Modelling and Simulation of Retort Processes

PTC Konolfingen

Bigelow‘s law

F_0-value

worst case scenario

heat transfer

modelling / simulation

analytical modelling

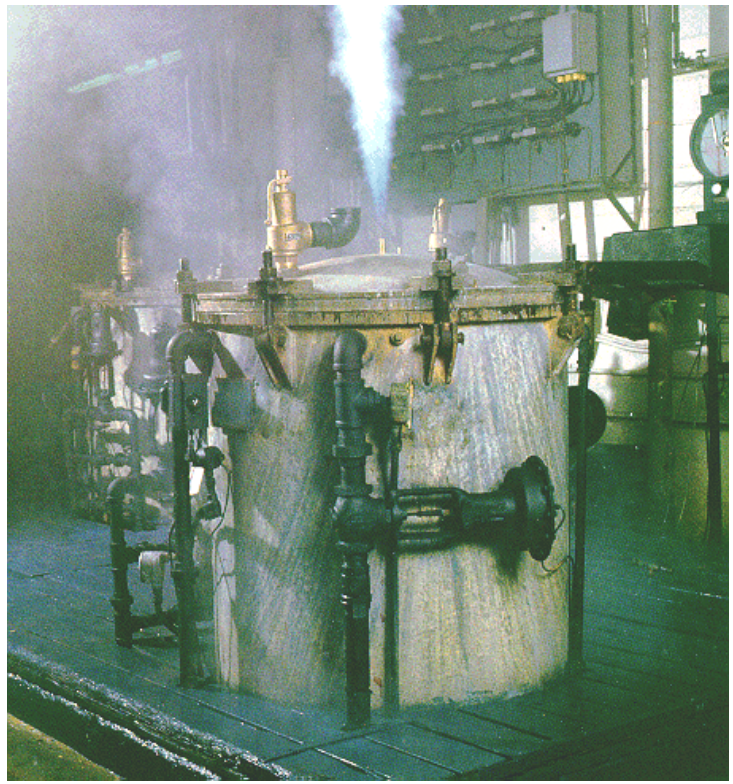
numerical modelling

summary

IFTPS *Institute For Thermal Processing Specialists*

1st European Conference:
Harmonization of Standards in Thermal Processing

October 30th and 31st, 2007
Grande Hotel do Porto
Porto, Portugal



Modelling and Simulation of Retort Processes

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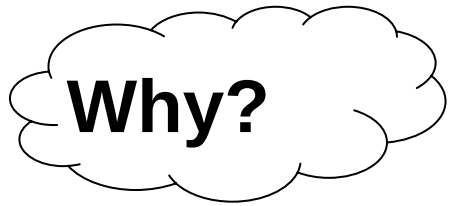

Are our retorted food products commercially sterile?

Bigelow's Law

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Modelling:

temperature time combination ~ microbiological reduction

Bigelow's Law ("General Method", W.D. Bigelow 1921)

$$F_z^{T_R} = \int_{t_B}^{t_E} 10^{\frac{T_C(t)-T_R}{z}} dt = D_{T_R} \cdot \log \frac{C_B}{C_E}$$

linear thermal death kinetics = first order reaction

$T_C(t)$ must be determined very accurate and precise

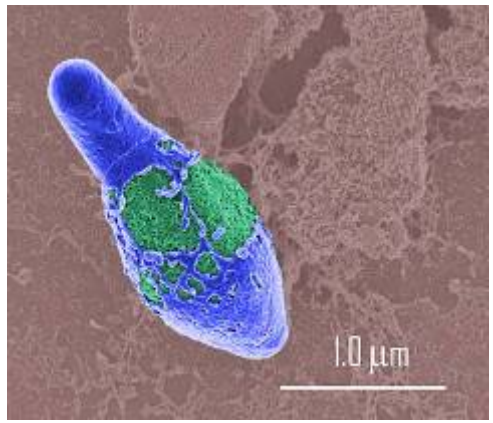
Bigelow's Law, F_0 - value

$$F_z^{T_R} = \int_{t_B}^{t_E} 10^{\frac{T_C(t)-T_R}{z}} dt = D_{T_R} \cdot \log \frac{C_B}{C_E}$$

example: "low acid canned food"
pH > 4.6 und a_w > 0.85 (FDA)

<u>food safety:</u>
Clostridium botulinum

decimal reduction time:	D_{TR} = 0.25 min
reference temperature:	T_R = 121.1°C
z-value:	z = 10°C
target: 12 decimal reductions:	log (C_B/C_E) = 12



$$F_0 = \int_{t_B}^{t_E} 10^{\frac{T_C(t)-121.1°C}{10°C}} dt = 0.25\,\text{min} \cdot 12 = 3\,\text{min}$$

F_0 - value

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$$F_0 = \int_{t_B}^{t_E} 10^{\frac{T_C(t) - 121.1°C}{10°C}} dt = 3\,\text{min}$$

with $dt = \Delta t \rightarrow 0$

and $\Delta t = \text{constant} = \Delta t_i = t_i - t_{i-1}$

and $n \cdot \Delta t = t_E - t_B$

$$\Rightarrow F_0 = \sum_{i=1}^{n} 10^{\frac{T_{Ci} - 121.1°C}{10°C}} \cdot \Delta t = 3\,\text{min}$$

$T_C(t)$ can be measured at different times t_i

it is defined as follows: $T_C(t_i) = T_{Ci}$

F_0 - value

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temperature measurement equipment for the use inside retorts ...

Worst Case Scenario

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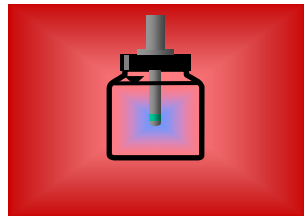
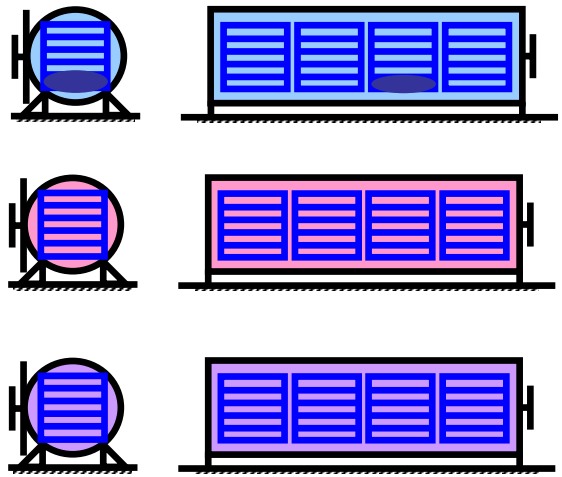
$$F_0 = \sum_{i=1}^{n} 10^{\frac{T_{Ci} - 121.1°C}{10°C}} \cdot \Delta t = 3\,\text{min}$$

T_{Ci} is defined as measured product temperature at the coldest spot inside the container.



This container is located at the cold spot of the retort,



which is heated slowest.

Worst Case Scenario

During production direct measurements of product temperature considering the worst case scenario are practically not possible.

Heat Transfer

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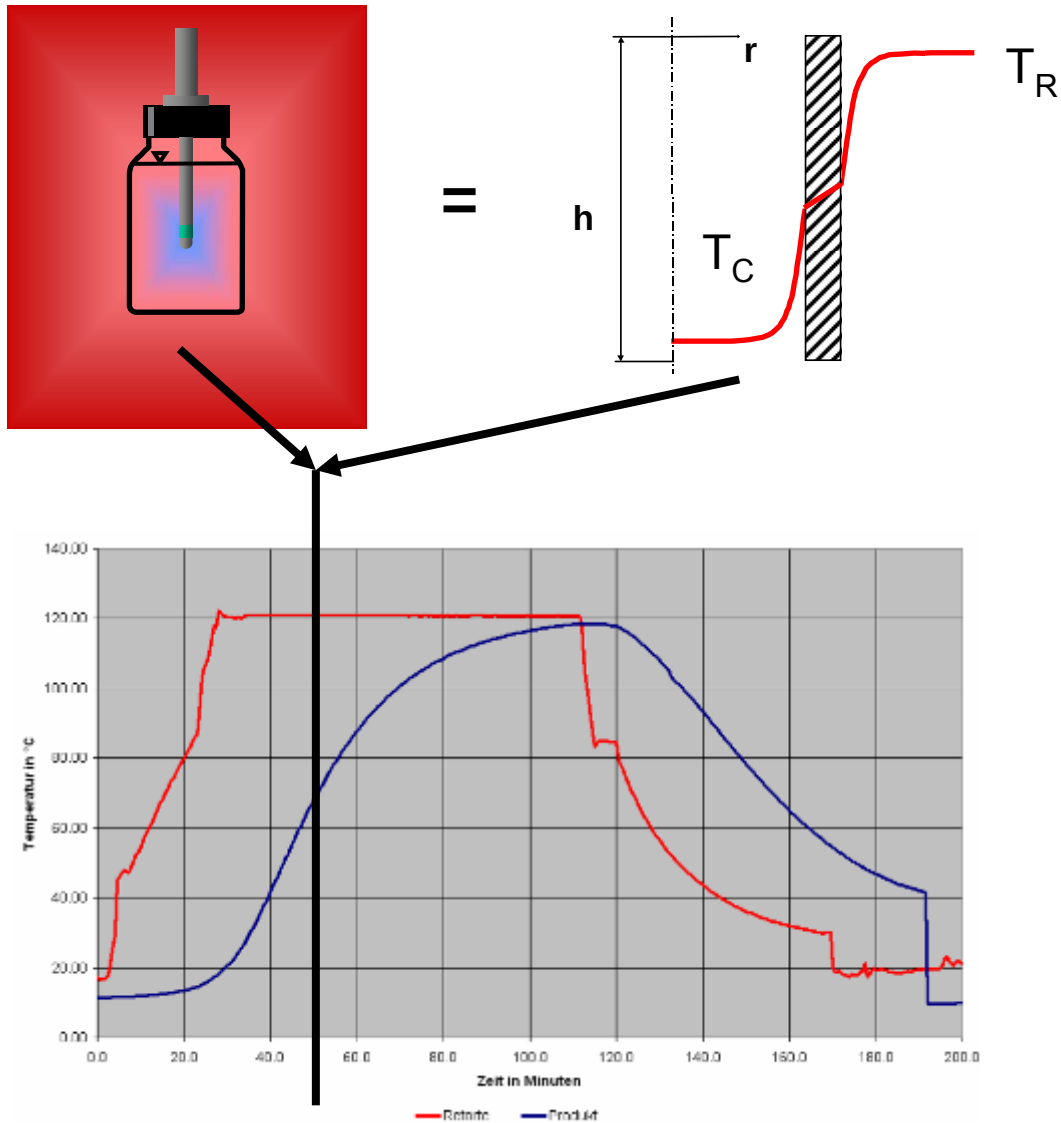
snapshot of information (photo)

chronological sequence of information (film)



1.

2.

heat penetration studies

measured or assumed scenario:
- retort temperature RT(t),
- initial product temperature IT,
- cooling water temperature RWT

→ model of heat transfer →

simulation of product temperature $T_C(t)$ at the coldest spot

Modelling / Simulation

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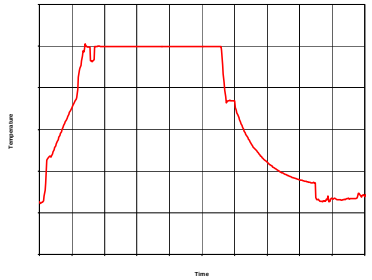


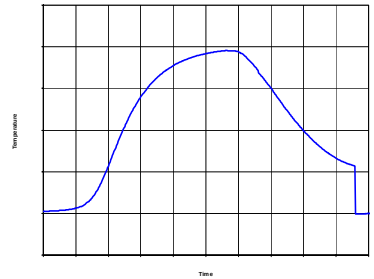
retort temperature must be measured (and controlled) during production

model:

heat transfer

retort temperature ~ product temperature

product temperature (considering the worst case scenario) cannot be measured during production



Modelling

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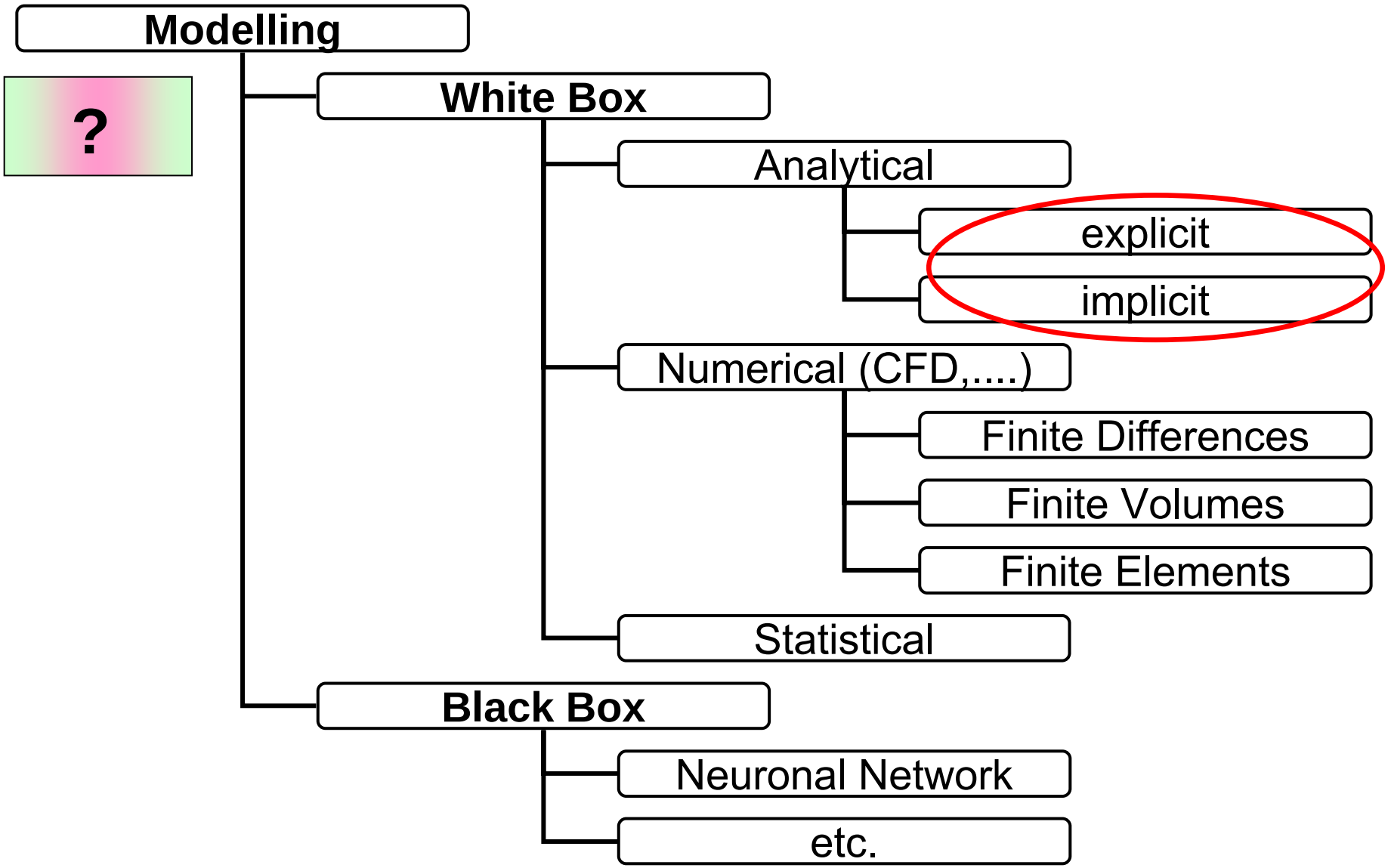

Analytical Modelling

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(formula methods):
examples: Ball, Stumbo, ...

logarithmic linear heating curve

$$T_C(t) = RT - j_h \cdot (RT - IT) \cdot 10^{\frac{-t}{f_h}}$$

hyperbolic cooling curve

$$\frac{\left[T_g + 0.3 \cdot (T_g - T_w) - T_C(t)\right]^2}{\left[0.3 \cdot (T_g - T_w)\right]^2} - \frac{t^2}{(0.175 \cdot f_h)^2} = 1$$

logarithmic linear cooling curve

$$T_C(t) = T_w - j_c \cdot (T_g - T_w) \cdot 10^{\frac{-t}{f_c}}$$

May, N.: “Guidelines for Performing Heat Penetration Trials for Establishing Thermal Processes in Batch Retort Systems”, Campden & Chorleywood Food Research Association, Guideline No. 16, 1997

Analytical Modelling

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$$T_C(t) = RT - j_h \cdot (RT - IT) \cdot 10^{\frac{-t}{f_h}}$$

logarithmic linear heating curve

$$\Leftrightarrow \log\left[RT - T_C(t)\right] = -\frac{1}{f_h} \cdot t + \log\left[j_h \cdot (RT - IT)\right]$$

with $j_h \cdot (RT - IT) = RT - T_A$

$$\Rightarrow \log\left[RT - T_C(t)\right] = -\frac{1}{f_h} \cdot t + \log(RT - T_A)$$

with $y = \log\left[RT - T_C(t)\right]$

and $t = x$

and $m = \frac{1}{f_h}$

and $n = \log(RT - T_A)$ mit $T_C(t = 0) = T_A \leq IT$

$$\Rightarrow y = -mx + n$$

linear equation

Analytical Modelling

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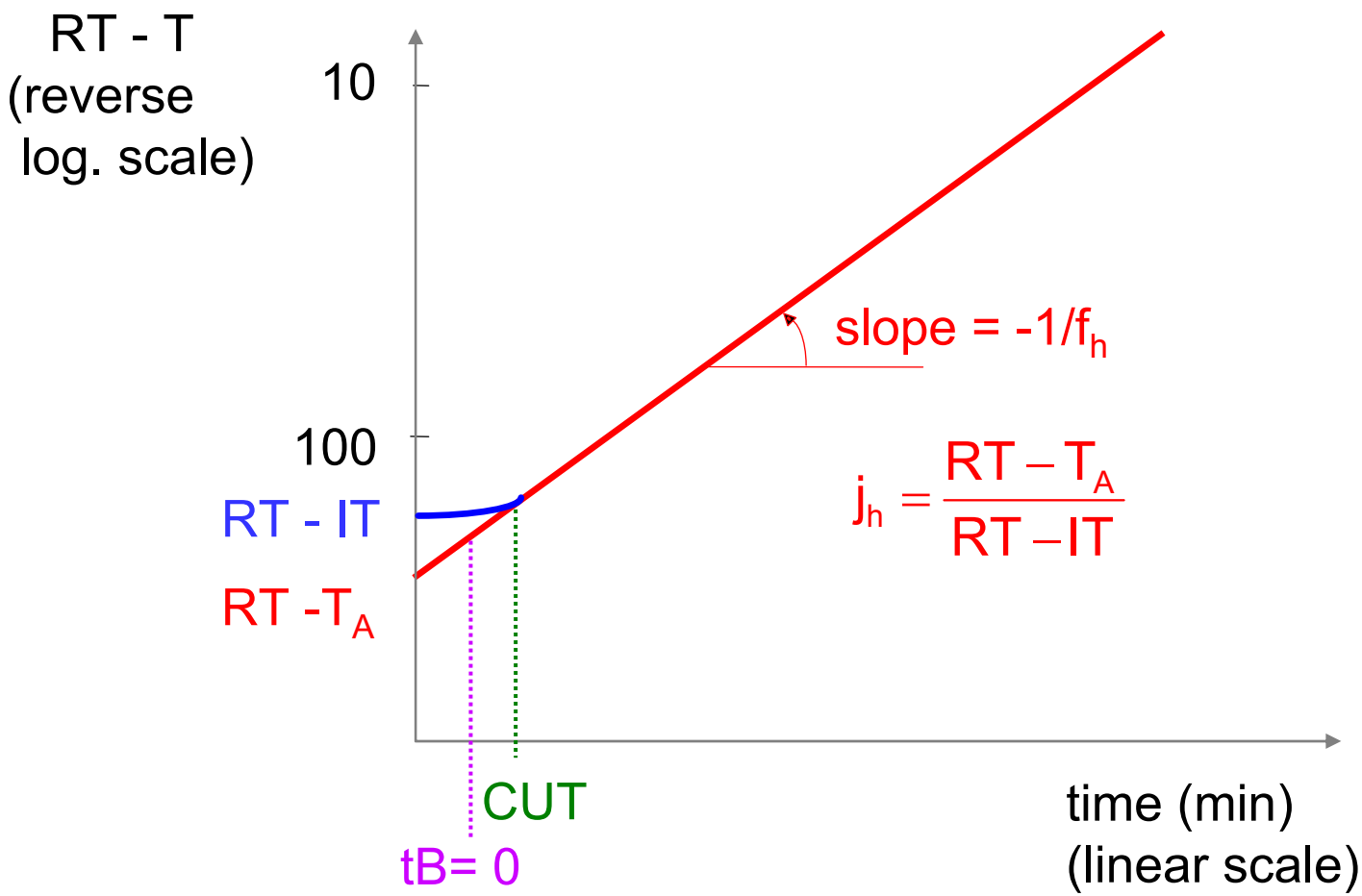
logarithmic linear heating curve



Analytical Modelling

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Ball's assumptions:

RT = constant

$t_{Ball} = t_{hold} + 0.42\ CUT$

RTW = constant

$f_h = f_c$

$j_c = 1.41$

Charles Olin Ball, 1957

Stumbo's assumptions:

RT = constant

$t_{Ball} = t_{hold} + 0.42\ CUT$

RTW = constant

f_h, f_c

j_h, j_c

Charles Raymond Stumbo, 1973

Charles Raymond Stumbo, the youngest child of FRED KING and IDA MAE STUMBO was born July 25, 1913 in Monmouth, Kansas. Charles held a PhD in Food Chemistry. He work for Heinz Corp., Michigan State College and the University of Massachusetts. He married Vi Brunk on April 4, 1936. They had two sons and one daughter. - Charles died in 1989.

Analytical Modelling

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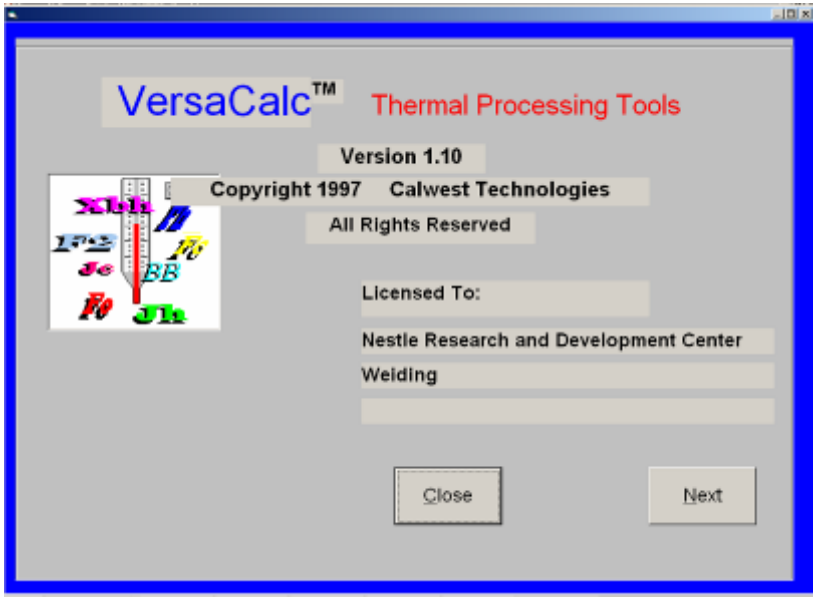
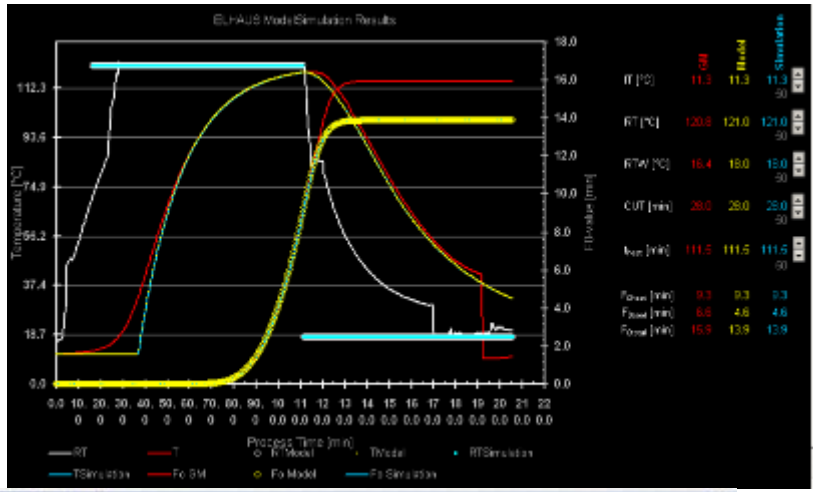
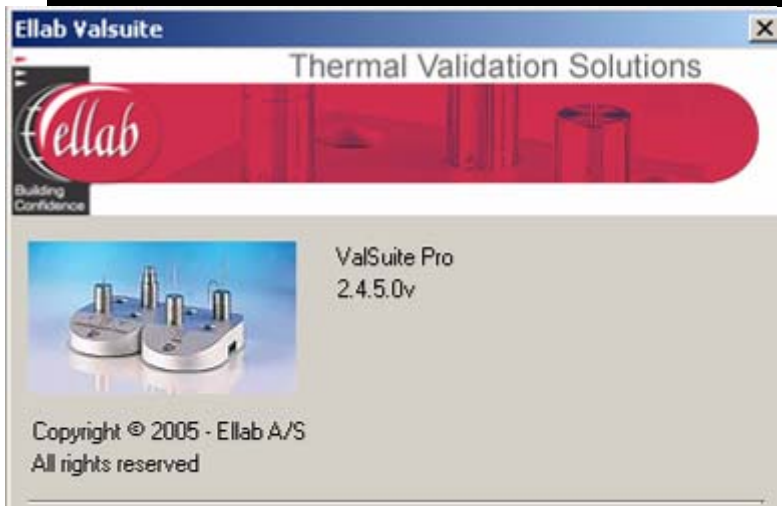
Analytical Modelling (Formula Methods):
Examples: Ball, Stumbo, ...







Modelling

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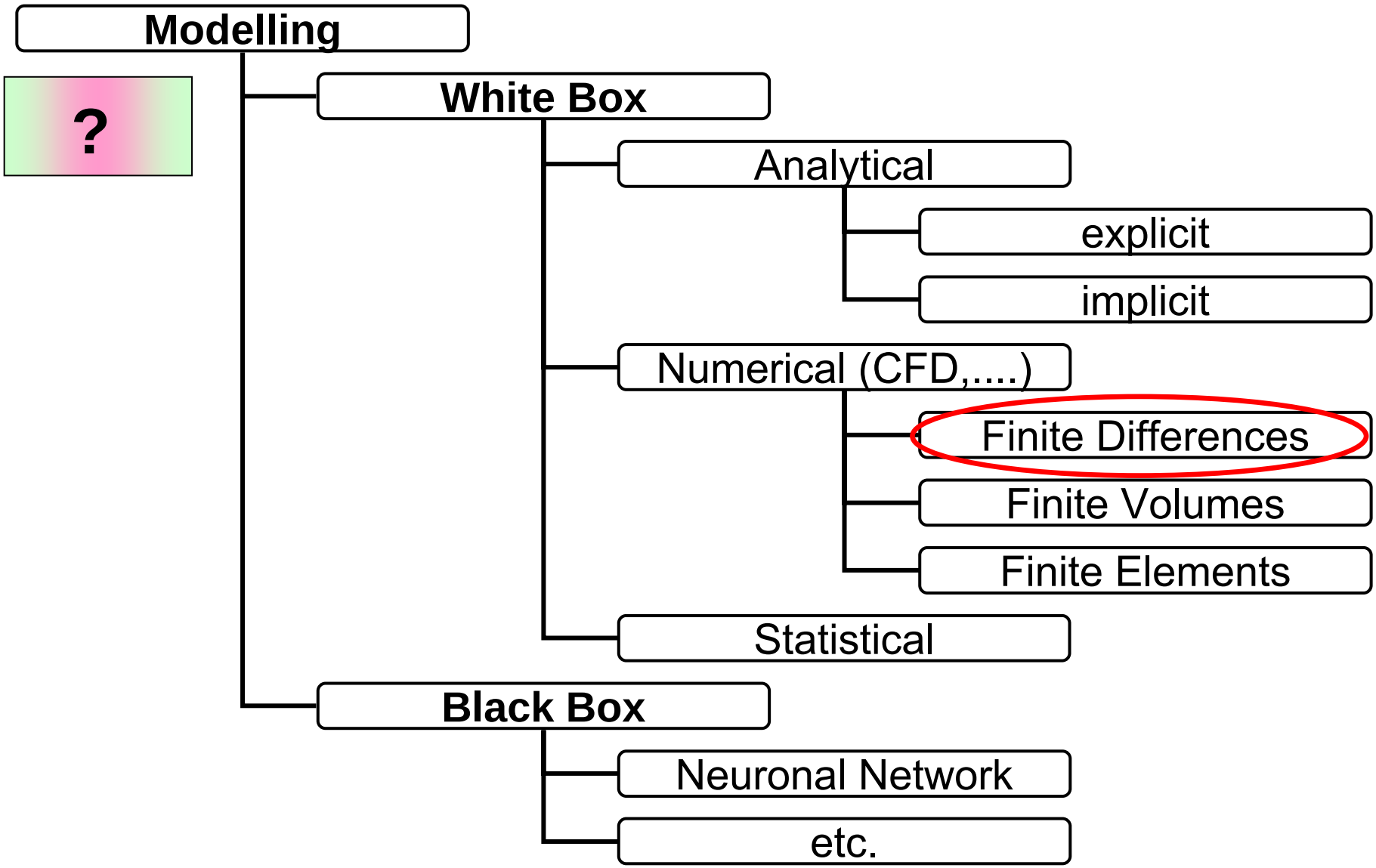

Numerical Modelling

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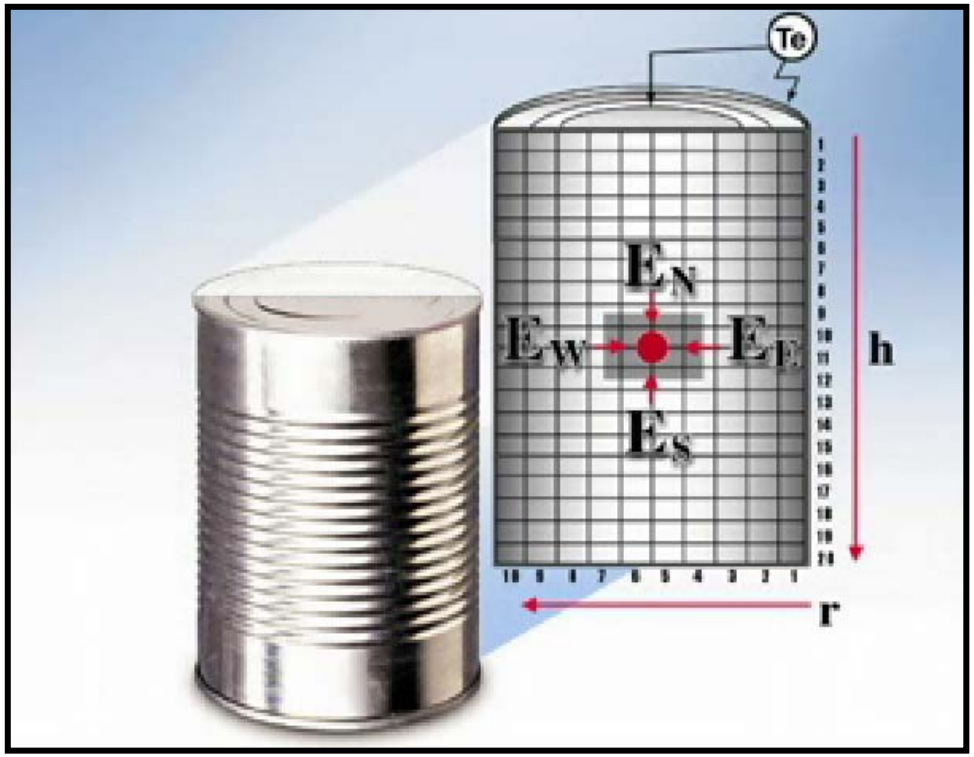
example: finite differences, ...



mass- and energy ballance at an infinitesimal volume

Numerical Modelling

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$$\frac{\partial T}{\partial t} = \alpha \left\{ \frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial h^2} \right\} \quad mit \quad \alpha = \frac{k}{\rho c_P}$$

Heat transfer equation

- conductive heat transfer in a finite cylinder
- twodimensional partiel differential equation of 2nd order
- can be solved numerically with methode of finite differences

T	temperature in K
t	time in s
r	radial coordinate in m
h	vertical coordinate in m
α	thermal diffusivity in m^2/s
k	heat conductivity in W/(mK)
ρ	density in kg/m^3
c_P	specific heat capacity at constant pressure in J/(kg K)

Numerical Modelling

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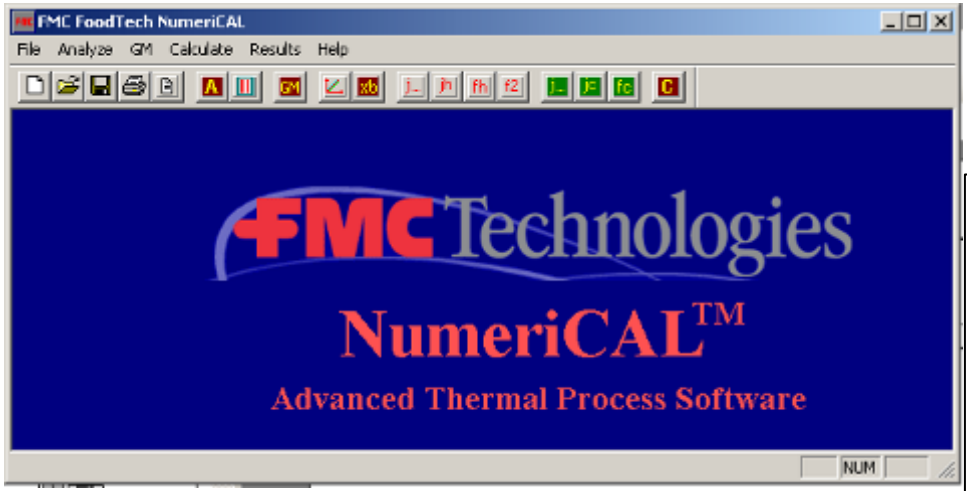
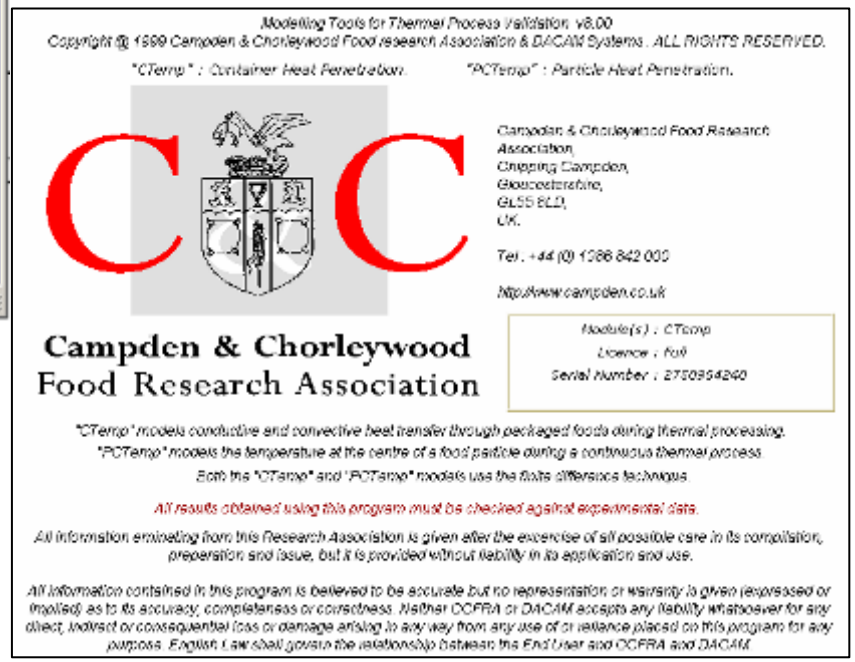
(Finite Differences):
Example: NumeriCal, CTemp, ...





Summary 1

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	General Method	**Formula Methods** (Ball, Stumbo, ...)	**Numerical Method** (finite Differences)
object	microbiological reduction – time temperature	heat transfer	heat transfer

Summary 1

PTC Konolfingen

	General Method	**Formula Methods** (Ball, Stumbo, ...)	**Numerical Method** (finite Differences)
object	microbiological reduction – time temperature	heat transfer	heat transfer
accuracy	most accurate (bench mark)	(very) conservative	very accurate

Summary 1

PTC Konolfingen

	General Method	Formula Methods (Ball, Stumbo, ...)	Numerical Method (finite Differences)
object	microbiological reduction – time temperature	heat transfer	heat transfer
accuracy	most accurate (bench mark)	(very) conservative	very accurate
advantages / disadvan-tages	simple calculation	a lot of assumptions	complex calculation
	not flexible (no deviations, no alternate processes predictable)	flexible (deviations, alternate processes predictable with some restrictions: IT, RT, RTW, CUT, t_{heat})	very flexible (deviations, alternate processes predictable)

Summary 2

PTC Konolfingen

	General Method	**Formula Methods** (Ball, Stumbo, ...)	**Numerical Method** (finite Differences)
software	data logging software (VersaCalc, CalSoft, Ellab, ... nearly all)	VersaCalc, CalSoft, Ellab, C-Temp, ...	NumeriCal, C-Temp, ...

Summary 2

PTC Konolfingen

	General Method	Formula Methods (Ball, Stumbo, ...)	Numerical Method (finite Differences)
software	data logging software (VersaCalc, CalSoft, Ellab, ... nearly all)	VersaCalc, CalSoft, Ellab, C-Temp, ...	NumeriCal, C-Temp, ...
criteria for selection	• validation of the software • recognized industrial standard • data import • data export • clearness, obvious handling • data security in compliance to 21CFR Part 11 • documentation		

Summary 3

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- There is a relation in between time temperature and microbiological reduction available.

- It is nearly impossible to determine the microbiological reduction during commercial production in retorts because of two reasons:
  1. In the above mentioned relation the microbiological reduction is affected very heavily by the measured temperature.
  2. The necessary consideration of the worst case scenario leads to not practical measurement requirements.

- That is why models for the heat transfer from outside to inside the containers are the method of choice.

- These models can demonstrate that a standard production lot has received a defined microbiological reduction (product release) and can simulate deviations.

- Both is reducing costs and is increasing product quality.

Modelling and Simulation of Retort Processes

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Education and training are an absolute must and a key for success ...

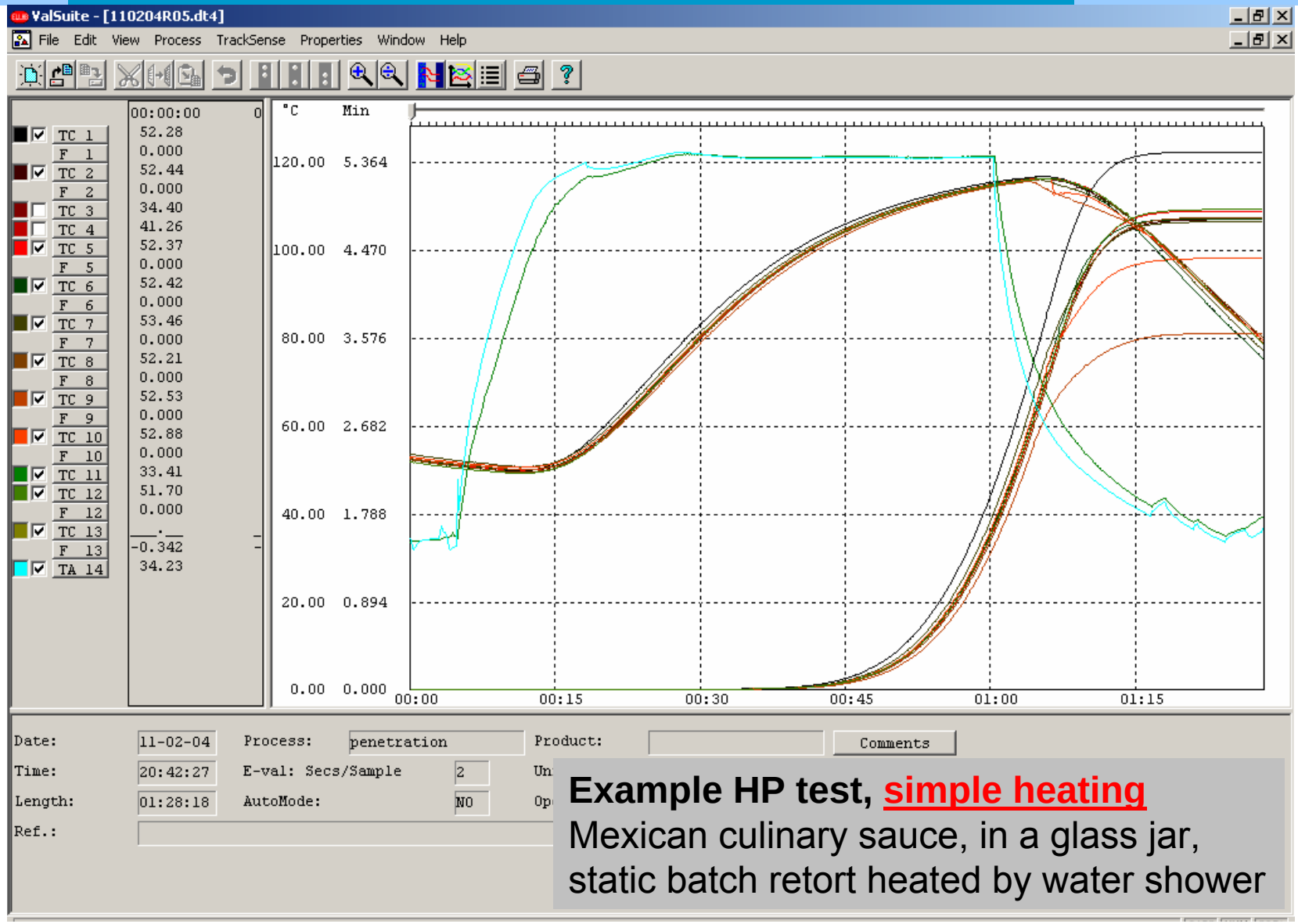
... the “blind use“ of each modelling software is dangerous.

... only good measured data lead to good models.

... thank you very much for your patience.

Modelling and Simulation of Retort Processes

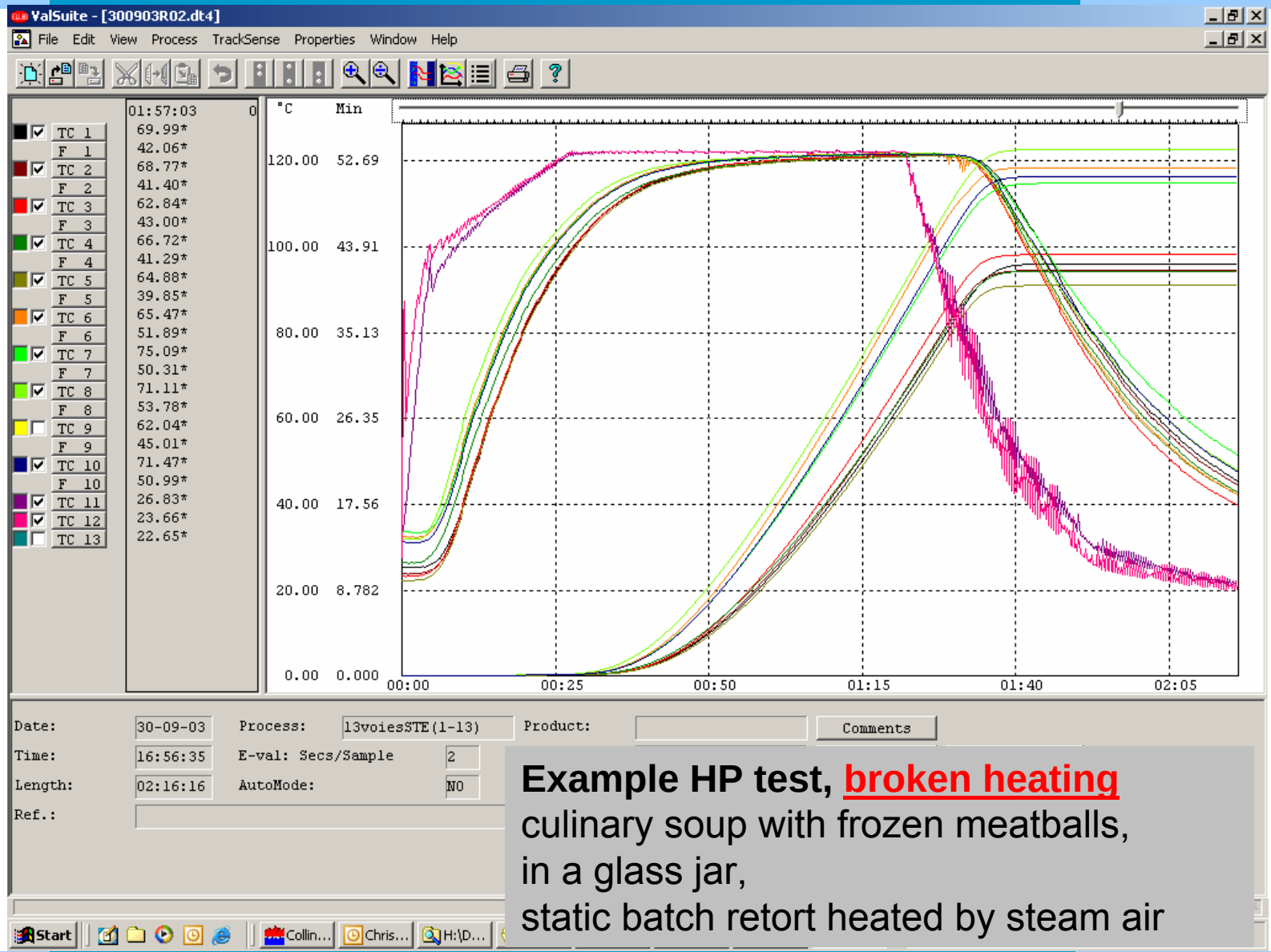
Nestlé
PTC Konolfingen



Example HP test, simple heating
Mexican culinary sauce, in a glass jar, static batch retort heated by water shower

Modelling and Simulation of Retort Processes

Nestlé
PTC Konolfingen



Example HP test, broken heating
culinary soup with frozen meatballs,
in a glass jar,
static batch retort heated by steam air