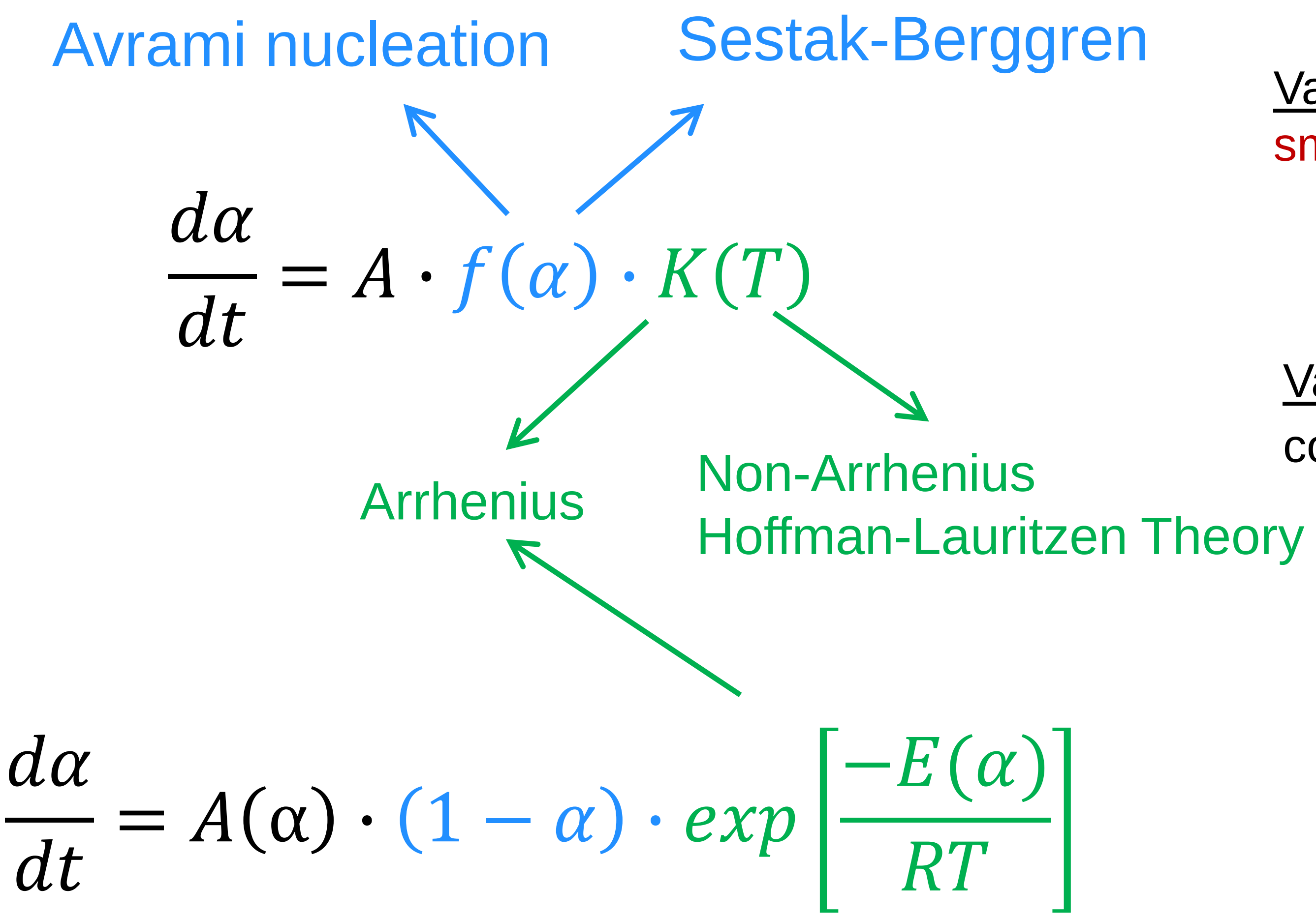
$$K(T) = exp\left(\frac{U^*}{R(T-T_\infty)}\right) \cdot exp\left(\frac{-K_G}{T\Delta T f}\right)$$

Solution for both isothermal and cooling crystallization
Works for complete crystallization range

Polymer: Heating and Cooling



Crystallization kinetics



Avrami nucleation

Sestak-Berggren

$$\frac{d\alpha}{dt} = A \cdot f(\alpha) \cdot K(T)$$

Arrhenius

Non-Arrhenius
Hoffman-Lauritzen Theory

$$\frac{d\alpha}{dt} = A(\alpha) \cdot (1-\alpha) \cdot exp\left[\frac{-E(\alpha)}{RT}\right]$$

Model based reaction type:

An: Avrami+ Arrhenius

SB: Sestak Berggren + Arrhenius

Valid: isothermal crystallization,
small temperature range

Nakamura: Avrami+ Hoffman-Lauritzen

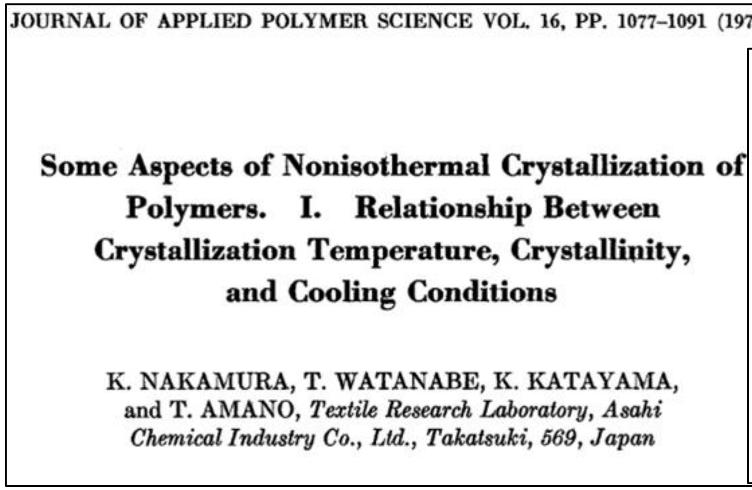
SBC: Sestak-Berggren+ Hoffman-Lauritzen

Valid: both isothermal and cooling crystallization
complete temperature range between T_∞ and Tm

Model free:

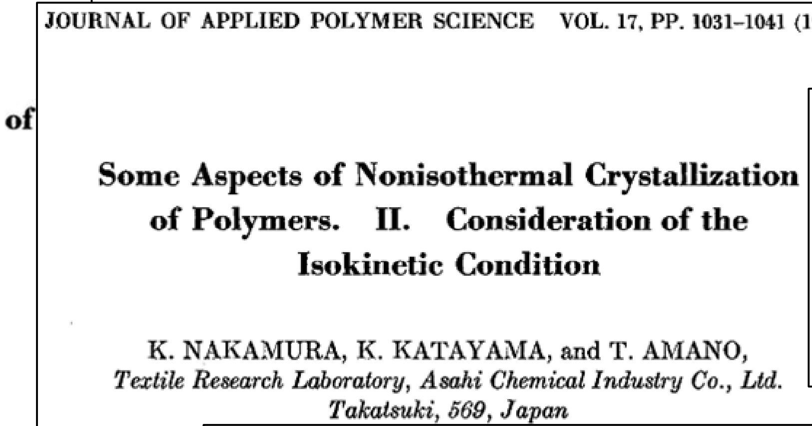
ASTM2070
Friedman
Numerical Optimization

Valid: isothermal crystallization,
small temperature range


JOURNAL OF APPLIED POLYMER SCIENCE VOL. 16, PP. 1077–1091 (1972)

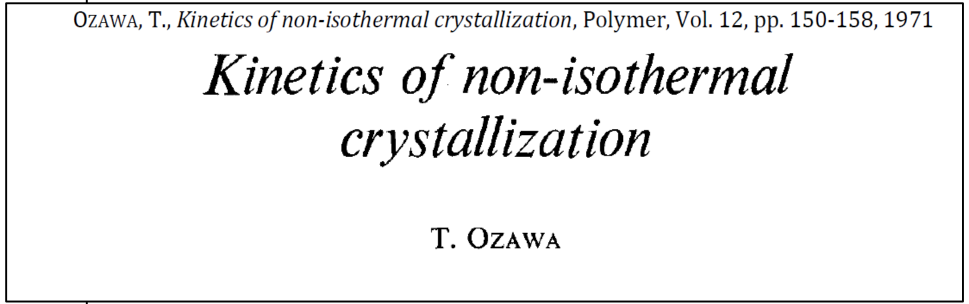
Some Aspects of Nonisothermal Crystallization of Polymers. I. Relationship Between Crystallization Temperature, Crystallinity, and Cooling Conditions

K. NAKAMURA, T. WATANABE, K. KATAYAMA, and T. AMANO, *Textile Research Laboratory, Asahi Chemical Industry Co., Ltd., Takatsuki, 569, Japan*


JOURNAL OF APPLIED POLYMER SCIENCE VOL. 17, PP. 1031–1041 (1973))

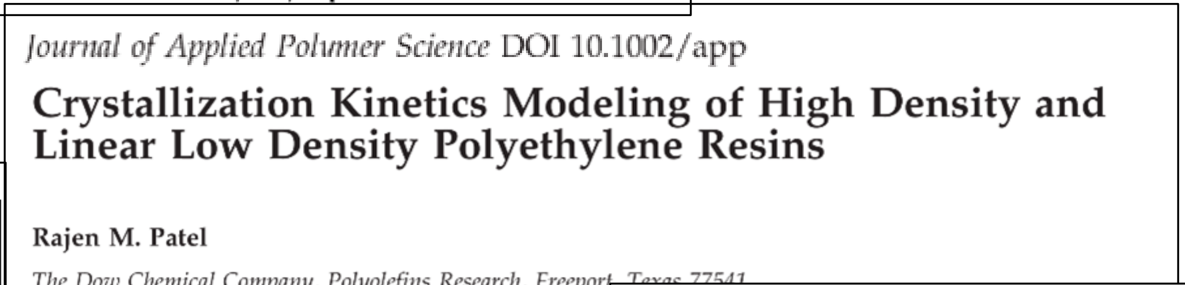
Some Aspects of Nonisothermal Crystallization of Polymers. II. Consideration of the Isokinetic Condition

K. NAKAMURA, K. KATAYAMA, and T. AMANO, *Textile Research Laboratory, Asahi Chemical Industry Co., Ltd. Takatsuki, 569, Japan*


OZAWA, T., *Kinetics of non-isothermal crystallization*, Polymer, Vol. 12, pp. 150-158, 1971

Kinetics of non-isothermal crystallization

T. OZAWA

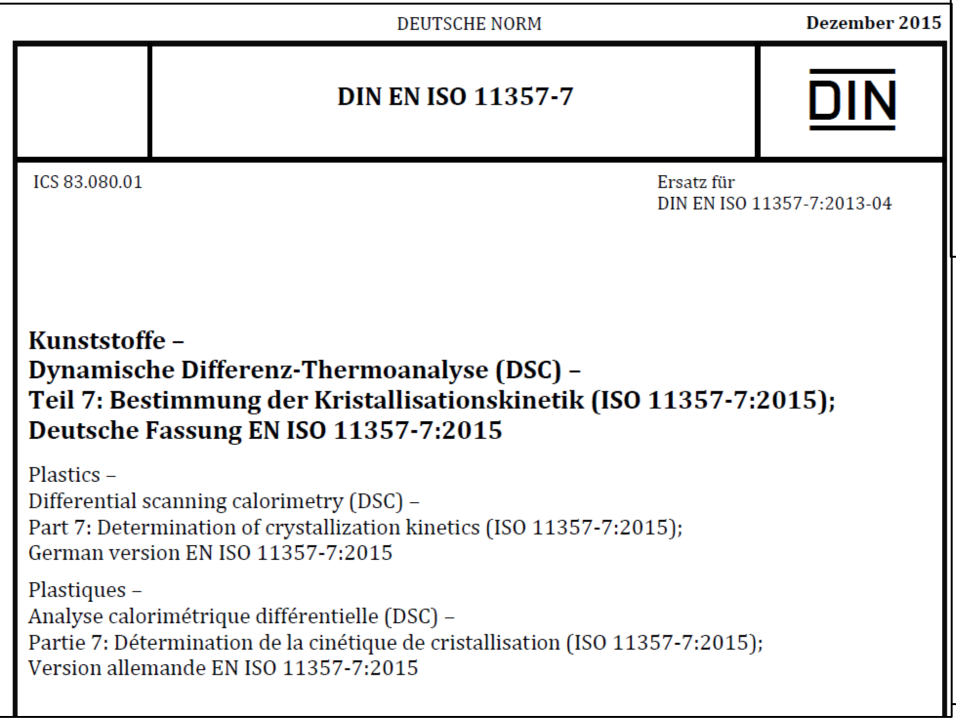

Journal of Applied Polymer Science DOI 10.1002/app

Crystallization Kinetics Modeling of High Density and Linear Low Density Polyethylene Resins

Rajen M. Patel

The Dow Chemical Company, Polyolefins Research, Freeport, Texas 77541

Received 21 February 2011; accepted 16 May 2011
DOI 10.1002/app.35177
Published online 20 October 2011 in Wiley Online Library (w


DEUTSCHE NORM **Dezember 2015**

DIN EN ISO 11357-7 DIN

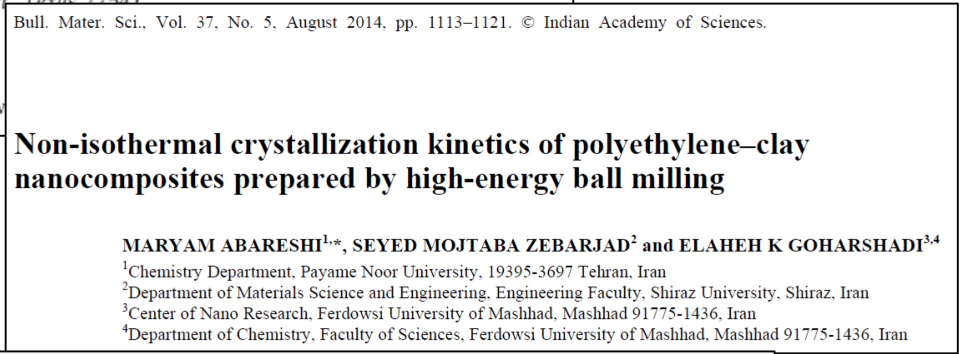
ICS 83.080.01

Ersatz für
DIN EN ISO 11357-7:2013-04

Kunststoffe –
Dynamische Differenz-Thermoanalyse (DSC) –
Teil 7: Bestimmung der Kristallisationskinetik (ISO 11357-7:2015);
Deutsche Fassung EN ISO 11357-7:2015

Plastics –
Differential scanning calorimetry (DSC) –
Part 7: Determination of crystallization kinetics (ISO 11357-7:2015);
German version EN ISO 11357-7:2015

Plastiques –
Analyse calorimétrique différentielle (DSC) –
Partie 7: Détermination de la cinétique de cristallisation (ISO 11357-7:2015);
Version allemande EN ISO 11357-7:2015


Bull. Mater. Sci., Vol. 37, No. 5, August 2014, pp. 1113–1121. © Indian Academy of Sciences.

Non-isothermal crystallization kinetics of polyethylene–clay nanocomposites prepared by high-energy ball milling

MARYAM ABARESHI[1,*], SEYED MOJTABA ZEBARJAD[2] and ELAHEH K GOHARSHADI[3,4]
[1]Chemistry Department, Payame Noor University, 19395-3697 Tehran, Iran
[2]Department of Materials Science and Engineering, Engineering Faculty, Shiraz University, Shiraz, Iran
[3]Center of Nano Research, Ferdowsi University of Mashhad, Mashhad 91775-1436, Iran
[4]Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad 91775-1436, Iran

---


Thermochimica Acta 650 (2017) 66–75

Modelling the non-isothermal crystallization of polymers: Application to poly(ethylene 2,5-furandicarboxylate)

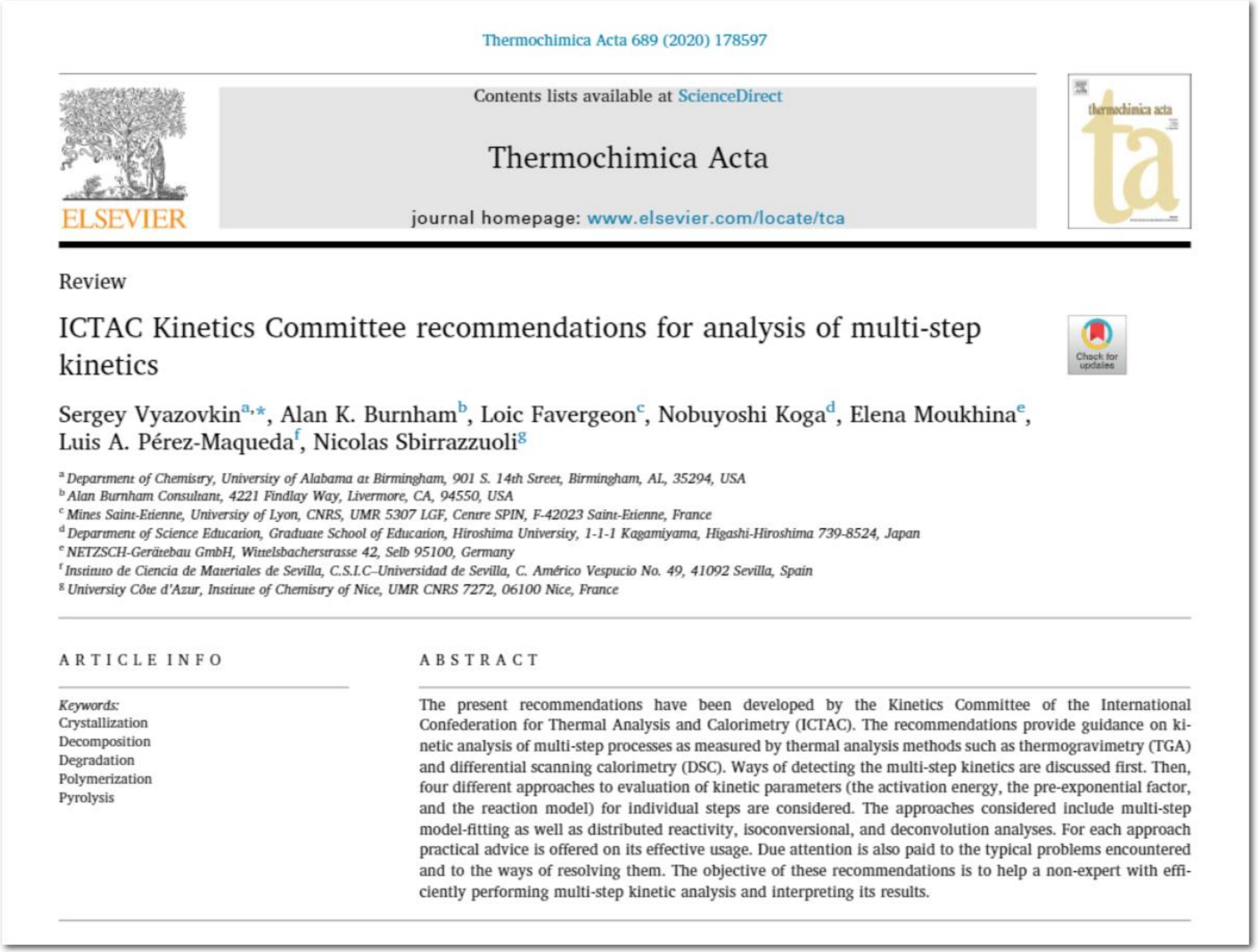
Nathanael Guigo[a], Jesper van Berkel[b], Ed de Jong[b], Nicolas Sbirrazzuoli[a,*]

[a] *Université Côte d'Azur, Institut de Chimie de Nice, UMR CNRS 7272, 06108 Nice, France*
[b] *Avantium Chemicals B.V., Zekeringstraat 29, 1014 BV, Amsterdam, The Netherlands*

Unique: Kinetics Analysis must fulfils ICTAC kinetics recommendations

NETZSCH

International Confederation for Thermal Analysis and Calorimetry



Thermochimica Acta 689 (2020) 178597

Contents lists available at ScienceDirect

Thermochimica Acta

journal homepage: www.elsevier.com/locate/tca

ELSEVIER

Review

ICTAC Kinetics Committee recommendations for analysis of multi-step kinetics

Sergey Vyazovkin[a,*], Alan K. Burnham[b], Loic Favergeon[c], Nobuyoshi Koga[d], Elena Moukhina[e], Luis A. Pérez-Maqueda[f], Nicolas Sbirrazzuoli[g]

[a] *Department of Chemistry, University of Alabama at Birmingham, 901 S. 14th Street, Birmingham, AL, 35294, USA*
[b] *Alan Burnham Consultant, 4221 Findlay Way, Livermore, CA, 94550, USA*
[c] *Mines Saint-Etienne, University of Lyon, CNRS, UMR 5307 LGF, Centre SPIN, F-42023 Saint-Etienne, France*
[d] *Department of Science Education, Graduate School of Education, Hiroshima University, 1-1-1 Kagamiyama, Higashi-Hiroshima 739-8524, Japan*
[e] *NETZSCH-Gerätebau GmbH, Wittelsbacherstrasse 42, Selb 95100, Germany*
[f] *Instituto de Ciencia de Materiales de Sevilla, C.S.I.C–Universidad de Sevilla, C. Américo Vespucio No. 49, 41092 Sevilla, Spain*
[g] *University Côte d'Azur, Institute of Chemistry of Nice, UMR CNRS 7272, 06100 Nice, France*

ARTICLE INFO

Keywords:
Crystallization
Decomposition
Degradation
Polymerization
Pyrolysis

ABSTRACT

The present recommendations have been developed by the Kinetics Committee of the International Confederation for Thermal Analysis and Calorimetry (ICTAC). The recommendations provide guidance on kinetic analysis of multi-step processes as measured by thermal analysis methods such as thermogravimetry (TGA) and differential scanning calorimetry (DSC). Ways of detecting the multi-step kinetics are discussed first. Then, four different approaches to evaluation of kinetic parameters (the activation energy, the pre-exponential factor, and the reaction model) for individual steps are considered. The approaches considered include multi-step model-fitting as well as distributed reactivity, isoconversional, and deconvolution analyses. For each approach practical advice is offered on its effective usage. Due attention is also paid to the typical problems encountered and to the ways of resolving them. The objective of these recommendations is to help a non-expert with efficiently performing multi-step kinetic analysis and interpreting its results.

- Model free analysis
- Multi-step model-fitting (model based)
- Diffusion control for curing
- Crystallization kinetics
- Kamal model for curing
- Deconvolution analysis (sum of peaks)

KINETICS
NEO

NETZSCH Kinetics Neo Web Site

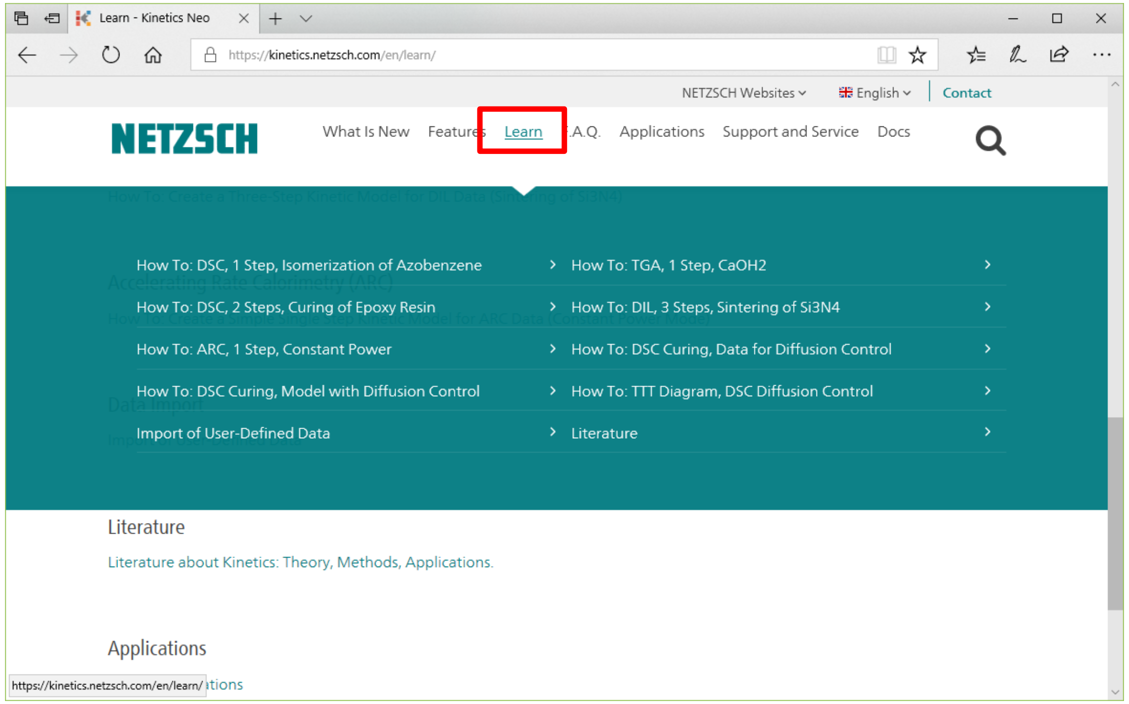
https://kinetics.netzsch.com

Users Guide, Training examples,

Webinars: Thermokinetics (pdf and video):

- *Advantages and disadvantages of different kinetics approaches.*
- *Unique and powerful features of NETZSCH Kinetics Neo software*

Trial Version 30 days



How To: DSC, 1 Step, Isomerization of Azobenzene

How To: TGA, 1 Step, CaOH2

How To: DSC, 2 Steps, Curing of Epoxy Resin

How To: DIL, 3 Steps, Sintering of Si3N4

How To: ARC, 1 Step, Constant Power

How To: DSC Curing, Data for Diffusion Control

How To: DSC Curing, Model with Diffusion Control

How To: TTT Diagram, DSC Diffusion Control

Import of User-Defined Data

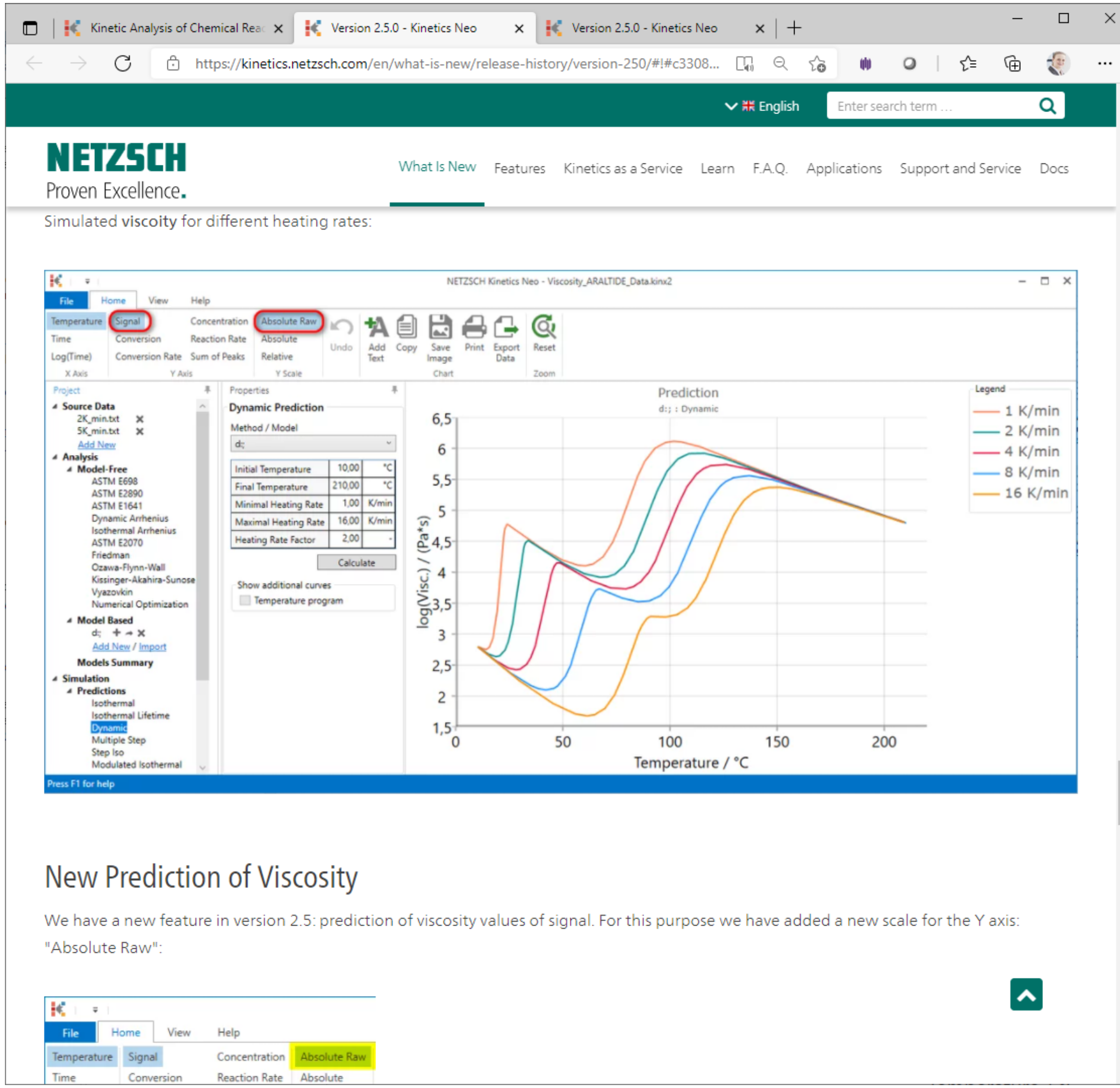
Literature

Literature

Literature about Kinetics: Theory, Methods, Applications.

Applications

https://kinetics.netzsch.com/en/learn/



Simulated viscosity for different heating rates:

New Prediction of Viscosity

We have a new feature in version 2.5: prediction of viscosity values of signal. For this purpose we have added a new scale for the Y axis: "Absolute Raw":

Conclusion

NETZSCH

KINETICS NEO is used to analyze kinetics of temperature dependent chemical processes.

Analysis

- one mathematical kinetic description for several measurements
- different approaches: model free (11 methods) and model based (unlimited number of models)
- model based: individual reaction steps, concentrations, kinetic triplet for each step, reaction mechanism
- standard reaction types (n-th order, Autocatalysis, diffusion, Avrami nucleation)
- unique reaction types (Kamal-Sourour, diffusion control, Nakamura nucleation, Hoffman-Lauritzen theory)
- Standard data types like TG or DSC
- Unique data types (Dilatometry, Rheometry, DEA)

Predictions and optimizations

- optimization of industrial chemical processes like debinding, curing, sintering
- standard predictions (isothermal, heating, multi-step, user-defined, TD24, climatic for 100 weather stations)
- unique predictions of individual peaks, concentrations, Tg, TTT diagram, temperature presets like fire presets)
- prediction of viscosity or ion viscosity for new temperature profile
- Optimization of temperature profile for constant or predefined conversion rate