SDT Society of Dairy Technology
Passion for Dairy

2023 SPRING CONFERENCE

Standard microbiological approach to calculating z values, and consequences of approximations

Dr Tomas Skoglund

Based on the article
On the common misuse of a constant z-value for calculations of thermal inactivation of microorganisms
https://doi.org/10.1016/j.jfoodeng.2021.110766

Outline

- Thermal inactivation of microorganisms – Basics
- Temperature dependence of kinetics
- Arrhenius – E_a vs. z-value
- Reference temperature, T_r, and
  Calculations with constant $z=z_r$ at $T \neq T_r$
- Examples

$$N = N_0 e^{-kt}$$

$$L = \log\left(\frac{N_0}{N}\right) = \frac{F}{D_r} = \frac{\int_0^t 10^{\frac{T(t)-T_r}{z}} dt}{D_r}$$

$$k = k_0 e^{-\frac{E_a}{RT}}$$
$$= k_0 10^{-\frac{E_a}{\ln(10)RT}}$$

$$F = \int_0^t 10^{\frac{T(t)-T_r}{z}} dt$$

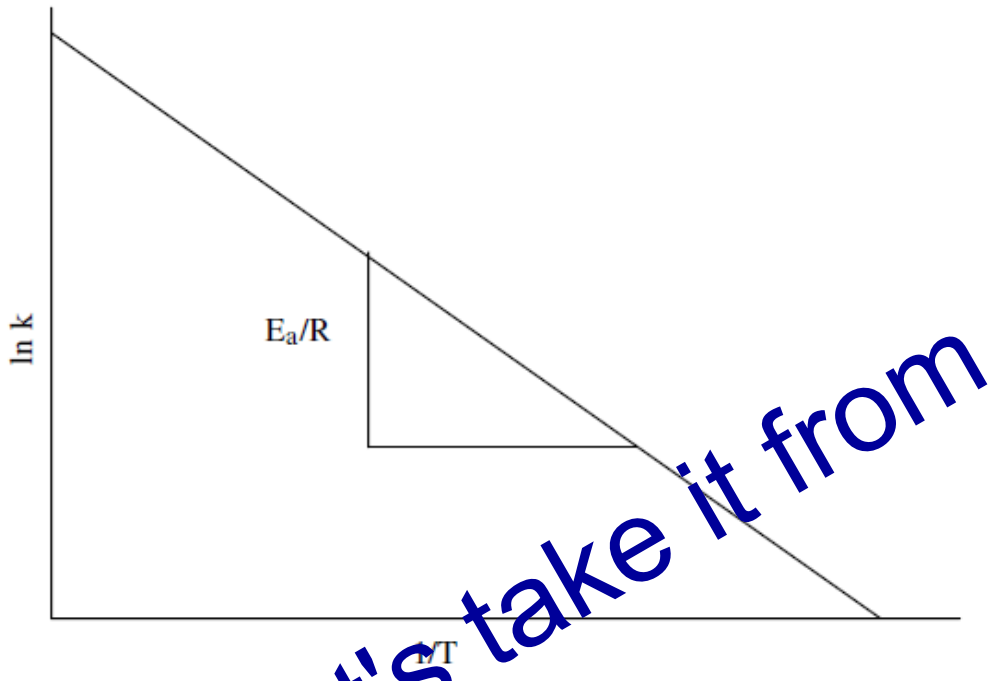
$$D = \ln(10)/k$$

$$z = \frac{\ln(10)\, RTT_r}{E_a}$$

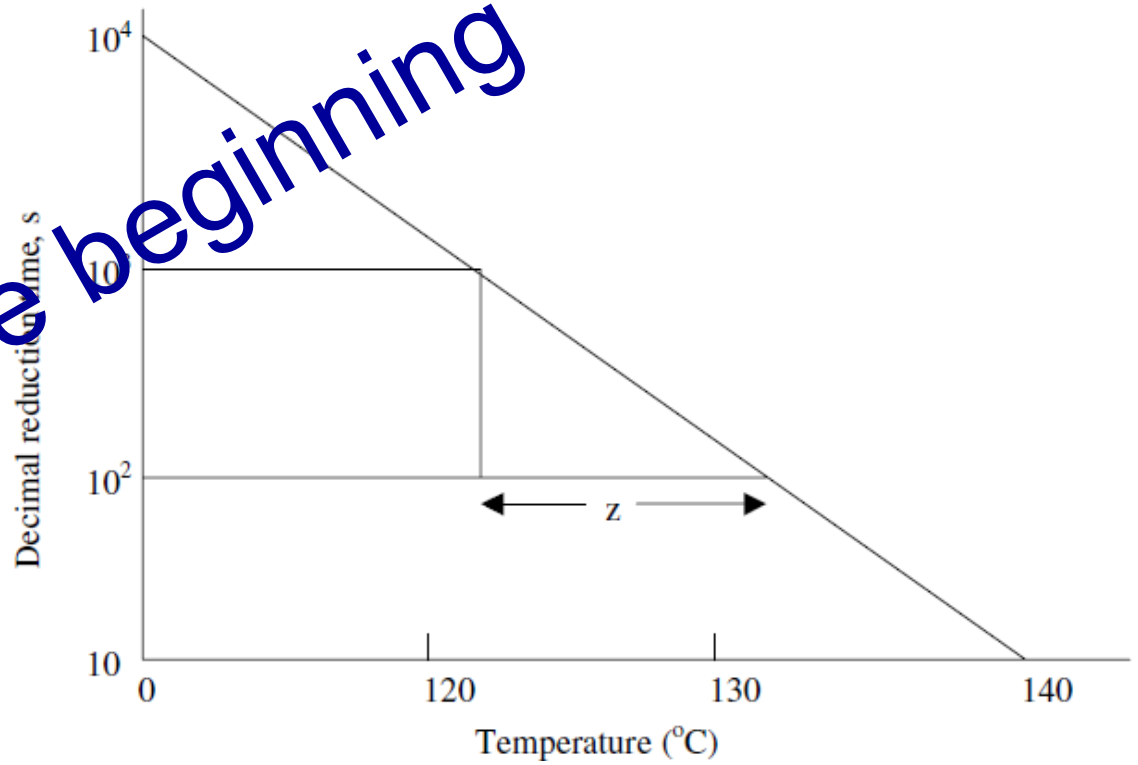
$$D_r = \ln(10)/k(T_r)$$

$$z_r = \frac{\ln(10)\, RT_r^2}{E_a}$$

Arrhenius' plot



Thermal Death Time (TDT) plot



Let's take it from the beginning

Thermal inactivation of microorganisms
Basics

- Target microorganism for the product?
  - Pathogen or
  - Food spoilage
- Kinetics
  - First order kinetics – Two representations
    - Reaction rate (frequency factor), k (SI-unit s^{-1})
    - Decimal reduction time, D (SI-unit s)

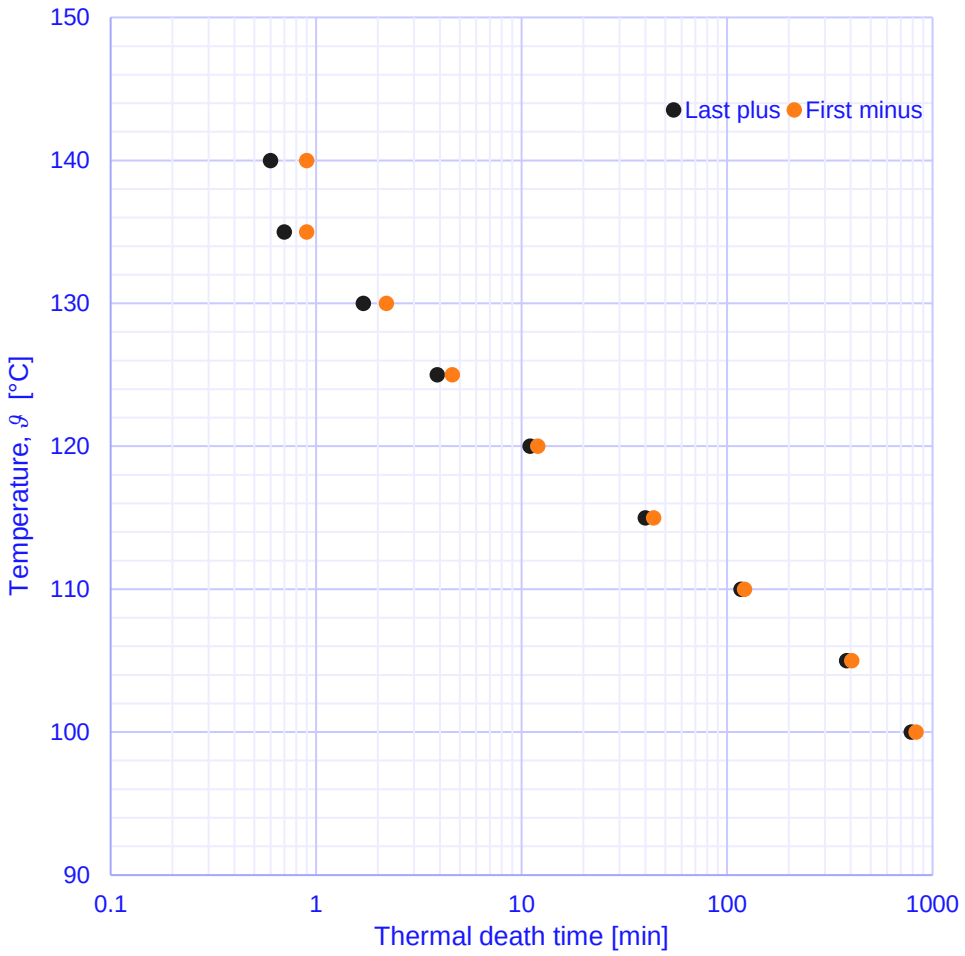
    $D = \ln(10)/k$
  - Temperature dependence – Two representations
    - Arrhenius activation energy, E_a (SI-unit J/mol)
    - z-value, (SI-unit K or °C)

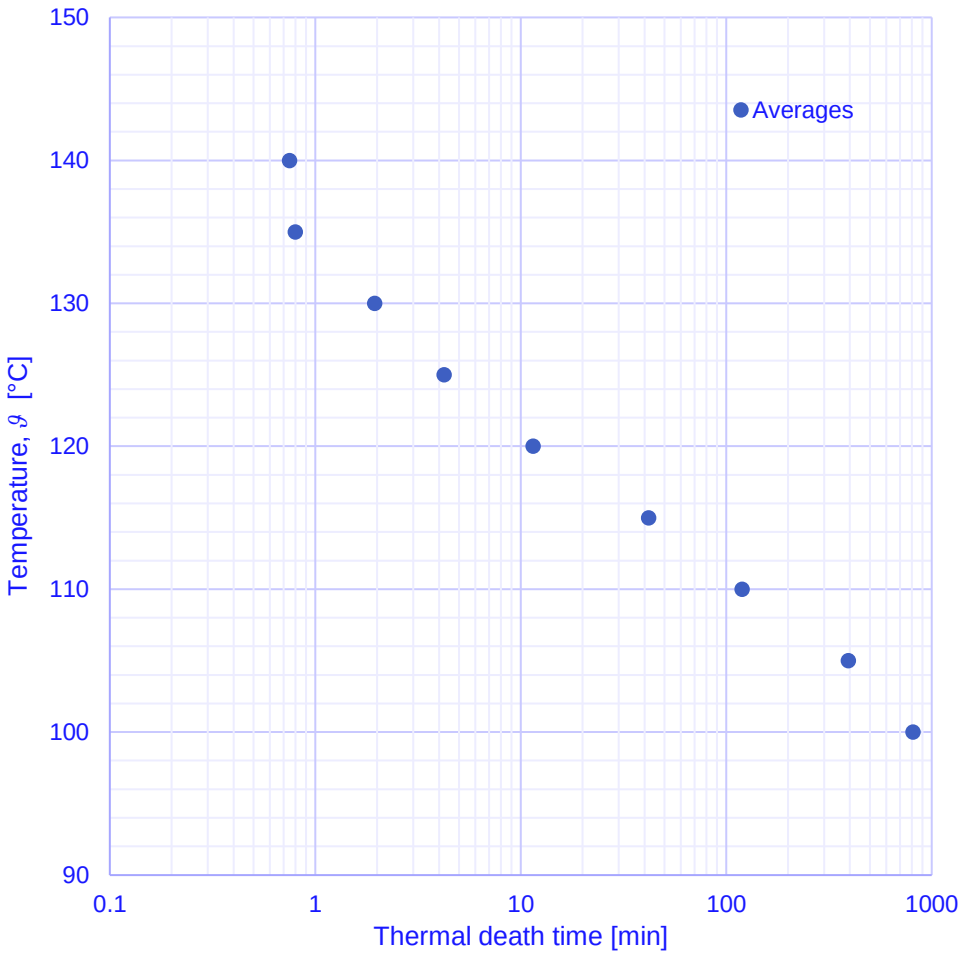
    $z = \ln(10)RT_rT/E_a$

    $z_r = \ln(10)RT_rT_r/E_a$

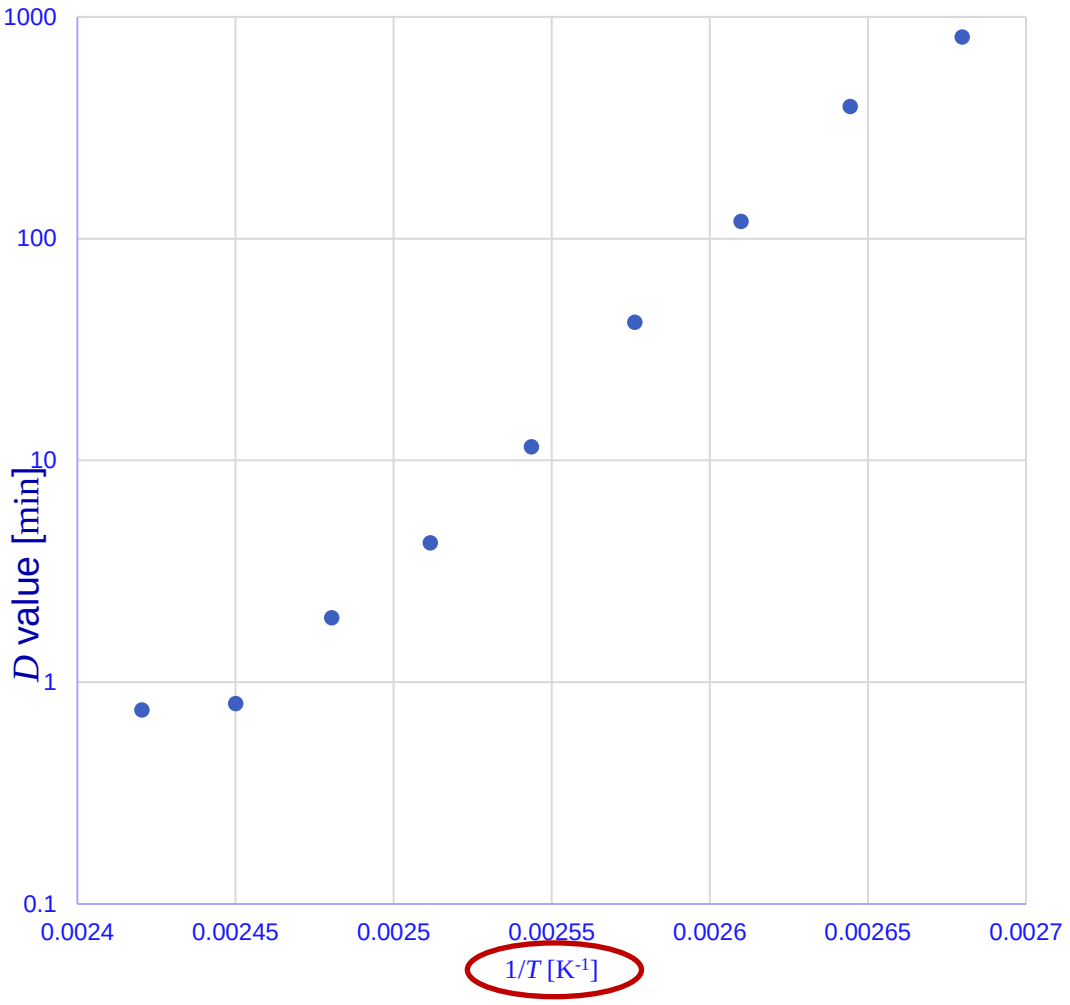
$\ln(10) \approx 2.303$

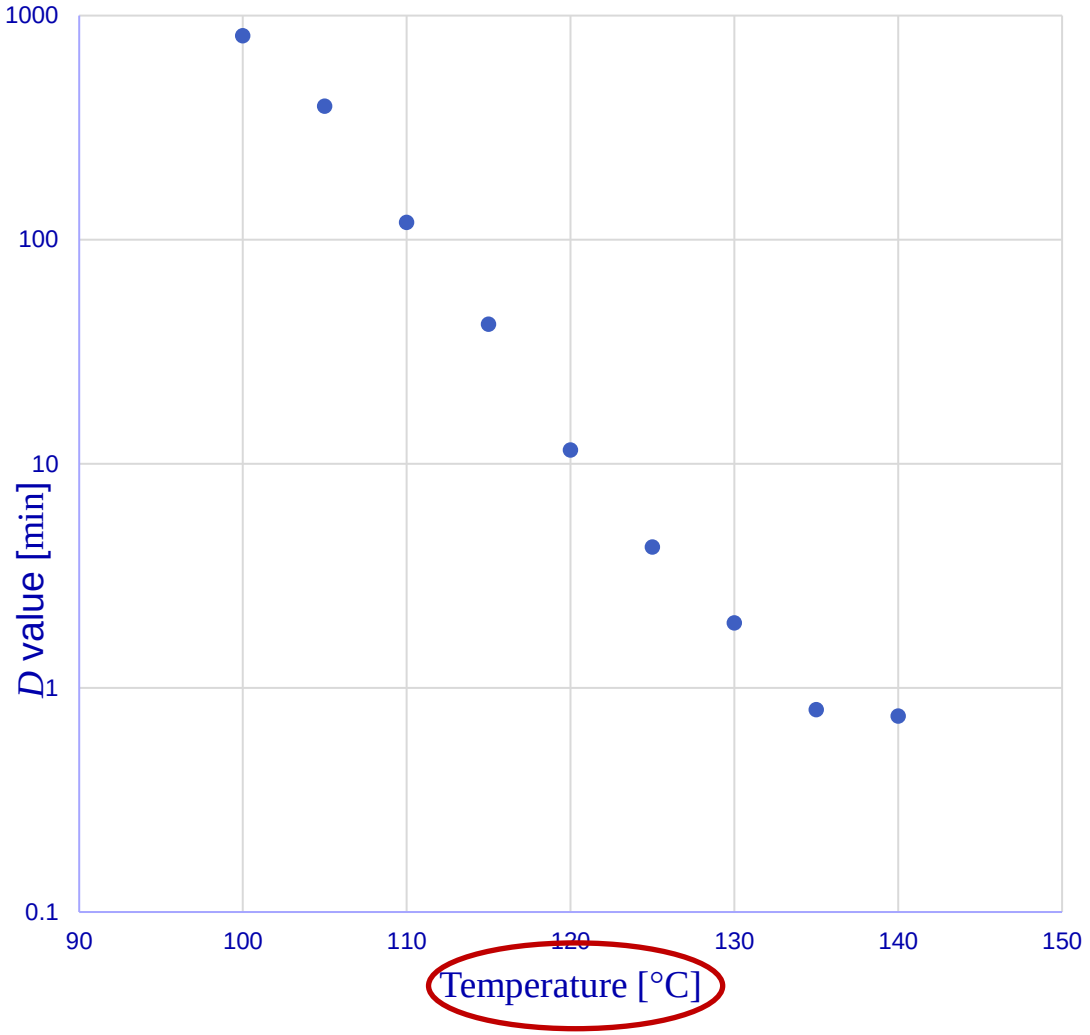
E_a vs. z-value (TDT (Thermal Death Time) plot from Bigelow 1921)





E_a vs. z-value (Data from Bigelow 1921)

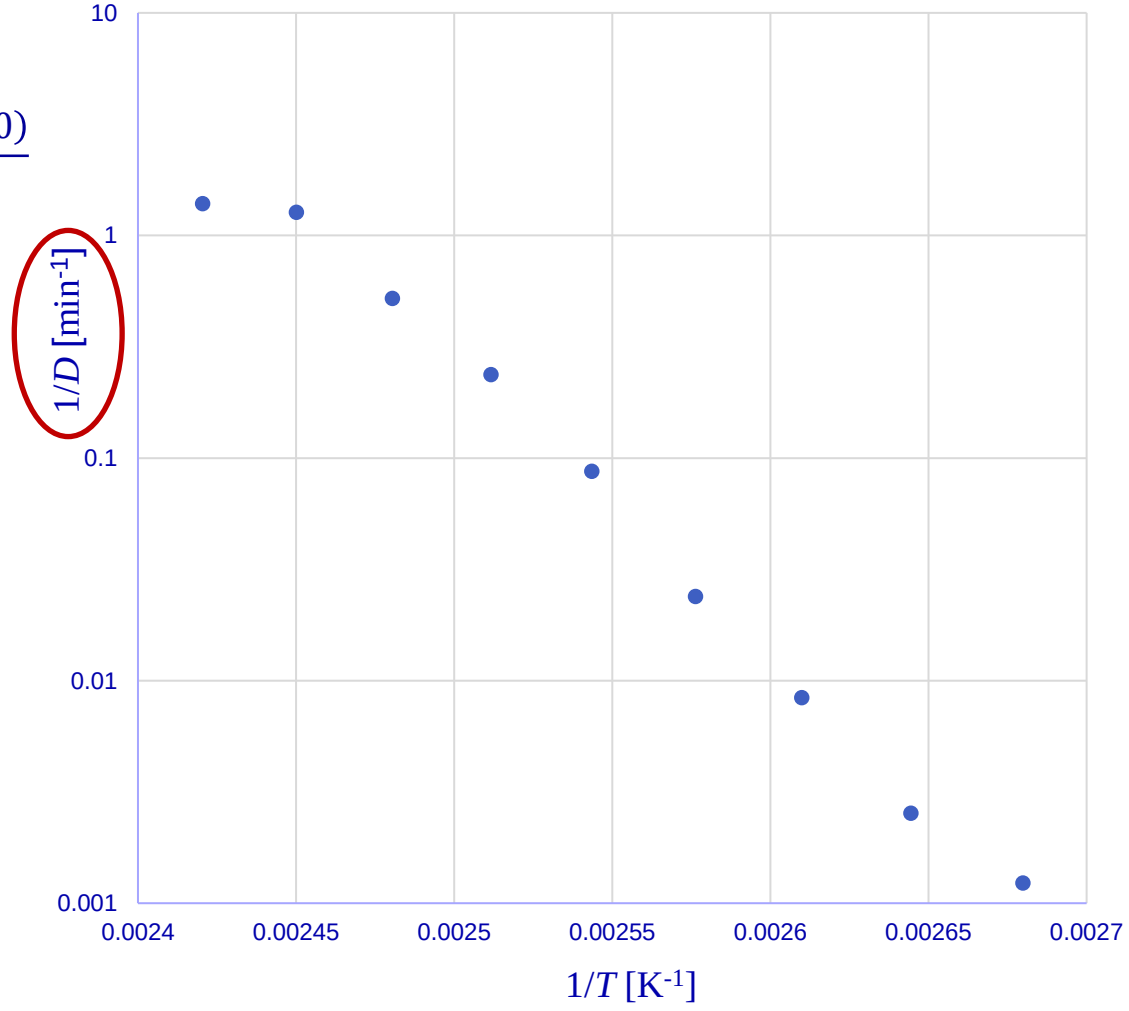




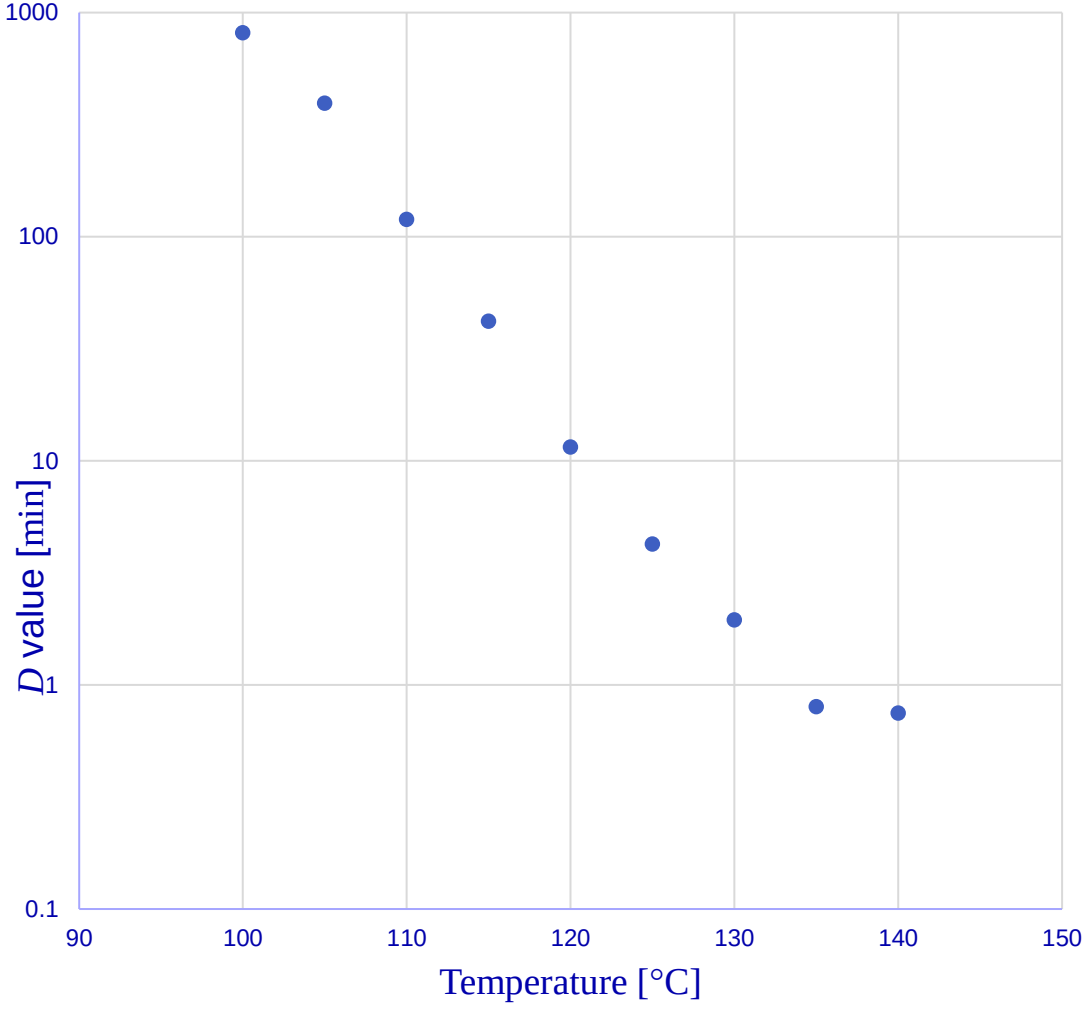
E_a vs. z-value (Data from Bigelow 1921)

$$D = \frac{\ln(10)}{k}$$

Arrhenius' plot

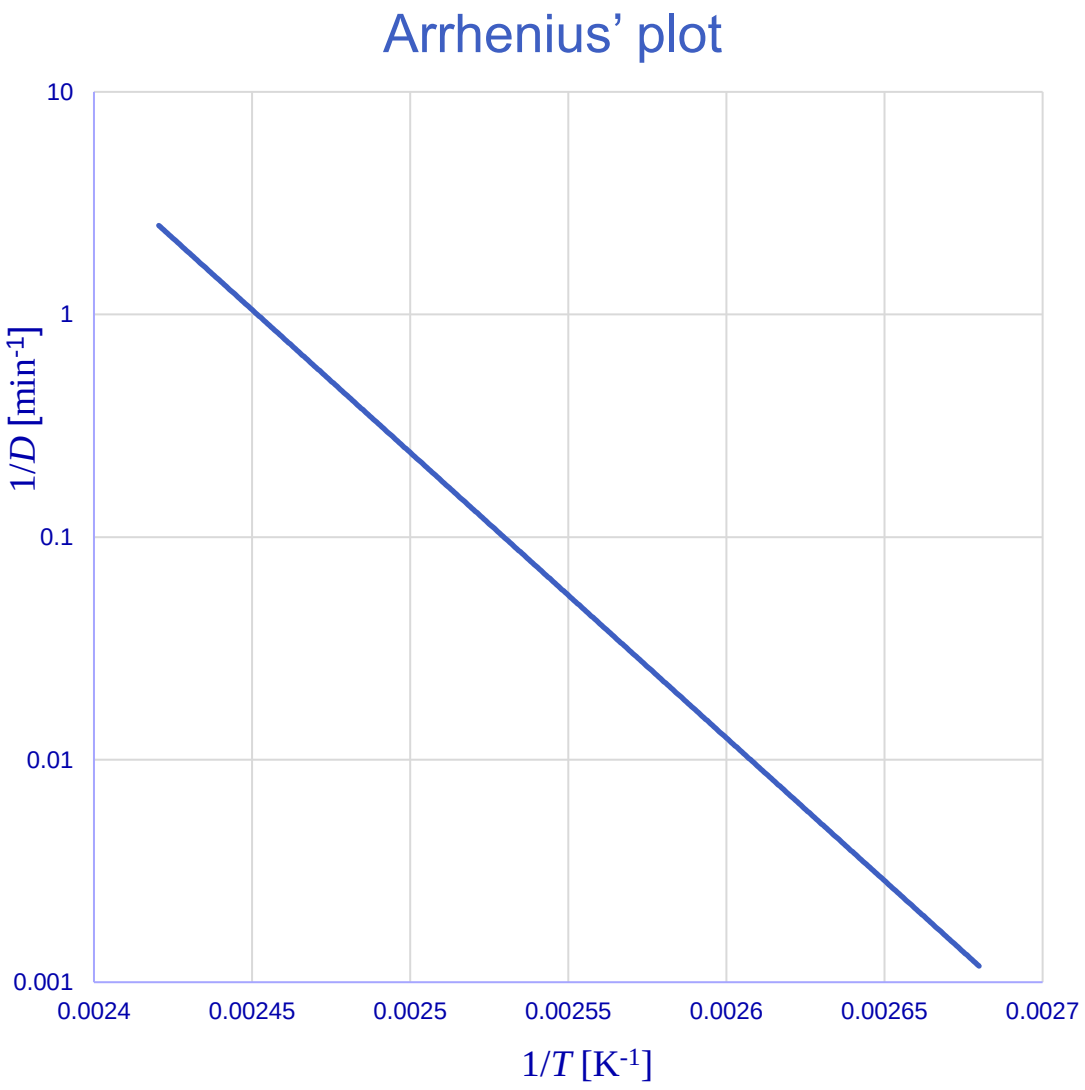


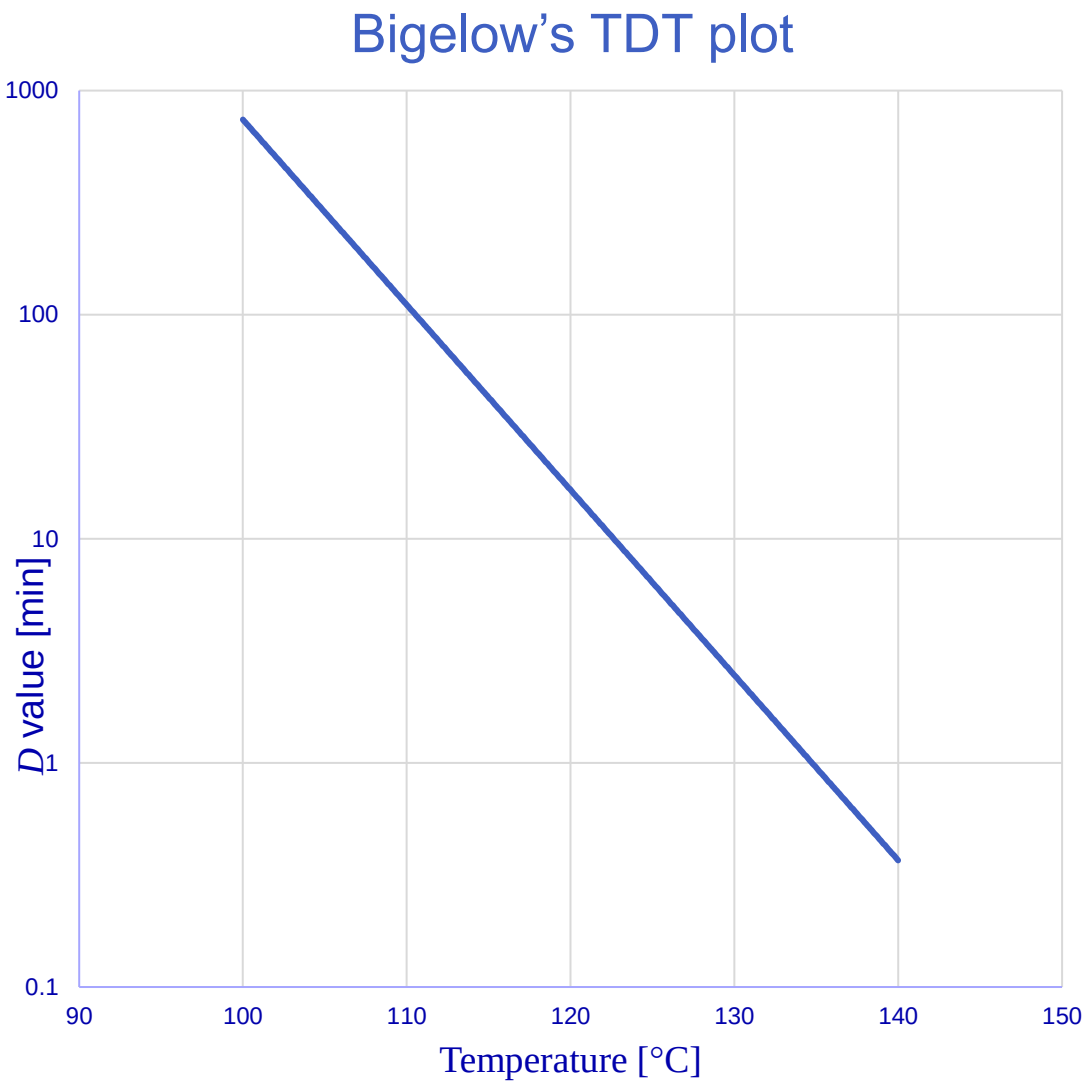
Bigelow's TDT plot



E_a vs. z-value – lin/log regression

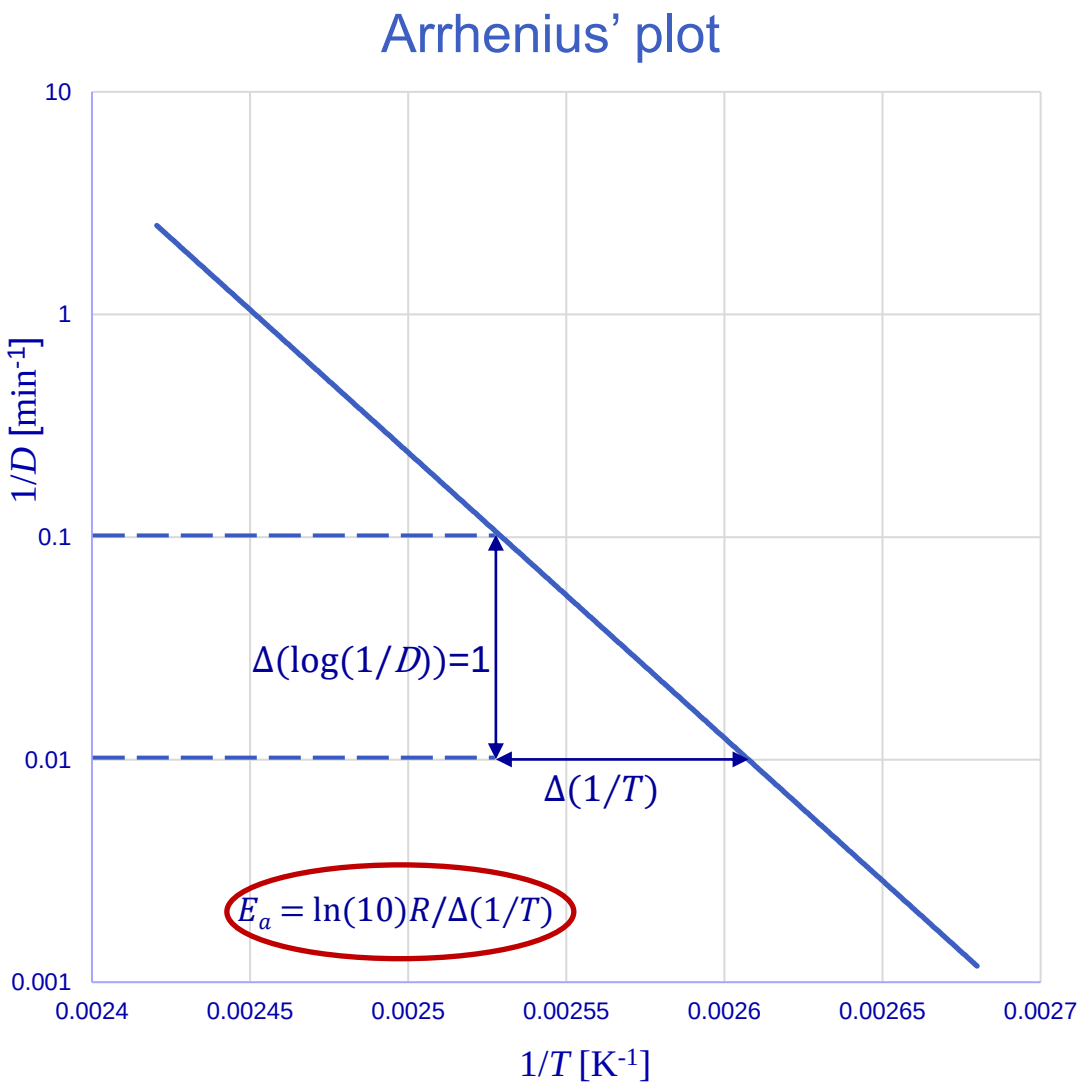
$$D = \frac{\ln(10)}{k}$$

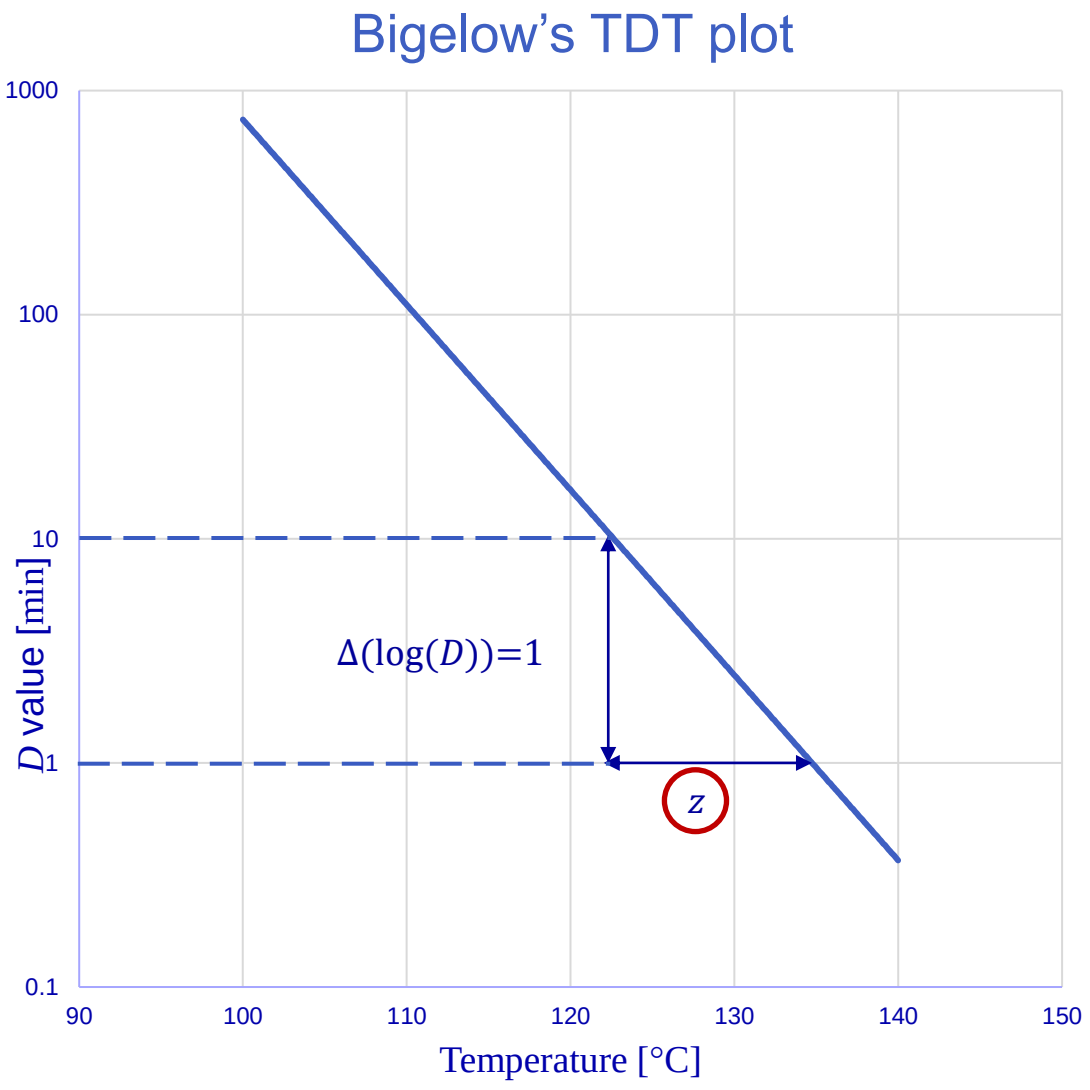




E_a vs. z-value – lin/log regression

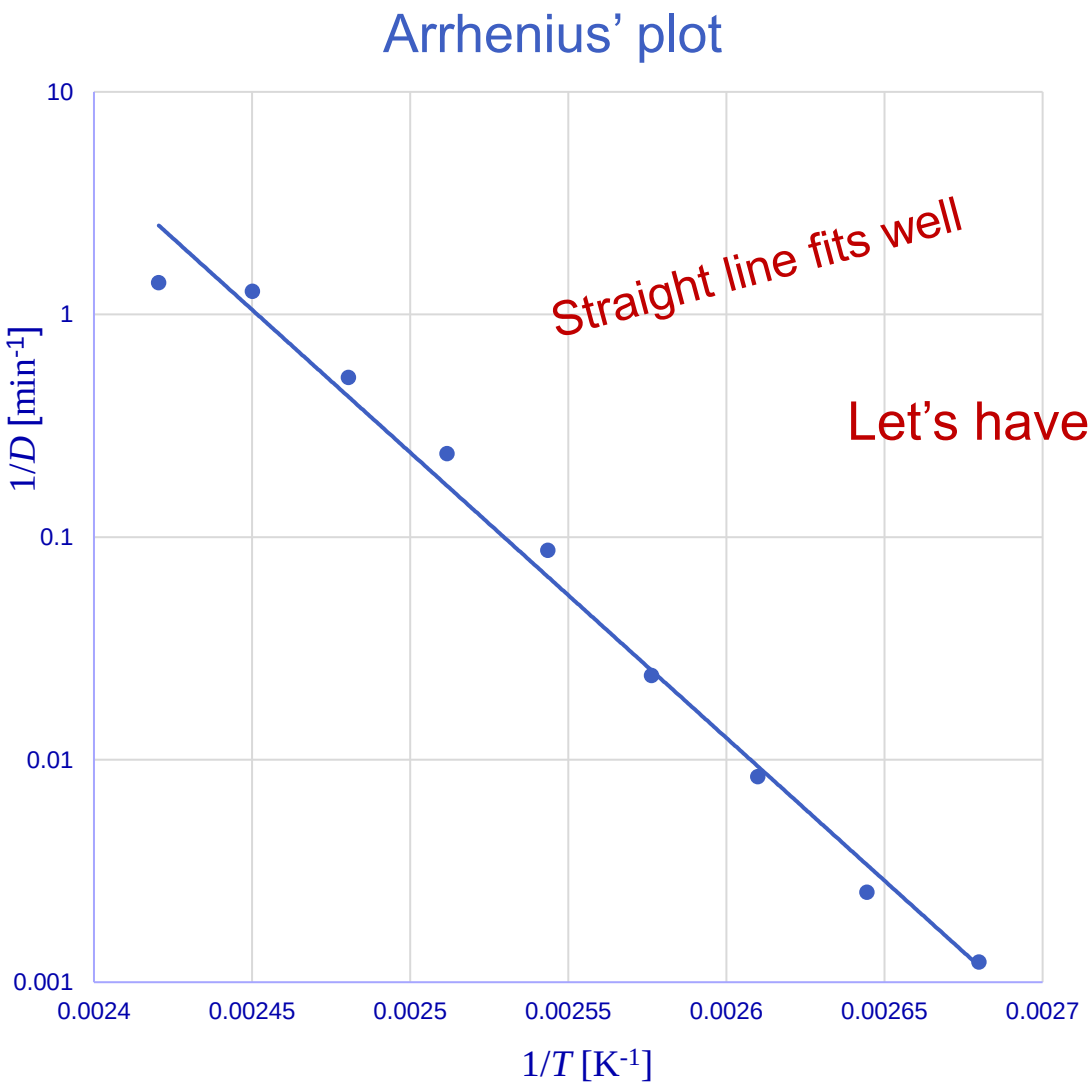
$$D = \frac{\ln(10)}{k}$$



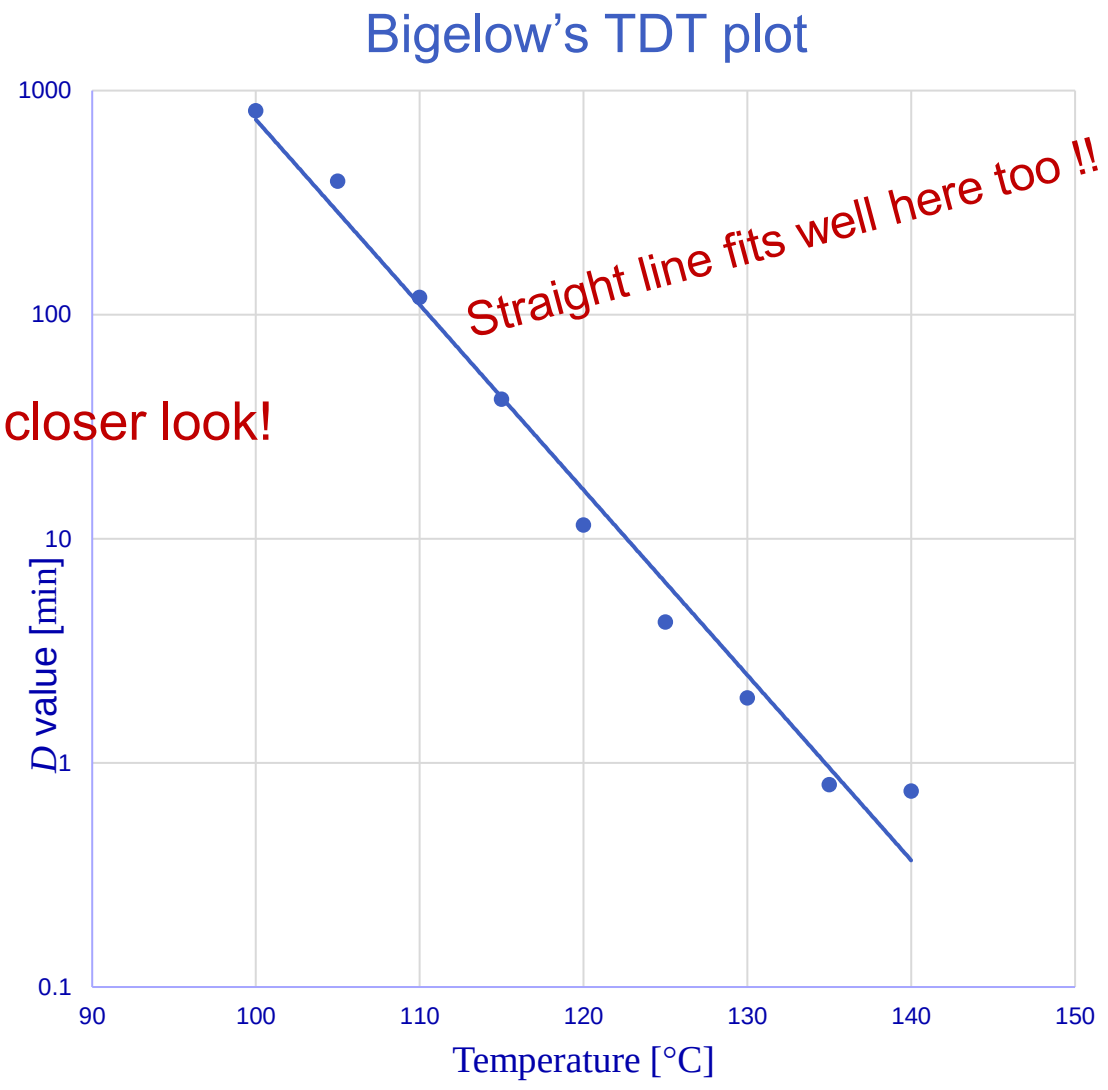


E_a vs. z-value – lin/log regression (Data from Bigelow 1921)

$$D = \frac{\ln(10)}{k}$$

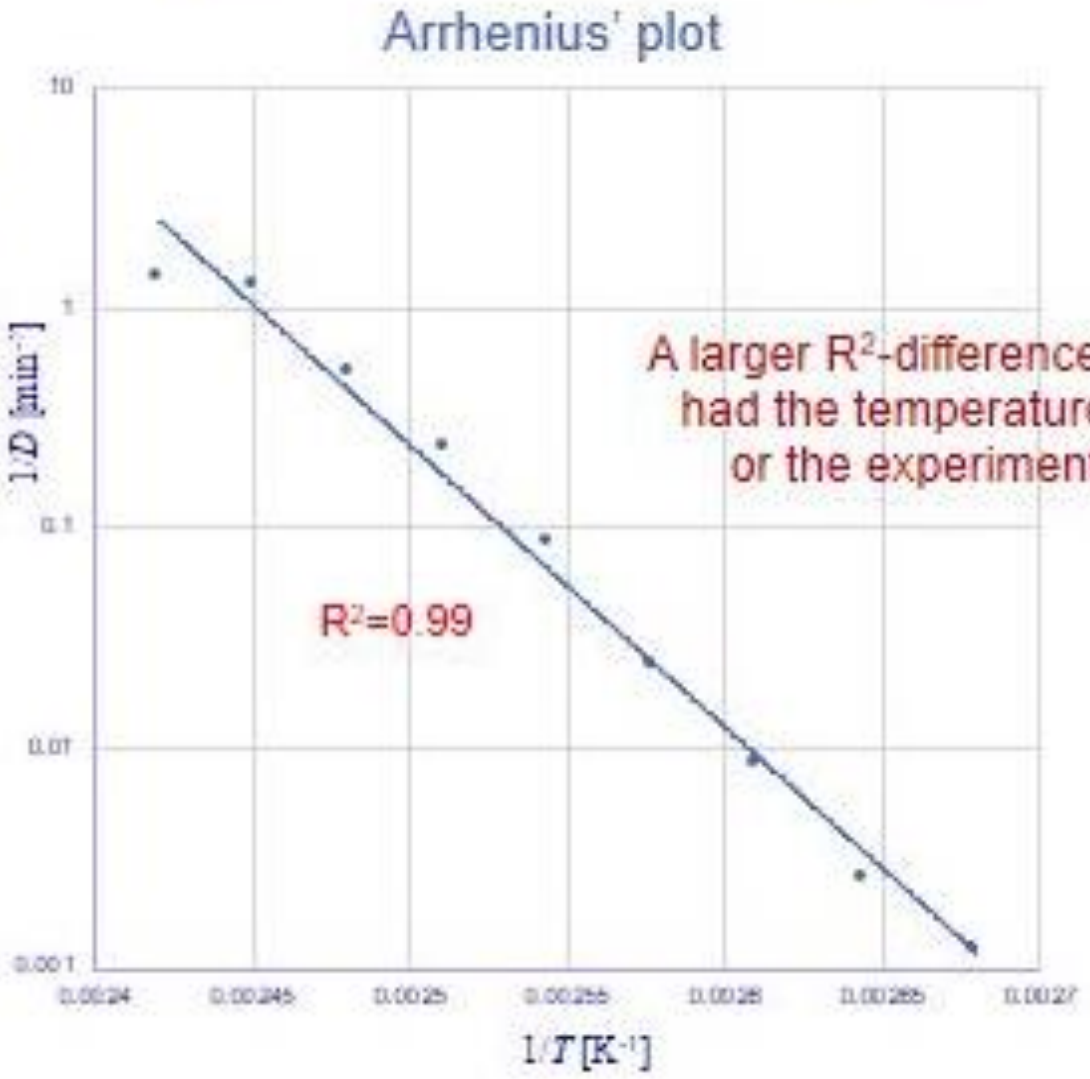


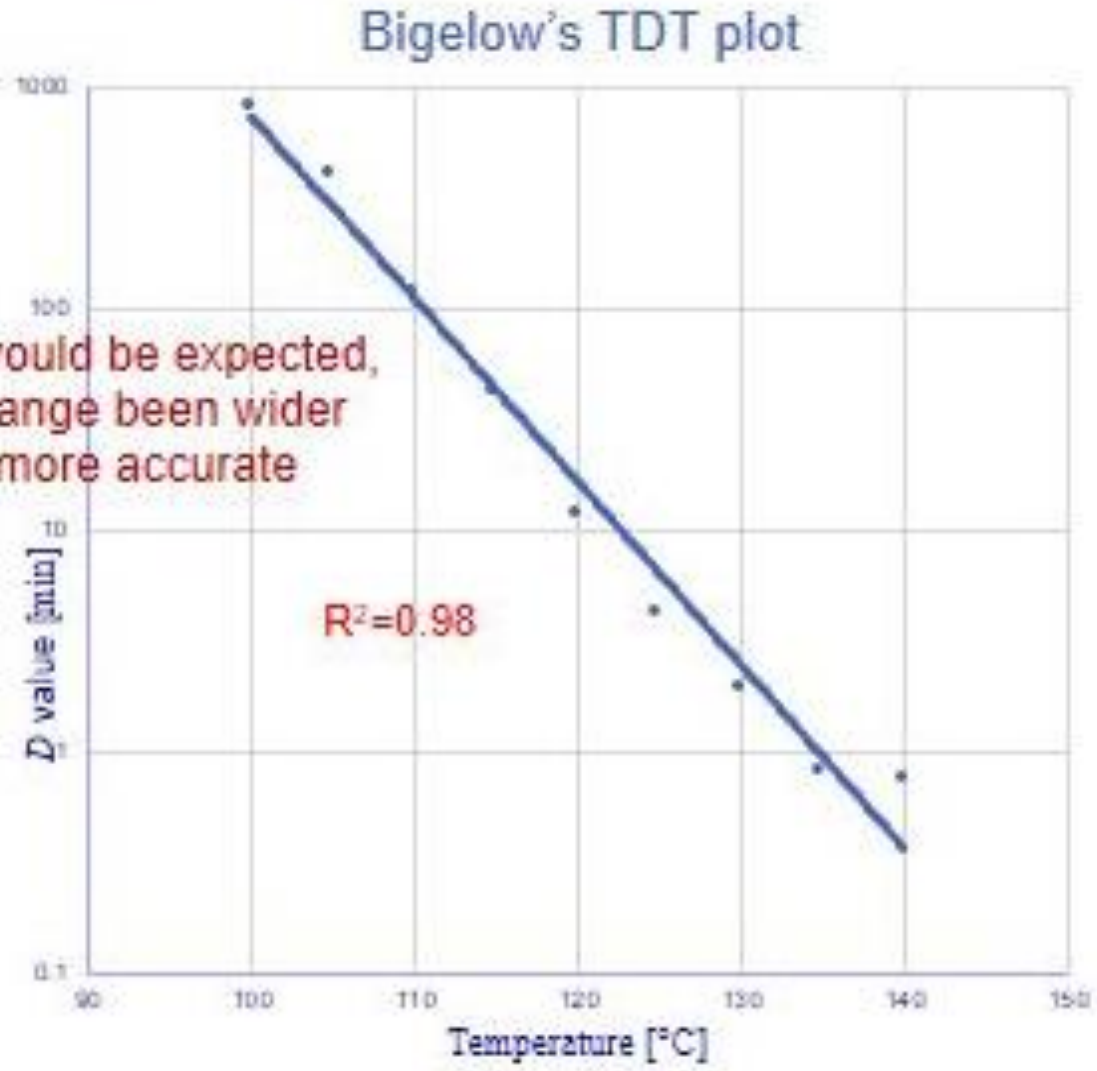
Let's have a closer look!



E_a vs. z-value – lin/log regression (Data from Bigelow 1921)

$$D = \frac{\ln(10)}{k}$$





A larger R^2-difference would be expected, had the temperature range been wider or the experiments more accurate

Comments on the representations/models

E_a vs. z-value

Activation energy (E_a)

- A bit hard to interpret
- Empirically proven and theoretically explained

z-value for decimal reduction time (D)

- Easy to interpret
- Established in calculations of process lethality (F values, also denoted "sterilization value")
- Often used inaccurately as constant, despite its temperature-dependent relationship to E_a

But does it matter?

Comments on the representations/models

E_a vs. z-value

H.-G. Kessler, Food and Bio Process Engineering: Dairy Technology, München: Verlag A. Kessler, 2002, p. 694.

For narrow temperature ranges within which the temperature dependence of the *z*-value can be neglected, the *z*-value expresses the increase in temperature [°C] necessary for obtaining the same effect in 1/10 of the time. In practice, however, the line is not straight (dotted line) and this cannot be neglected in the discussion of larger temperature ranges, as will be shown later. Many investigations have demonstrated the constancy of the energy of activation in a large number of reactions. The representation in Fig. 6.11 should therefore be used in calculations.

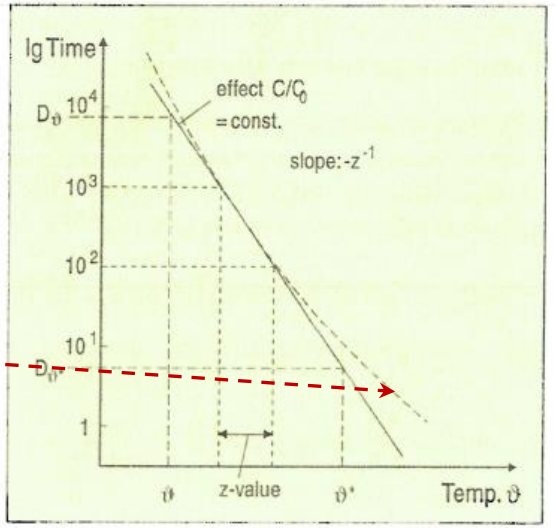


Fig. 6.12. Diagram of a decomposition reaction proceeding at a constant rate. Plot of lg time against temperature [C°]

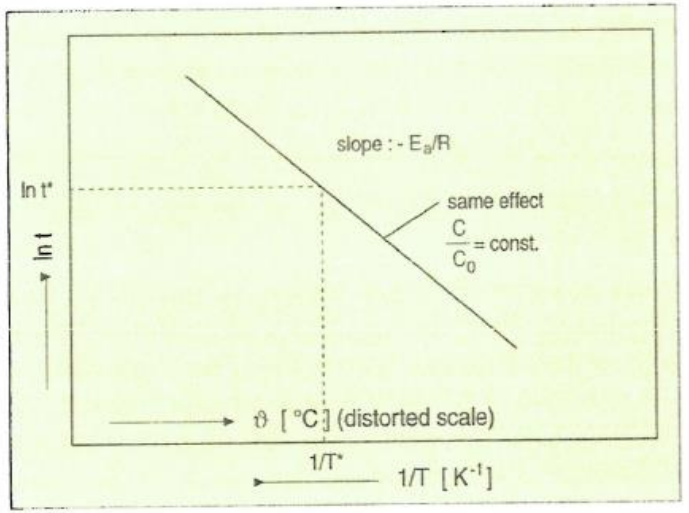


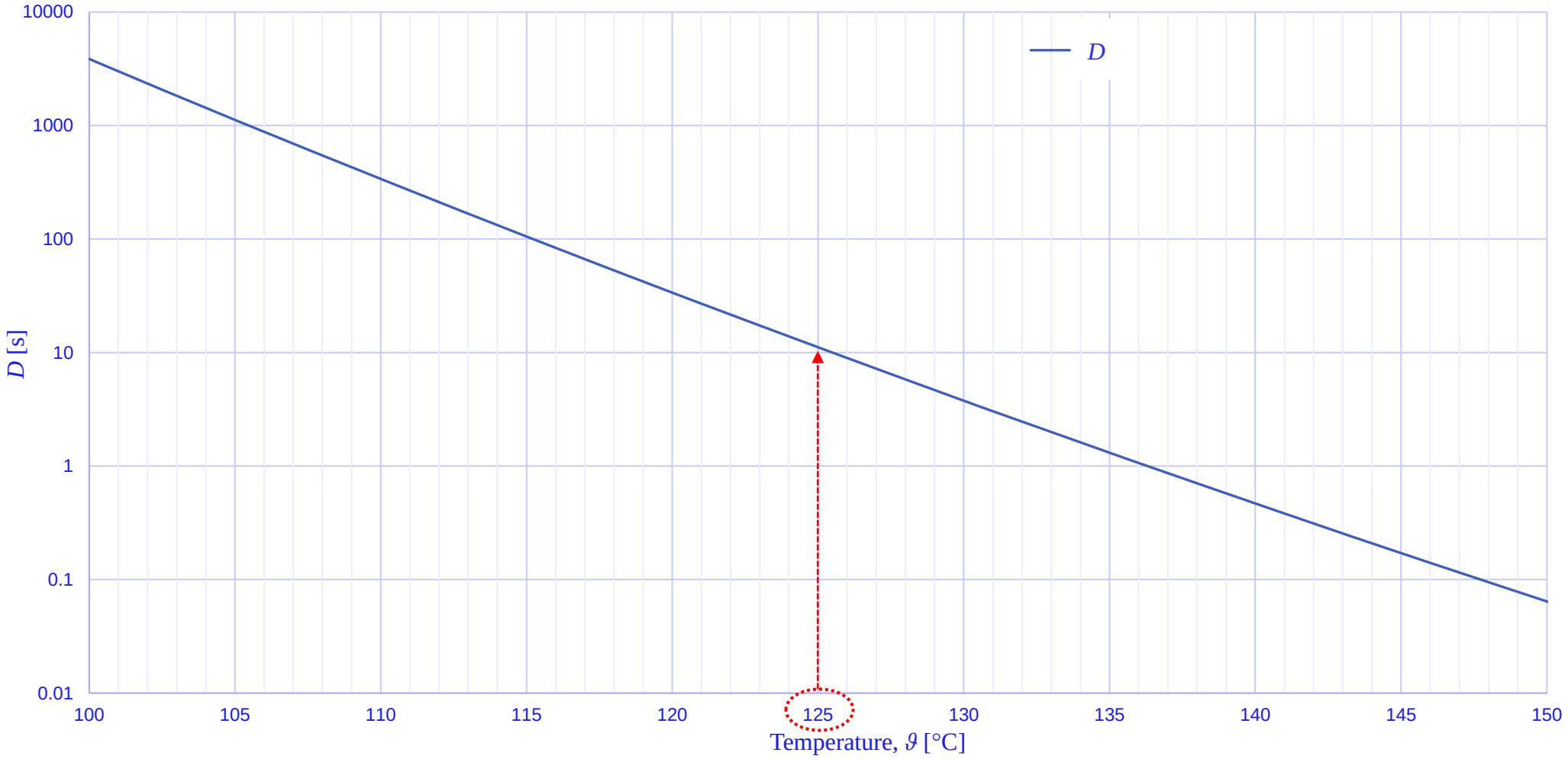
Fig. 6.11. Illustration of a decomposition process proceeding at a constant rate by a plot of the natural logarithm of the time against the reciprocal of the absolute temperature

But how narrow?

As we will see, ”narrow” is narrow indeed!

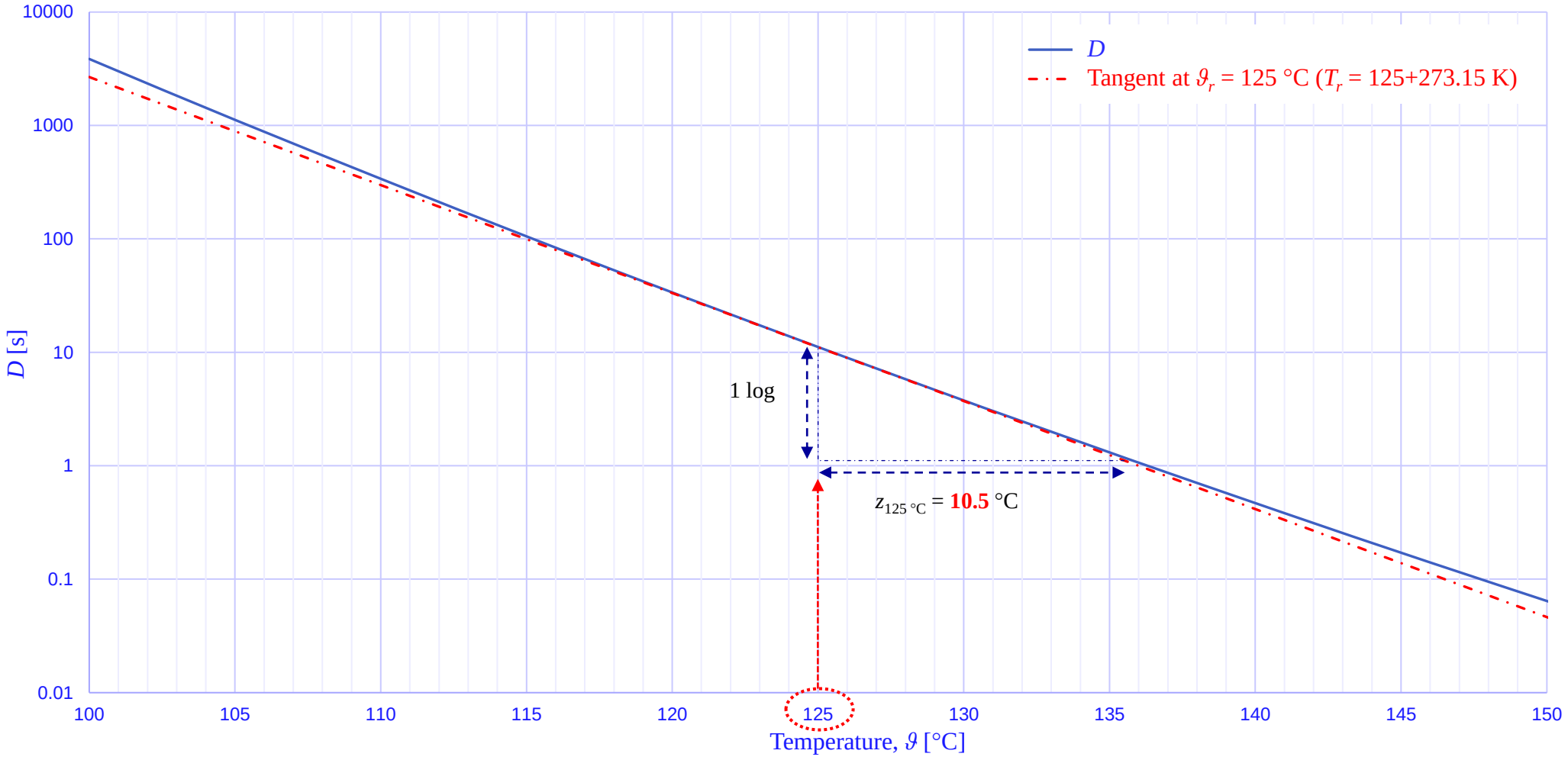
The problem with constant z – An example

D plot vs. temperature based on Arrhenius (constant E_a) for Natural thermophilic flora, Milk (high D)



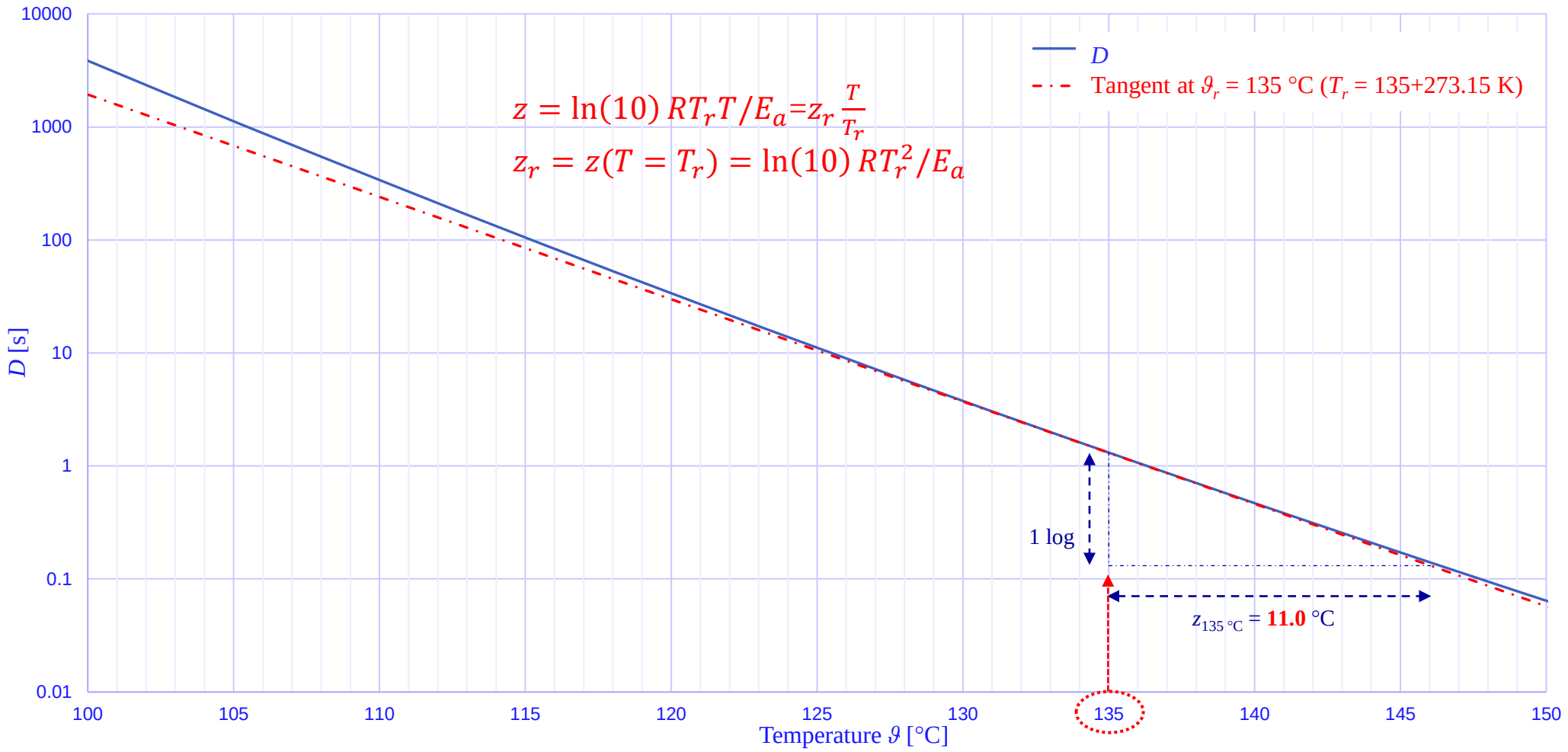
The problem with constant z – An example

D plot vs. Temperature based on Arrhenius (constant E_a) for Natural thermophilic flora, Milk (high D)



The problem with constant z – An example

D plot vs. Temperature based on Arrhenius (constant E_a) for Natural thermophilic flora, Milk (high D)



Example – Calculation of holding time in a UHT line

Direct-steam injection with flash cooling: Temperature profile 80 °C – 138 °C – 81 °C

$$L = \frac{F}{D_r} = \frac{\int_0^{t_h} 10^{\frac{T-T_r}{z}} dt}{D_r} = \frac{\int_0^{t_h} 10^{\frac{T-T_r}{z_r}\frac{T_r}{T}} dt}{D_r}$$

Constant temperature $\Longrightarrow L = \frac{t_h 10^{\frac{\vartheta-\vartheta_r}{z_r}\frac{T_r}{T}}}{D_r}$ $\Longrightarrow t_h = \frac{LD_r}{10^{\frac{T-T_r}{z_r}\frac{T_r}{T}}} = \frac{LD_r}{10^{\frac{\vartheta-\vartheta_r}{z_r}\frac{T_r}{T}}}$

		μ-organisms (pathogen and spoilage)	
		Clostridium botulinum spores	Natural thermophilic flora, Milk (high D)
Kinetic data provided in the literature	ϑ_r	121.1 °C	121.1 °C
	D_r	12 s	26.4 s
	z_r	10.0 °C	10.3 °C
	Reference	Text books, e.g. H.-G. Kessler, Food and Bio Process Engineering	W. G. Bigelow, "The logarithmic nature of thermal death curves,"
Target logred, L		12	6
Accurate holding time		$\frac{12 * 12\ \text{s}}{10^{\frac{138-121.1}{10}\frac{121.1+273.15}{138+273.15}}} = 3.5\ \text{s}$	$\frac{6 * 26.4\ \text{s}}{10^{\frac{138-121.1}{10.3}\frac{121.1+273.15}{138+273.15}}} = 4.2\ \text{s}$
Inaccurate holding time		$\frac{12 * 12}{10^{\frac{138-121.1}{10}}} = 2.9\ \text{s}$	$\frac{6 * 26.4}{10^{\frac{138-121.1}{10.3}}} = 3.6\ \text{s}$

$T_r = \vartheta_r + 273.15\ \text{K}$

Example – Calculation of holding time in a UHT line

Direct-steam injection with flash cooling: Temperature profile 80 °C – 138 °C – 81 °C

$$L = \frac{F}{D_r} = \frac{\int_0^{t_h} 10^{\frac{T-T_r}{z}} dt}{D_r} = \frac{\int_0^{t_h} 10^{\frac{T-T_r}{z_r}\frac{T_r}{T}} dt}{D_r}$$

Constant temperature $\Longrightarrow L = \frac{t_h 10^{\frac{\vartheta-\vartheta_r}{z_r}\frac{T_r}{T}}}{D_r}$ $\Longrightarrow t_h = \frac{LD_r}{10^{\frac{T-T_r}{z_r}\frac{T_r}{T}}} = \frac{LD_r}{10^{\frac{\vartheta-\vartheta_r}{z_r}\frac{T_r}{T}}}$

		μ-organisms (pathogen and spoilage)	
		Clostridium botulinum spores	Natural thermophilic flora, Milk (high D)
Kinetic data provided in the literature	ϑ_r	121.1 °C	121.1 °C
	D_r	12 s	26.4 s
	z_r	10.0 °C	10.3 °C
	Reference	Text books, e.g. H.-G. Kessler, Food and Bio Process Engineering	W. G. Bigelow, "The logarithmic nature of thermal death curves,"
Target logred, L		12	6
Accurate holding time		$(F_0 = 2.40 \text{ min})$ 3.5 s	$(F = 2.64 \text{ min})$ 4.2 s
Inaccurate holding time		2.9 s	3.6 s

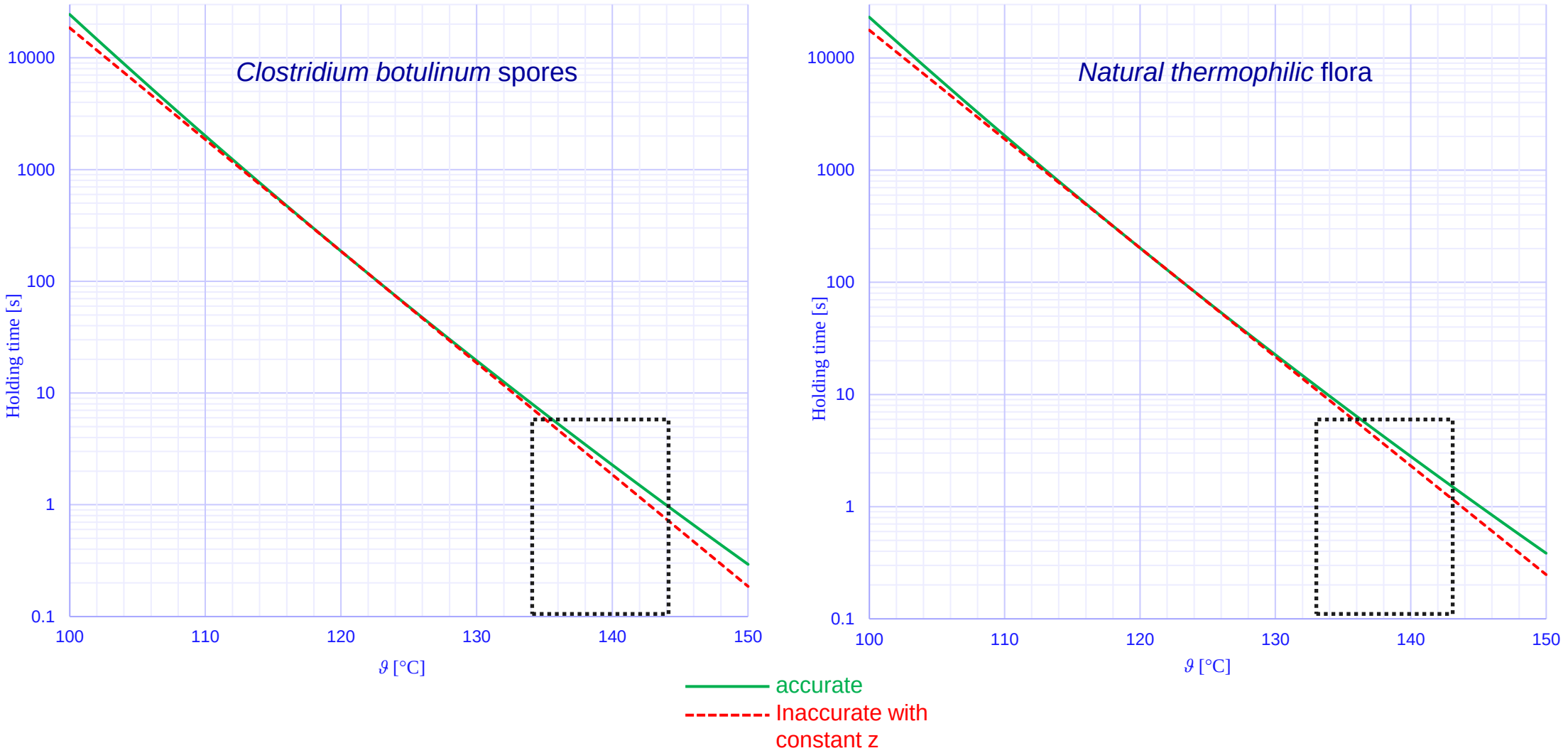
$T_r = \vartheta_r + 273.15$ K

14% TOO SHORT

Example – Calculation of holding time

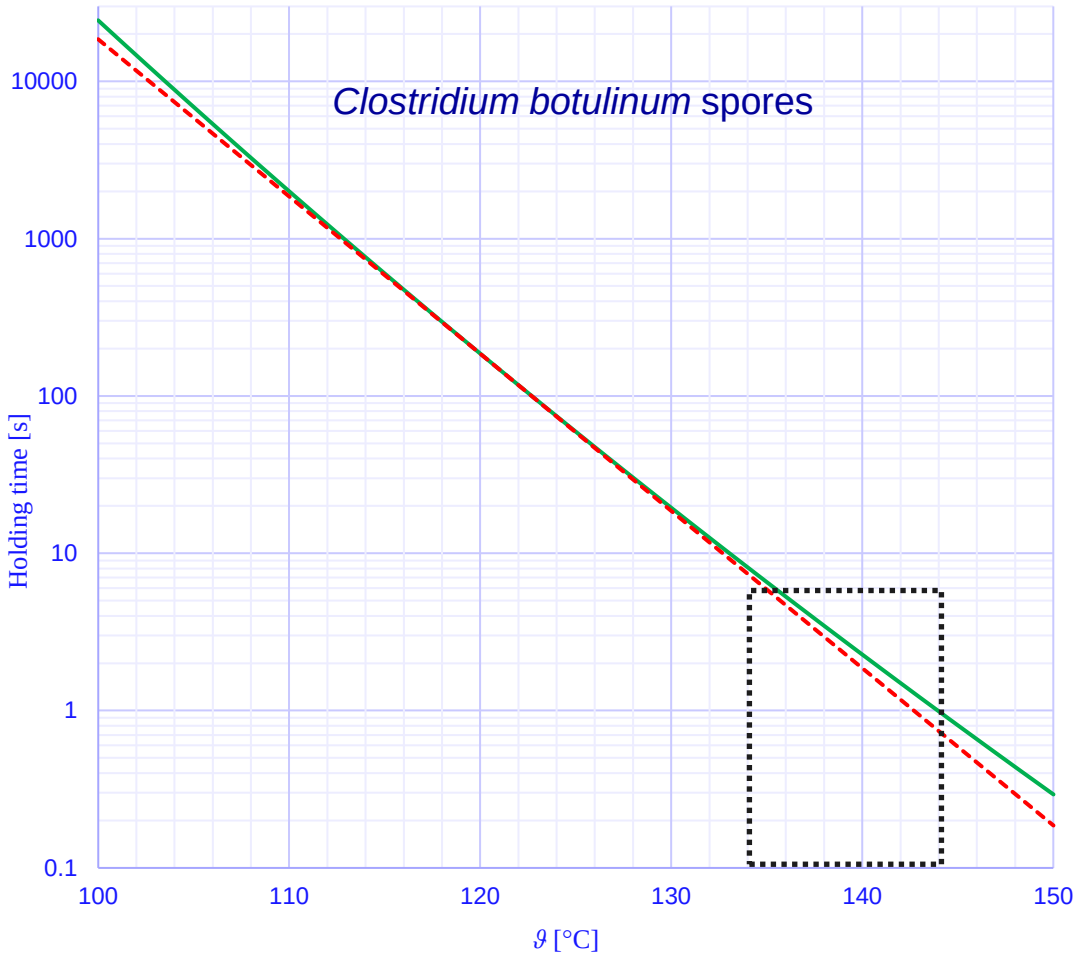
$$\text{Relative error of } t_h = 10^{-\frac{(T-T_r)^2}{Tz_r}} - 1$$

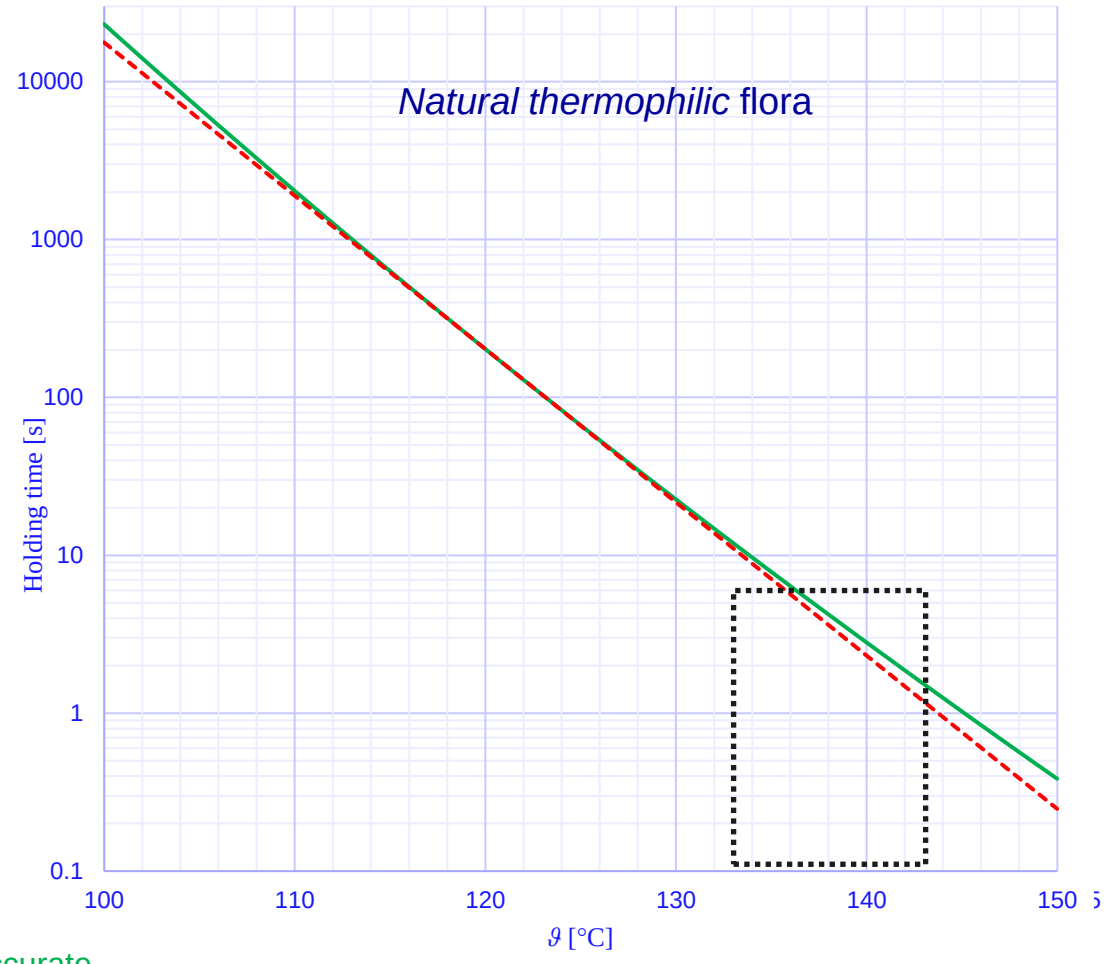
Difference between using approximation with constant z=z_r and temperature dependence of z



Example – Calculation of holding time

Difference between using approximation with constant $z=z_r$ and temperature dependence of z



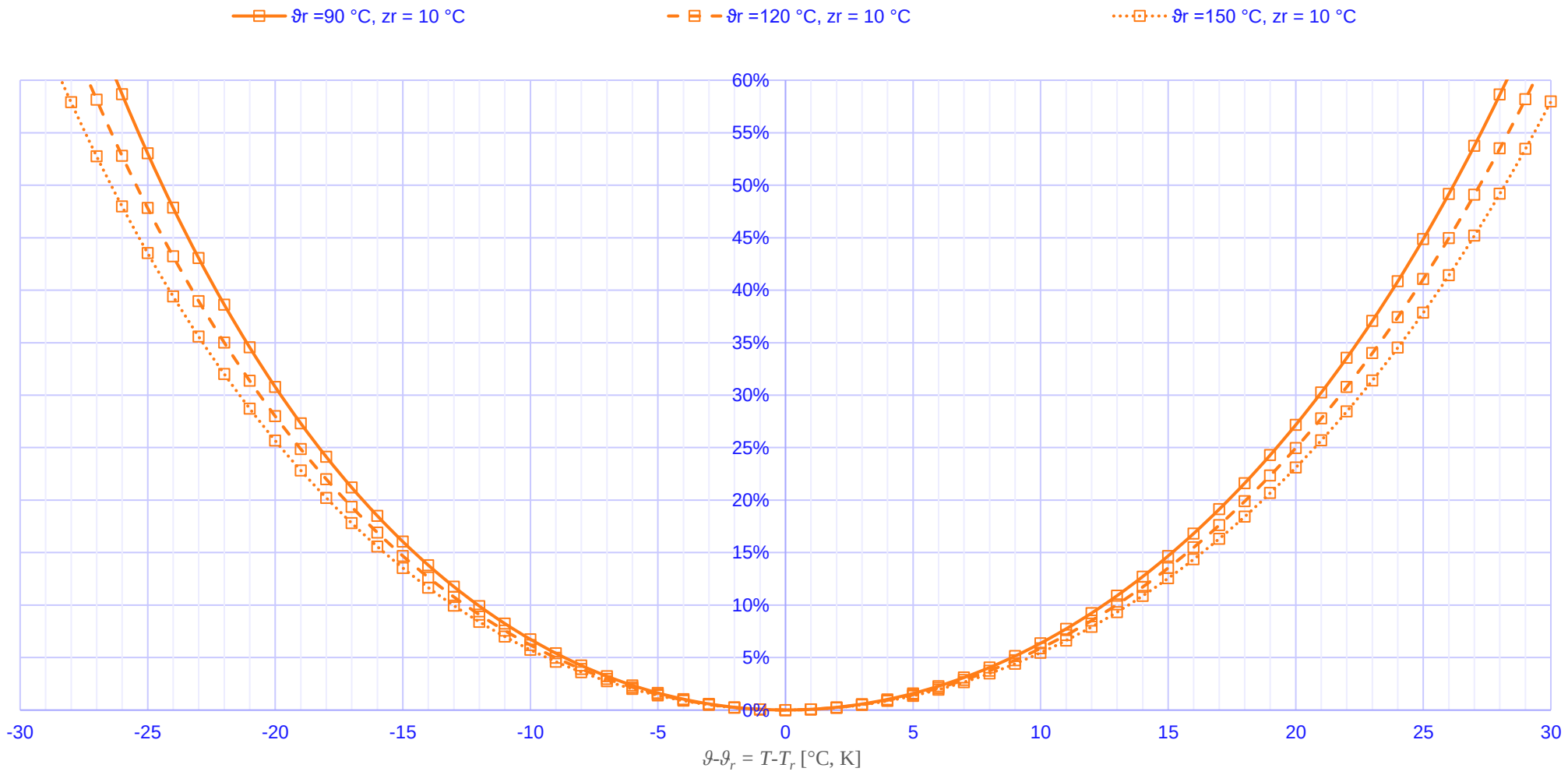


accurate

Inaccurate with constant z

Error calculations of F

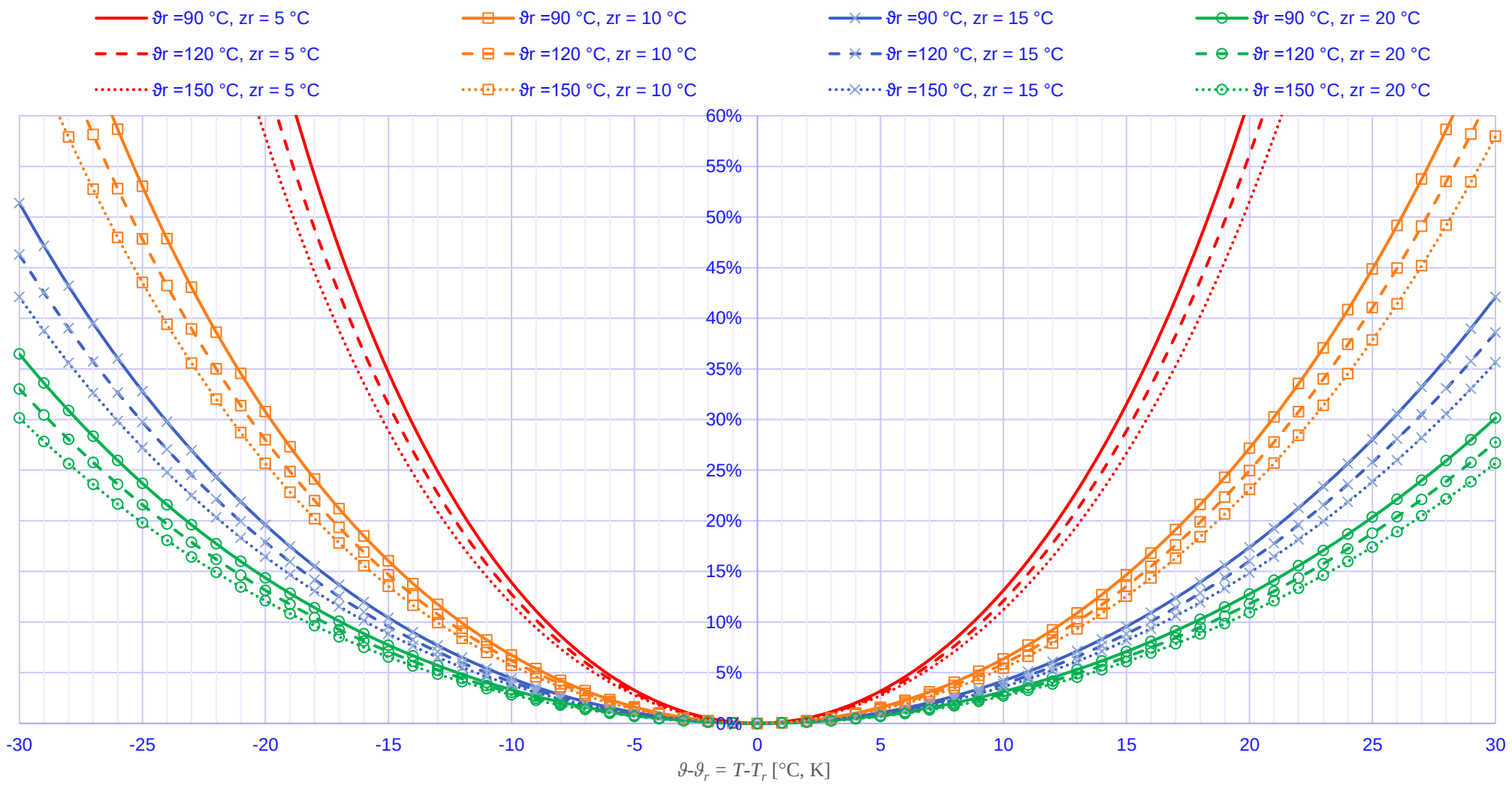
T deviation from T_r for different T_r and with z_r = 10.0 °C



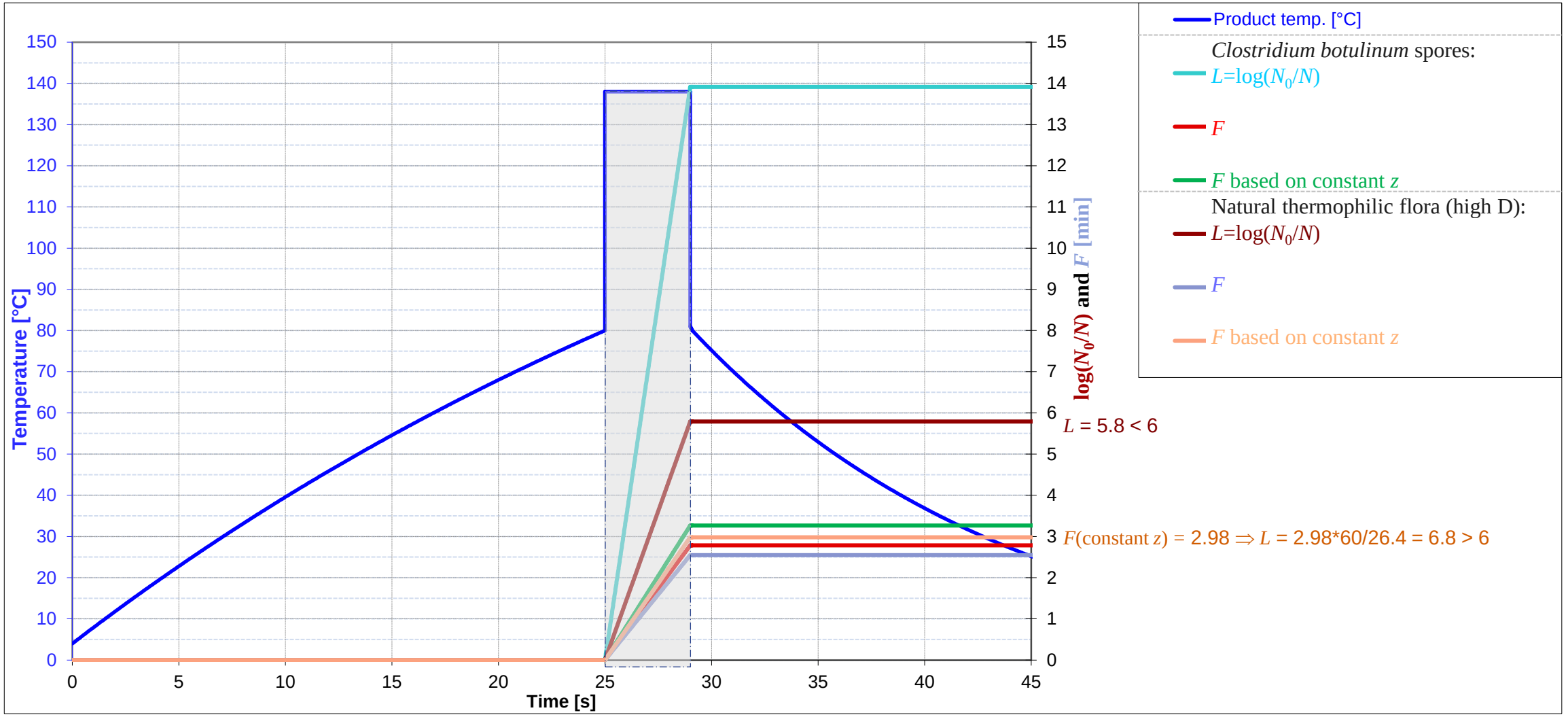
Error calculations of F

$$\text{Relative error of } F = 10^{\frac{(T-T_r)^2}{Tz_r}} - 1$$

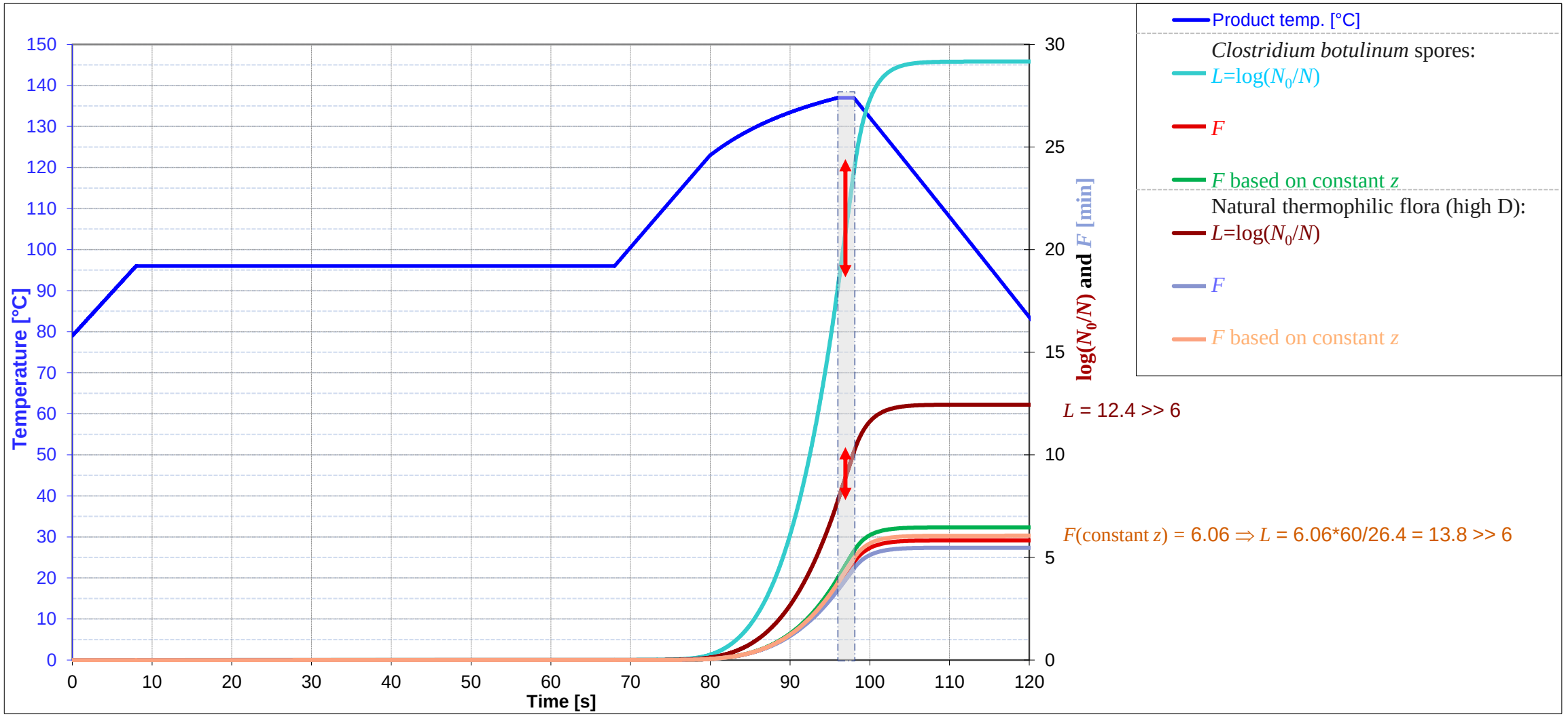
T deviation from T_r for different T_r and z_r



A direct heating & flash cooling system
80 – 138 (4 s) – 81 °C



An indirect heating & cooling system
96 – 123 – 137 (2 s) – 29 °C



Conclusion

- Temperature dependence
  - Follows Arrhenius equation, linear log(k) vs. 1/T
  - Seemingly, but inaccurately linear log(D) vs. T
- Constant $z = z_r$ (for $T \neq T_r$) $\Rightarrow$
  - overestimation of L and F
  - underestimation of required holding times
  - not negligible errors
- To avoid compromising food safety and quality: Use $z = \ln(10) R T_r T / E_a = z_r T / T_r$!
  - Particularly important for direct heating systems

Thank you!
Questions?

Tomas Skoglund's professional background

I studied engineering physics at the Faculty of Engineering (Lund Institute of Technology, LTH) at Lund University and obtained my Master of Science degree (Eng. Phys) 1978. The year 2007 a PhD degree was obtained. During my early years after education I worked with automatic control engineering (at Volvo Aero), acoustics and vibrations consultations (at Ingemansson Akustik) and with research and education (at the Department of Physics at Lund University / Faculty of Engineering, LTH).

From 1982 I was employed at Alfa-Laval and Tetra Pak with a range of assignments and studies:

- 2012 – 2020 Senior Technology Specialist (Heat Treatment & Math. Modeling & Simulation)
- 2001 – 2012 Senior Development engineer and project manager
- 2004 – 2007 PhD studies (part time) at the Faculty of Engineering at Lund University
- 1982 – 2001 Department manager, Environmental manager, Technical product manager, Project manager, Food plant and line automation engineer.

After retirement 2020 I have worked as self-employed consultant in combination with independent private researcher at NovaUmbra.

I am married since 1978 and have three grown-up children with their own families.

LinkedIn

Research

Lund University

Inventions & patents

Education & research