Applications of Finite Difference Analyses to Assess Lethality and Quality

IFTPS – Bangkok
November 4, 2014

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- Calculation Methods
    - The General Method
    - Ball Formula Method
    - Finite Difference Model (NumeriCAL™)
- Cook Value
- Process Optimization Approach
- Case Study Example

Thermal Processing
– Scientific Development

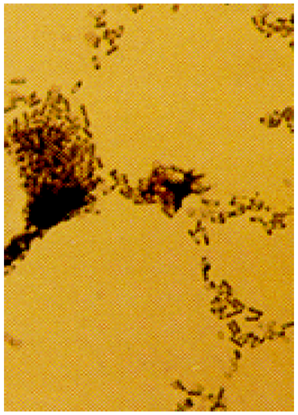
- 1810
  N. Appert published his treatise on canning
  P. Durand introduced the patented “tin canisters”

- 1864
  - Pasteur discovered the relationship between heat and death of microbial cells and food spoilage

Thermal Processing – Scientific Development

- 1874 – First use of pressure cooker

- 1910 - Importance of controlling C. Botulinum in canned foods was established



Thermal Processing
– Process Calculation Methods

- 1920
  - Bigelow established the relationship between pH of foods and heat resistance of bacterial spores
  - Developed first scientifically based method to calculate the minimum safe sterilization of canned foods
- 1923 - C. Olin Ball developed a mathematical method for the determination of sterilization processes.

Thermal Processing
– Process Calculation Methods

- 1952 - General Method - Modified by Patashnik
- 1953 - Gillespy Formula Method
- 1966 - Stumbo Formula Method
- 1988 - NumeriCAL™ - thermal process finite difference model released for industry use

Thermal Processing
– Process Calculation Methods

- Today the three most widely used thermal process calculation methods are:
  - General Method
  - Ball Formula Method
  - NumeriCAL (finite difference method)

The General Method - Attributes

- Advantages
  - It can be a very accurate method
  - Relatively simple to use
- Disadvantages
  - Based on direct temperature measurement
  - Temperature measurement system and thermocouples <u>must be calibrated</u> to a known standard.

Improved General Method

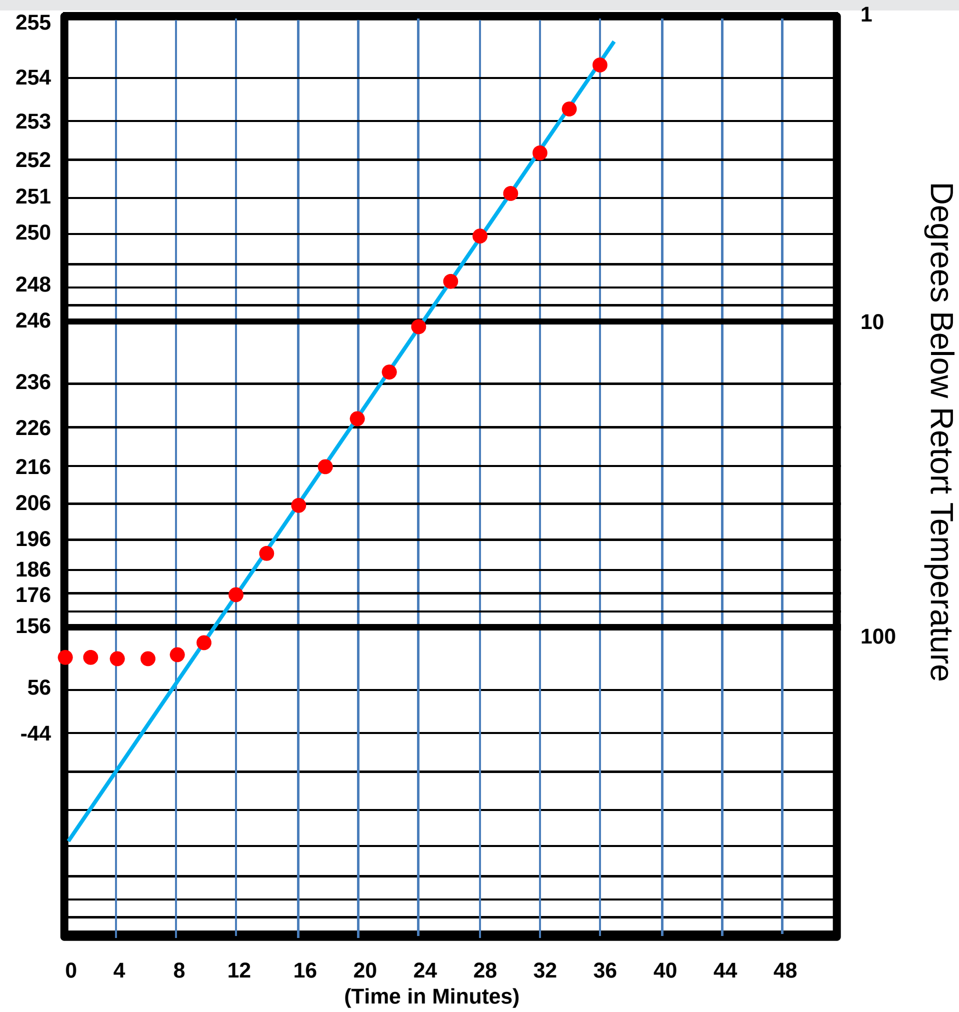
- Unlike the Ball Formula and Finite Difference Methods, the General Method only allows the determination of the lethality delivered from a specific set of test/process conditions.
- Cannot be used to accurately design processes at initial temperatures and retort temperatures that are different from what was tested
- **What you test is what you get**

The Ball Formula

- Developed in the 1923 by C. Olin Ball
- Based on temperature differences (difference between cold spot temperature in the container and retort temperature) instead of absolute temperature readings
- A "formula method" that allows for the determination of process time or lethality independent of a direct temperature measurement
- The Ball Formula Method is one of most widely used process calculation methods

The Ball Formula - Attributes

- Allows use of semi-log curves for detailed analysis of time temperature data
- Provides some correction for come up time
- Utilizes heating factors that facilitate the calculation of processes over a range of IT and RT
- Generally viewed as a conservative thermal process model



Ball Formula Assumptions

- 42% of the Come-Up Time may be considered as time at process temperature.
- No additional heating once cooling begins.
- Cooling lag (j_c) is fixed at 1.41.
- Cooling slope (f_c) is fixed at the faster of the f_h or f_2 values.
- Containers are immediately exposed to cooling water temperature of 100ºC below the retort temperature

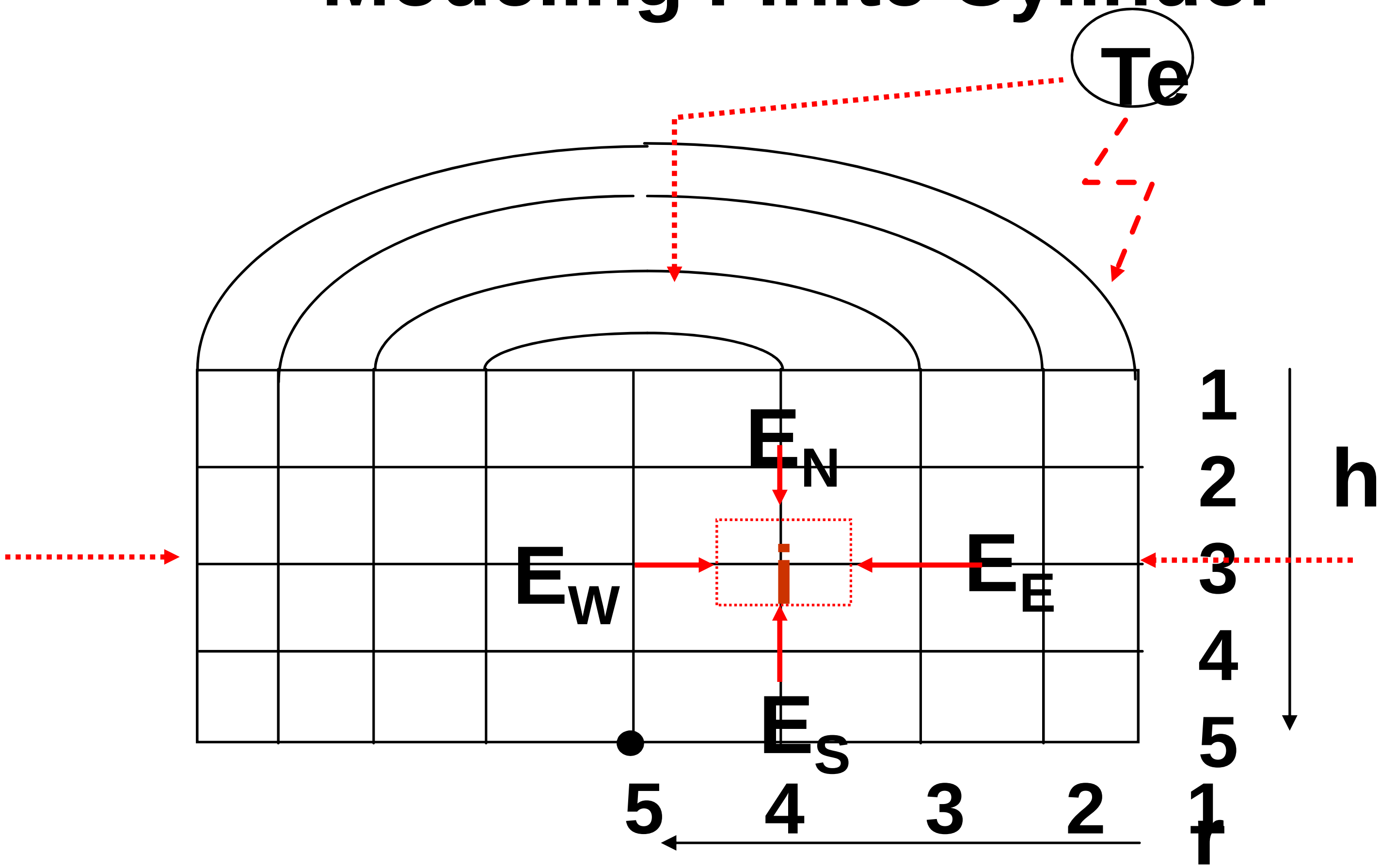
Finite Difference Model

- The finite difference method (Explicit Alternating Direction) is used to solve the governing partial differential equations of unsteady state heat transfer problems.

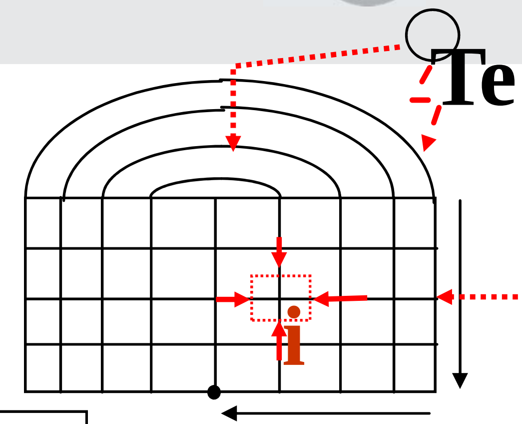
- By adding heat penetration and sterility characteristics of the product, as well as the time and retort temperature during each stage of the thermal process, the finite difference model accurately simulates the cold point temperature of a thermally processed food as it passes through various stages of sterilization and cooling.

Finite Difference Method - “Grid”

Modeling Finite Cylinder



Finite Difference Method Simulation



Initial Input, Runtime = 0

↓

Runtime = Runtime + dt

↓

Read Boundary Temp at Runtime

↓

Simulate the Surface Node Temperatures

↓

Simulate the interior node temperatures, node by node, layer by layer towards the cold spot

↓

Calculate the accumulated lethality, Fo(t) at cold spot

(loop back to: Runtime = Runtime + dt)

NumeriCAL™

- NumeriCAL™ is a finite difference model which is designed to overcome many of the limitations of the General Method and the Ball Formula Method.
- Provides Ball Method flexibility (ranging RT, IT).
- Utilizes Ball "type" heating and cooling factors (f_h, j_h, etc.)
- Models the container cold spot temperature for any type of heat transfer mode.
- Handles variable retort temperatures.
- Accurate for all container shapes and sizes.
- Delivers General Method accuracy for the calculated F_o-value of both the heating and cooling portions of the process.

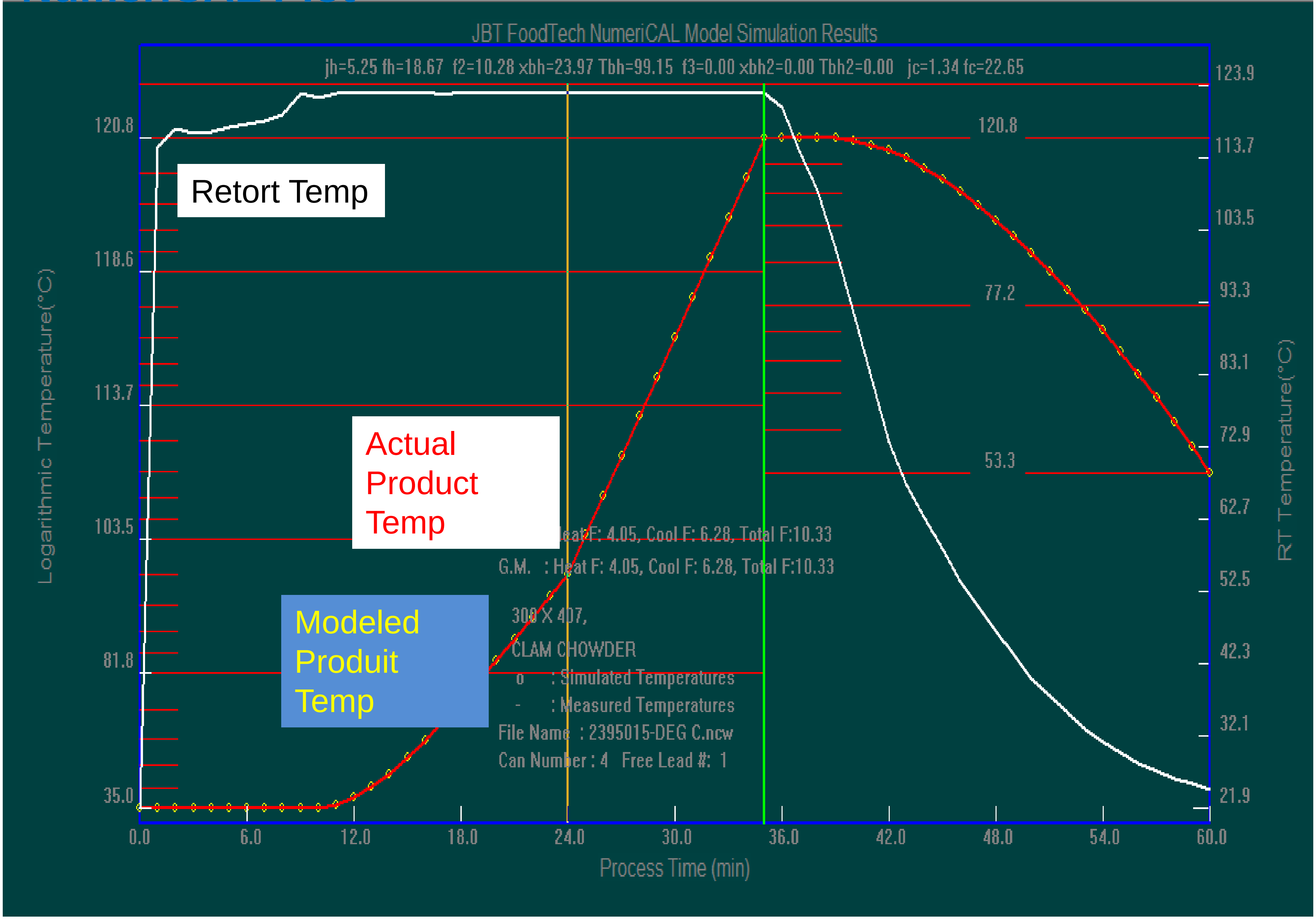
Summary - NumeriCAL

- Can be used for:
  - Initial temperatures different from HP test.
  - Varying retort temperatures
    - Ramped come-up.
    - Temperature deviations
  - Modeling the cooling portion of the process.
  - Process optimization, utilizing come-up, cook and cool.

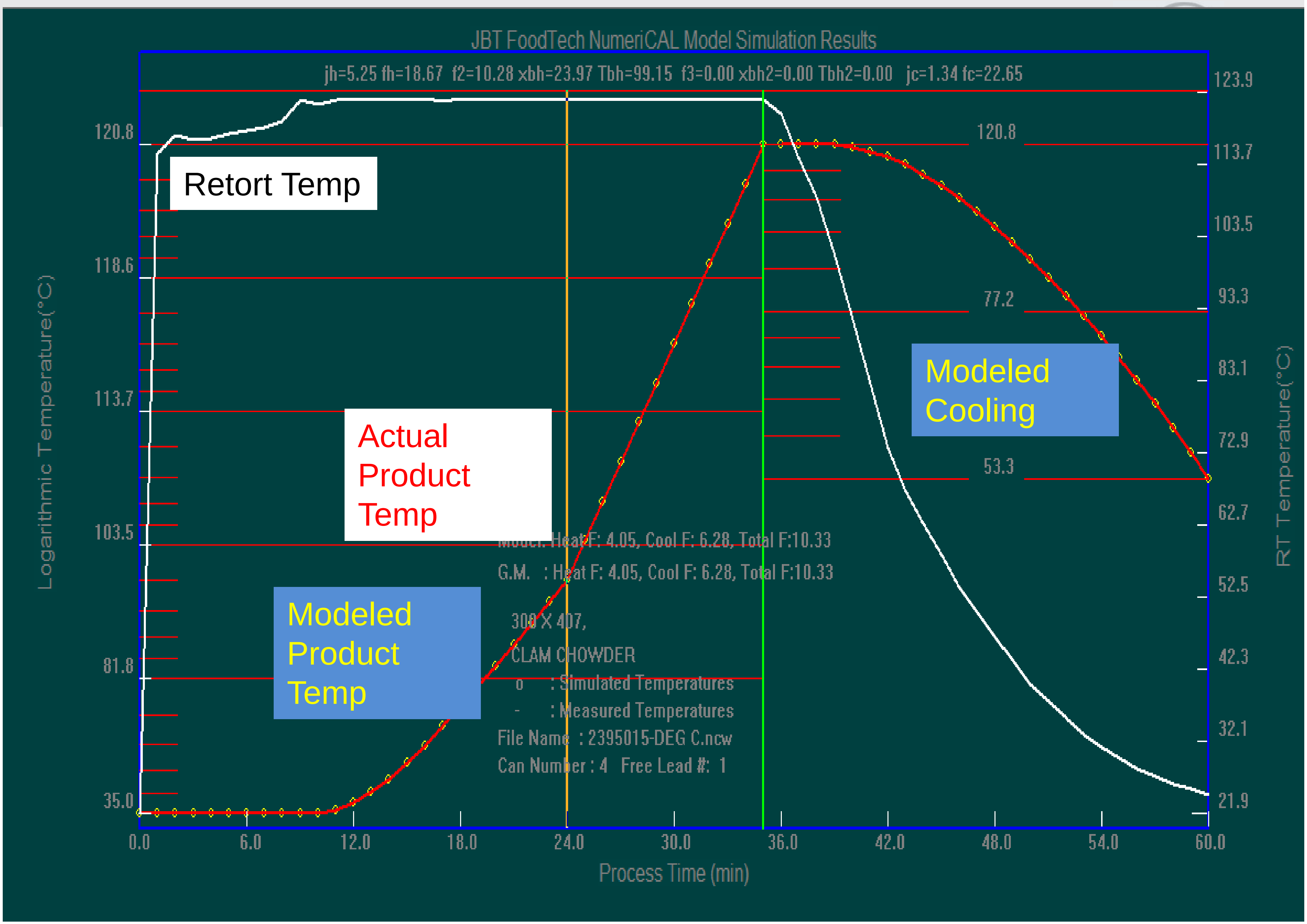
NumeriCAL™ - Attributes

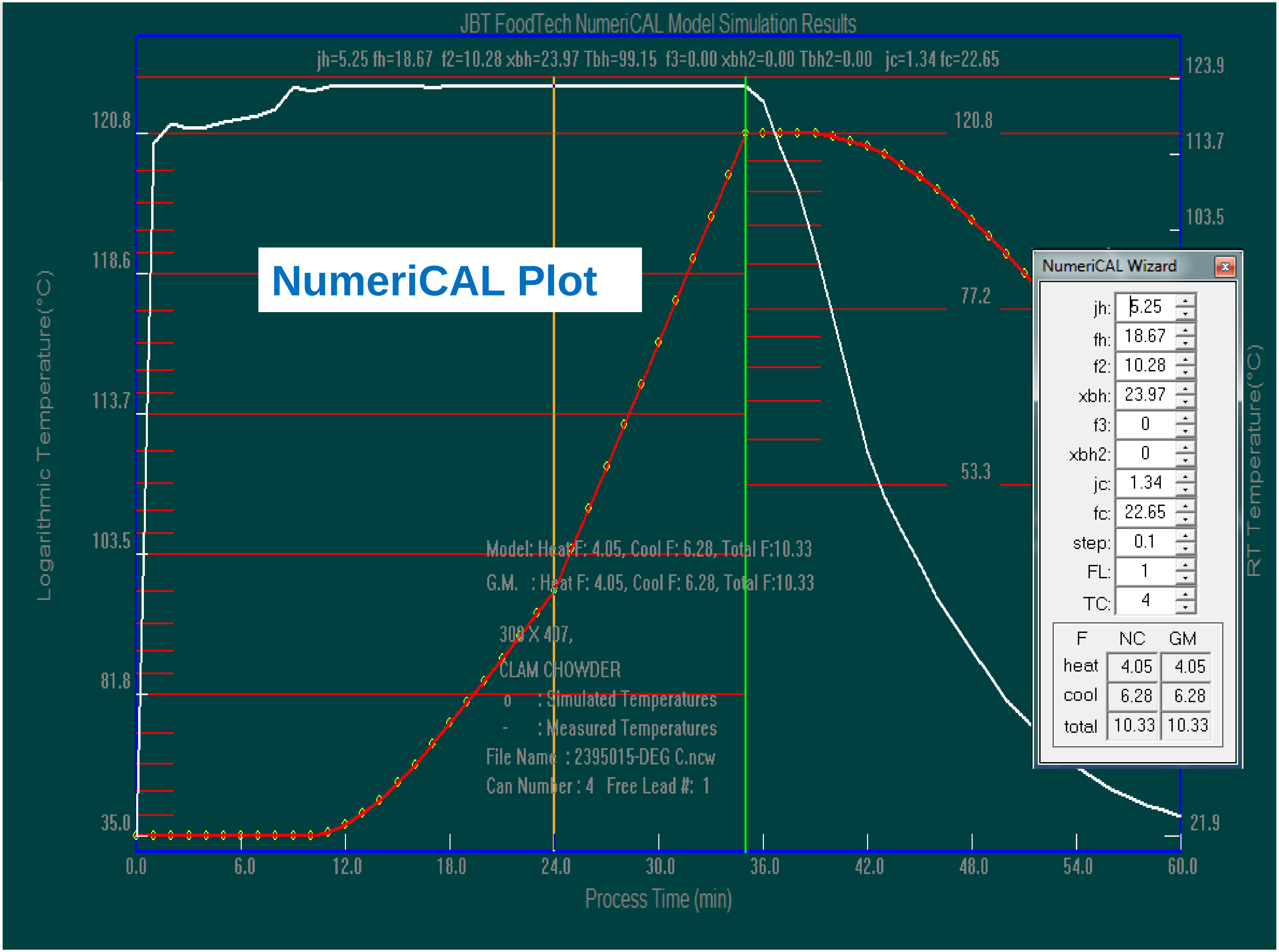
- Accurately models all phases of the process; Come-up, Cook, and Cool
  - Can be used to reduce process time without sacrificing product safety. determine best process approach for a particular product.
  - Can evaluate the effect a process change will have on product quality or cook value.

NumeriCAL Plot



NumeriCAL Plot





JBT FoodTech NumeriCAL Model Simulation Results
jh=5.25 fh=18.67 f2=10.28 xbh=23.97 Tbh=99.15 f3=0.00 xbh2=0.00 Tbh2=0.00 jc=1.34 fc=22.65
NumeriCAL Plot
Logarithmic Temperature(°C)
120.8
118.6
113.7
103.5
81.8
35.0
123.9
113.7
103.5
120.8
77.2
53.3
21.9
RT Temperature(°C)
Model: Heat F: 4.05, Cool F: 6.28, Total F:10.33
G.M. : Heat F: 4.05, Cool F: 6.28, Total F:10.33
300 X 407,
CLAM CHOWDER
o : Simulated Temperatures
- : Measured Temperatures
File Name : 2395015-DEG C.ncw
Can Number : 4 Free Lead #: 1
0.0
6.0
12.0
18.0
24.0
30.0
36.0
42.0
48.0
54.0
60.0
Process Time (min)
NumeriCAL Wizard
jh: 5.25
fh: 18.67
f2: 10.28
xbh: 23.97
f3: 0
xbh2: 0
jc: 1.34
fc: 22.65
step: 0.1
FL: 1
TC: 4
F NC GM
heat 4.05 4.05
cool 6.28 6.28
total 10.33 10.33

Thermal Process Development

- Determine critical factors
- Design HP test conditions based on:
  - Product related critical factors
  - Retort type
  - Control system’s ability to accurately control all aspects of the heating and cooling process
- Conduct heat penetration studies
- Evaluate heat penetration results
- Calculate the process
- Issue process to the plant.

Thermal Process Development

- But what if you have a heat sensitive product
- Is there a way to design a safe process while optimizing for cook time or product quality

Process Optimization

- Use general method and continually repeat tests under different process conditions
- Use Ball formula to calculate processes at different initial temperatures and retort temperatures … but that is not really optimization

OR

- Use a finite difference method to accurately model the thermal process (time and temperature) and calculate more optimum processes

Process Opriomization

- How can we determine how the process conditions might affect product quality.
  - Evaluate based on the actual Fo delivered
  - Evaluate based on the “Cook Value” delivered

Cook Value

- Cook Value - is a concept that is used to describe the degradation of product sensory or nutrient attributes based on the products exposure to elevated temperatures

$$\mathbf{C_{100}} = 10^{(T-100)/z}$$

- Where
  - 100 C is the reference temperature
  - Z relates to the number of degrees C to make a ten fold change in the destruction rate of the nutrient

- **The lower the cook value delivered to a product the less nutrient degradation**

Cook Value

- Cook Value is a simple method to help determine the most suitable process conditions, ie time temperature profile, for achieving the retention of a specified vitamin or best retention of color or flavor

Cook Value

- Generally the rate of a chemical reaction (such as the destruction of a vitamin) doubles for a 10 C rise in temperature. However, the rates of bacterial destruction typically increase 10 fold for each 10 C

Cook Value

- Historically the destruction of thiamine has been used to evaluate the “cook value” of a process.

- Z = 33.0 C
- T_{ref} = 100 C

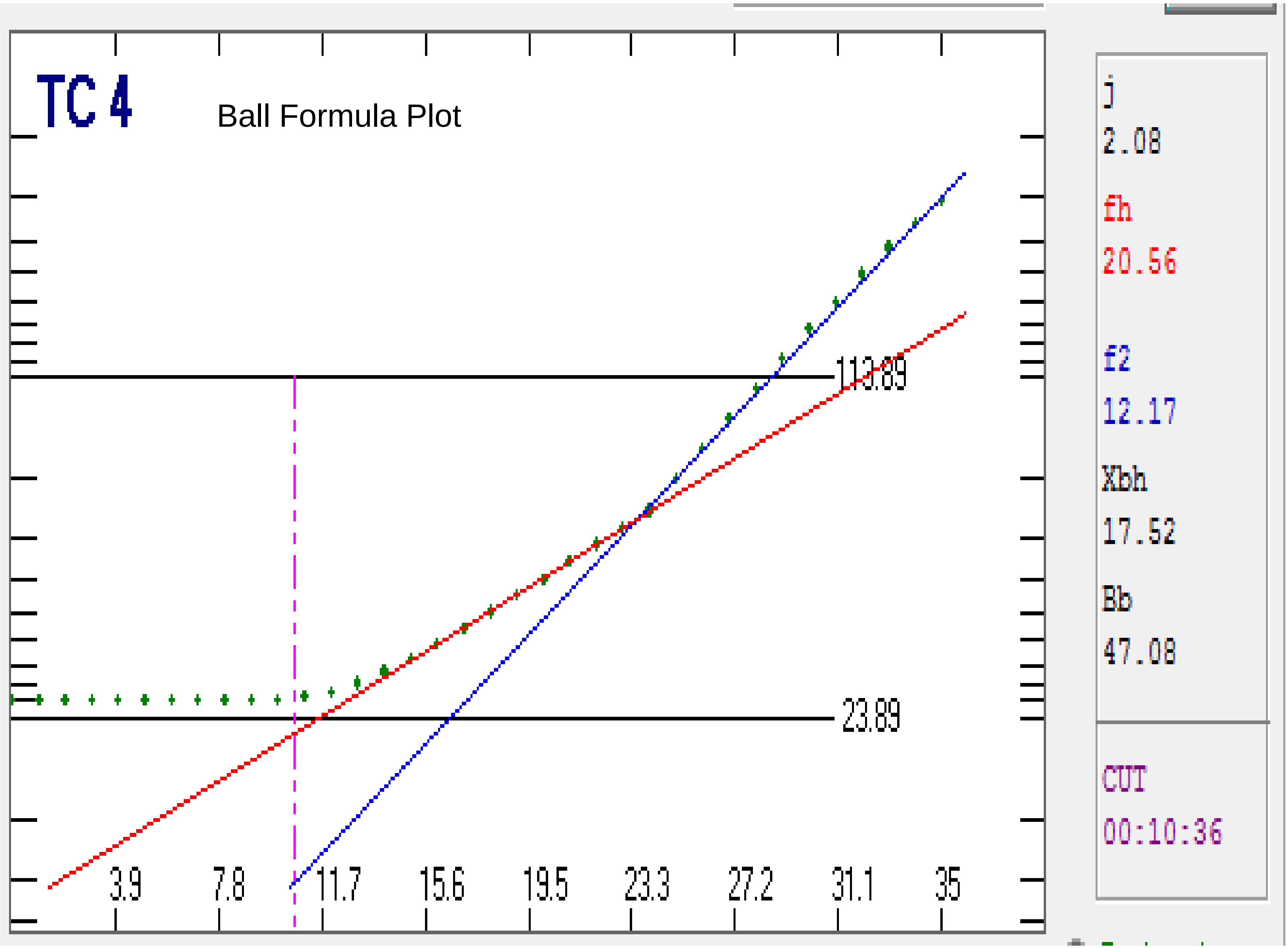
- **Goal – design a process to deliver the required Fo value while maximizing nutrient retention …. and therefore provide for both process safety and product quality**

Case Study

Determine optimum retort temperature for Clam Chowder in
76 X 110 can

Thermal Process Development

- Determine critical factors
- Design HP test conditions based on:
  - Product related critical factors
  - Retort type
  - Control system's ability to accurately control all aspects of the heating and cooling process
- Conduct heat penetration studies
- **Evaluate heat penetration results**
- **Calculate the process**
- Issue process to the plant.



TC 4
Ball Formula Plot
113.89
23.89
3.9
7.8
11.7
15.6
19.5
23.3
27.2
31.1
35
j
2.08
fh
20.56
f2
12.17
Xbh
17.52
Bb
47.08
CUT
00:10:36

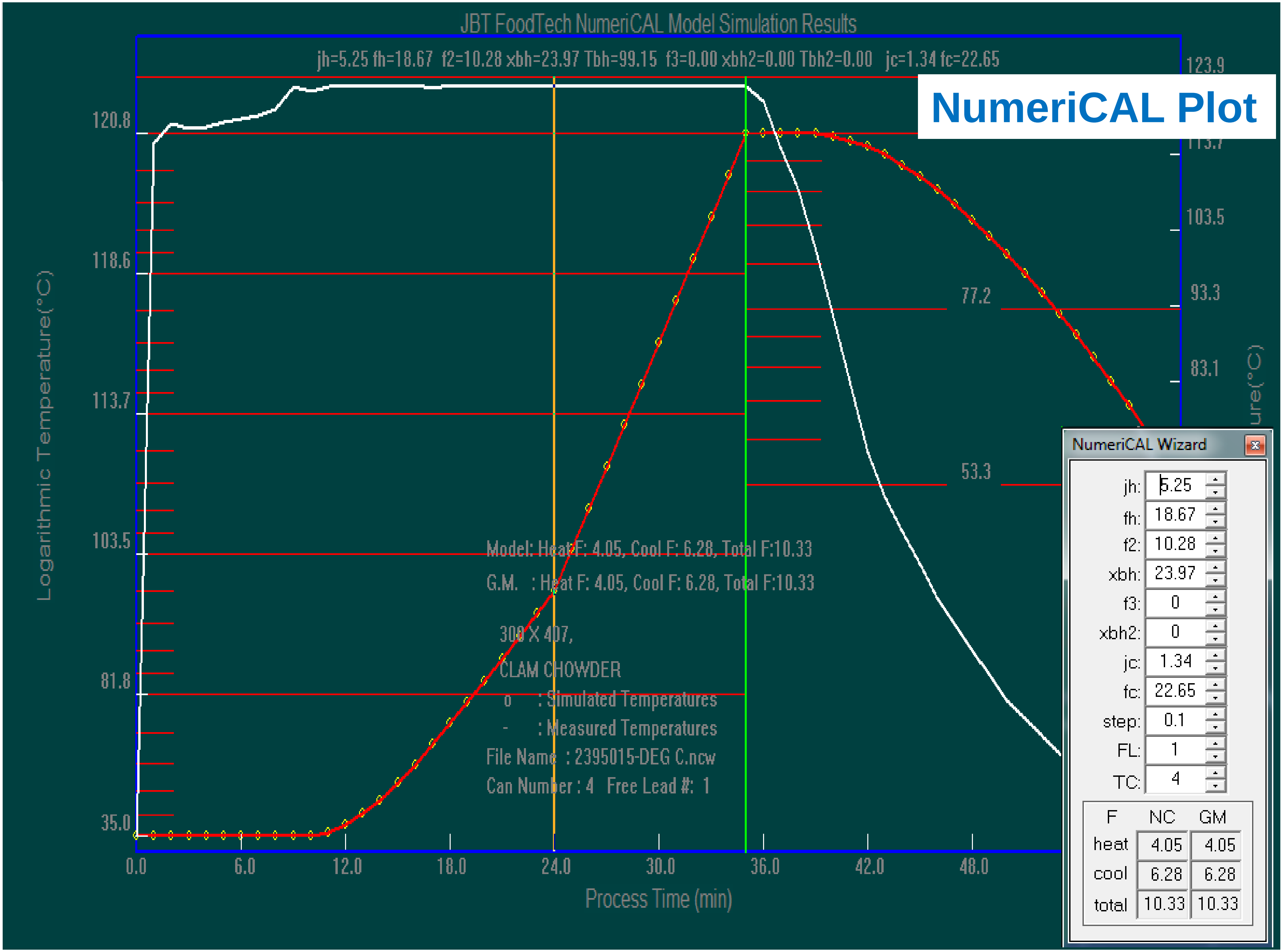
Ball Formula
Process Times - Fo = 8.0

jh = 2.08 fh = 20.56 f2 = 12.17 xbh = 17.52
jc = 1.41 fc = 12.17 F(10.00/121.11) = 8.00
m+g =100 Come-Up-Time used for Credit Calculat

9th Degree Ball Formula Used

I.T. (deg. C)	R.T. (deg. C)	Calculated Process Time (minutes)
35.00	121.00	36.32
35.00	122.00	34.39
35.00	123.00	32.76
35.00	124.00	31.36
35.00	125.00	30.15

NumeriCAL Plot



Example:
NumeriCAL - Process Calculation

PRODUCT IDENTIFICATION | PROCESS DATA

z-Value: 10 Reference Temp: 121.1 Initial Temp: 35 Temp Unit: °C Simple or Broken: B

Evaluation: 11-3-2014 Container Type: Container Dimension: Today: 11/ 3/20

Segments	1S	2S	3B	4C	5C	6C	7C	8C	9C
Duration (min)	12.00	11.97	10.58	5.00	10.00	15.00	0.00	0.00	0.00
RT Begin	85.00	123.00	123.00	123.00	70.00	25.00	0.00	0.00	0.00
RT End	123.00	123.00	123.00	70.00	25.00	25.00	0.00	0.00	0.00
jh or jc	5.25	5.25	5.25	1.34	1.34	1.34	0.00	0.00	0.00
fh, f2, f3 or fc	18.67	18.67	10.28	22.65	22.65	22.65	0.00	0.00	0.00
Elapsed Time	12.00	23.97	34.55	39.55	49.55	64.55	0.00	0.00	0.00
Retort Temp	123.00	123.00	123.00	70.00	25.00	25.00	0.00	0.00	0.00
Product Temp	39.45	98.20	120.62	117.11	70.44	36.79	0.00	0.00	0.00
Accum F Value	0.000	0.007	3.572	7.477	8.017	8.017	0.000	0.000	0.000

Example:
NumeriCAL - Process Calculation

z Value: 10.00 Reference Temp: 121.10 Initial Temp: 35.00
Temp Unit: °C Simple/Broken: B

Seg No	Segment Type	Duration (min)	Accum Time	Start RT	Final RT	Seg jh/jc	Seg fh/f2/fc	Cold Spot	Accum F (min)
1	Simple	12.00	12.00	85.00	123.00	5.25	18.67	39.45	0.000
2	Simple	11.97	23.97	123.00	123.00	5.25	18.67	98.20	0.007
3	Broken1	10.58	34.55	123.00	123.00	5.25	10.28	120.62	3.572
4	Cooling	5.00	39.55	123.00	70.00	1.34	22.65	117.11	7.477
5	Cooling	10.00	49.55	70.00	25.00	1.34	22.65	78.44	8.017
6	Cooling	15.00	64.55	25.00	25.00	1.34	22.65	36.79	8.017

Accumulated F(10.00/121.10) contributed by all heating segments (min): 3.572

Accumulated F(10.00/121.10) contributed by all cooling segments (min): 4.445

Calculated Cook Time Comparison NumeriCAL vs Ball Formula

Retort Temperature	NumeriCAL Cook Time Total Fo = 8	Ball Formula Cook Time Fo = 8
	Time in Minutes	
121	25.7	36.3
122	24.0	34.4
123	22.6	32.8
124	21.4	31.4
125	20.6	30.2

Calculated Cook Time Comparison
NumeriCAL vs Ball Formula

Retort Temperature	NumeriCAL Cook Time Fo = 8 (total)	Ball Formula Cook Time Fo = 8 (Calculated)	Actual Fo Delivered by NC Cook Time	Actual Fo Delivered by Ball Cook Time
121	25.7	36.3	8.0	18.2
122	24.0	34.4	8.0	20.6
123	22.6	32.8	8.0	23.2
124	21.4	31.4	8.0	26.3
125	20.6	30.2	8.0	30.0

Cook Value Comparison

- Determine the resultant cook value obtained from a range of NumeriCAL calculated and Ball Formula calculated cook times

Example:
NumeriCAL - Cook Value Calculation

z Value: 33.00   Reference Temp: 100.00   Initial Temp: 35.00
Temp Unit: °C   Simple/Broken: B

Seg No	Segment Type	Duration (min)	Accum Time	Start RT	Final RT	Seg jh/jc	Seg fh/f2/fc	Cold Spot	Accum F (min)
1	Simple	12.00	12.00	85.00	123.00	5.25	18.67	39.45	0.132
2	Simple	11.97	23.97	123.00	123.00	5.25	18.67	98.20	3.245
3	Broken1	10.58	34.55	123.00	123.00	5.25	10.28	120.62	32.710
4	Cooling	5.00	39.55	123.00	70.00	1.34	22.65	117.11	52.814
5	Cooling	10.00	49.55	70.00	25.00	1.34	22.65	78.44	65.117
6	Cooling	15.00	64.55	25.00	25.00	1.34	22.65	36.79	65.935

Accumulated F(33.00/100.00) contributed by all heating segments (min): 32.710

Accumulated F(33.00/100.00) contributed by all cooling segments (min): 33.225

Example:
NumeriCAL - Cook Value Calculation

PRODUCT IDENTIFICATION | PROCESS DATA

z-Value: 33 Reference Temp: 100 Initial Temp: 35 Temp Unit: °C Simple or Broken: B

Evaluation: 11-3-2014 Container Type: Container Dimension: Today: 11/ 3/20

Segments	1S	2S	3B	4C	5C	6C	7C	8C	9C
Duration (min)	12.00	11.97	10.58	5.00	10.00	15.00	0.00	0.00	0.00
RT Begin	85.00	123.00	123.00	123.00	70.00	25.00	0.00	0.00	0.00
RT End	123.00	123.00	123.00	70.00	25.00	25.00	0.00	0.00	0.00
jh or jc	5.25	5.25	5.25	1.34	1.34	1.34	0.00	0.00	0.00
fh, f2, f3 or fc	18.67	18.67	10.28	22.65	22.65	22.65	0.00	0.00	0.00
Elapsed Time	12.00	23.97	34.55	39.55	49.55	64.55	0.00	0.00	0.00
Retort Temp	123.00	123.00	123.00	70.00	25.00	25.00	0.00	0.00	0.00
Product Temp	39.45	98.20	120.62	117.11	78.44	36.79	0.00	0.00	0.00
Accum F Value	0.132	3.245	32.710	52.814	65.117	65.935	0.000	0.000	0.000

Example:
NumeriCAL - Cook Value Calculation

z-Value: 33 | Reference Temp: 100 | Initial Temp: 35 | Temp Unit: °C | Simple or Broken: B

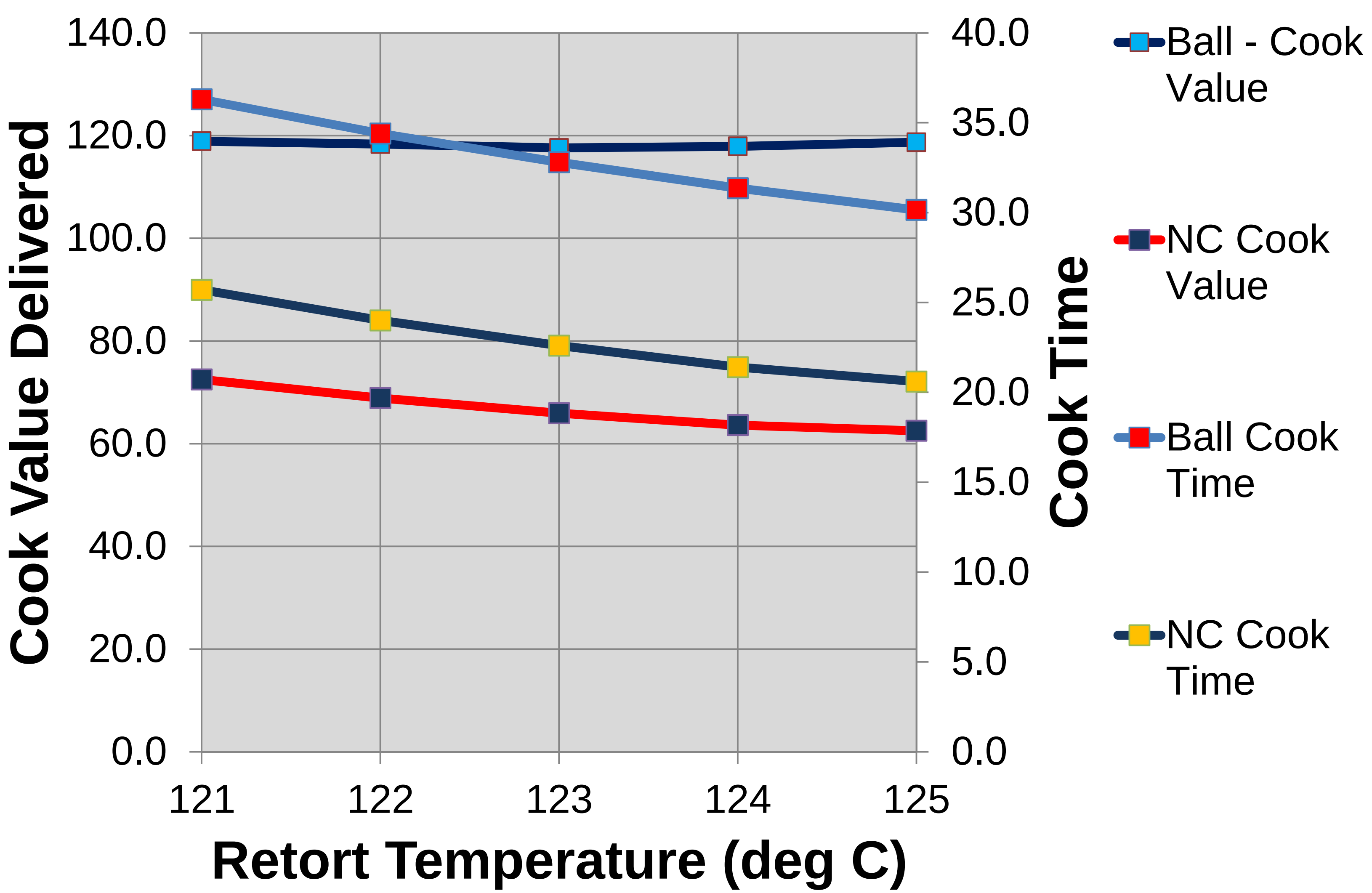
Evaluation: 11-3-2014 | Container Type: | Container Dimension: | Today: 11/ 3/20

Segments	1S	2S	3B	4C	5C	6C	7C	8C	9C
Duration (min)	12.00	11.97	20.83	5.00	10.00	15.00	0.00	0.00	0.00
RT Begin	85.00	123.00	123.00	123.00	70.00	25.00	0.00	0.00	0.00
RT End	123.00	123.00	123.00	70.00	25.00	25.00	0.00	0.00	0.00
jh or jc	5.25	5.25	5.25	1.34	1.34	1.34	0.00	0.00	0.00
fh, f2, f3 or fc	18.67	18.67	10.28	22.65	22.65	22.65	0.00	0.00	0.00
Elapsed Time	12.00	23.97	44.80	49.80	59.80	74.80	0.00	0.00	0.00
Retort Temp	123.00	123.00	123.00	70.00	25.00	25.00	0.00	0.00	0.00
Product Temp	39.45	98.20	122.76	118.68	79.46	37.56	0.00	0.00	0.00
Accum F Value	0.132	3.245	80.562	103.402	116.926	117.798	0.000	0.000	0.000

Cook Value Comparison - NumeriCAL vs Ball Formula Process Times

Retort Temperature	NumeriCAL Cook Value Delivered	Ball Formula Cook Value - Delivered
121	72.5	118.9
122	68.9	118.3
123	65.9	117.6
124	63.6	117.9
125	62.5	118.7

Cook Value and Cook Time vs Retort Temperature



Summary –

- Process optimization can be achieved by carefully studying the affect of process conditions on product quality.
- The calculation method used for process determination can have a large affect on the resultant process.
  - The **General Method** can be used to provide information needed for process optimization but it would require repeated studies and may be costly.
  - For many products the **Ball Formula Method** cannot provide the detailed analysis required for optimization and may result in higher than expected lethality and cook values

Summary –

- A **finite difference method** such as **NumeriCAL™** provides a means to determine the affect of different process profiles on product quality attributes.
- By modeling all phases of the process one can achieve General Method accuracy of lethality and cook value calculations and use this information to help optimize the process for both cook time and product quality.
- Allows for highest level of process safety
- Reduces testing required to achieve the desired result.

Summary - NumeriCAL

- NumeriCAL is a finite difference model that can accurately reproduce the cold spot temperature history in a container regardless of the product type or the container shape or size.
- By recreating the cold spot time-temperature history and then applying the lethal rate equation to these temperatures, NumeriCAL provides a calculation with the accuracy of the General Method but with the ease of using Ball Formula type heating factors.

Thank You