ISEKI Food Association

CATÓLICA
FACULTY
OF BIOTECHNOLOGY
PORTO

Integrative predictive modeling for food safety and quality:

Tools and applications

Cristina L.M. Silva

European FooD-STA

www.food-sta.eu

Erasmus+

554312-EPP-1-2014-1-AT-EPPKA2-KA

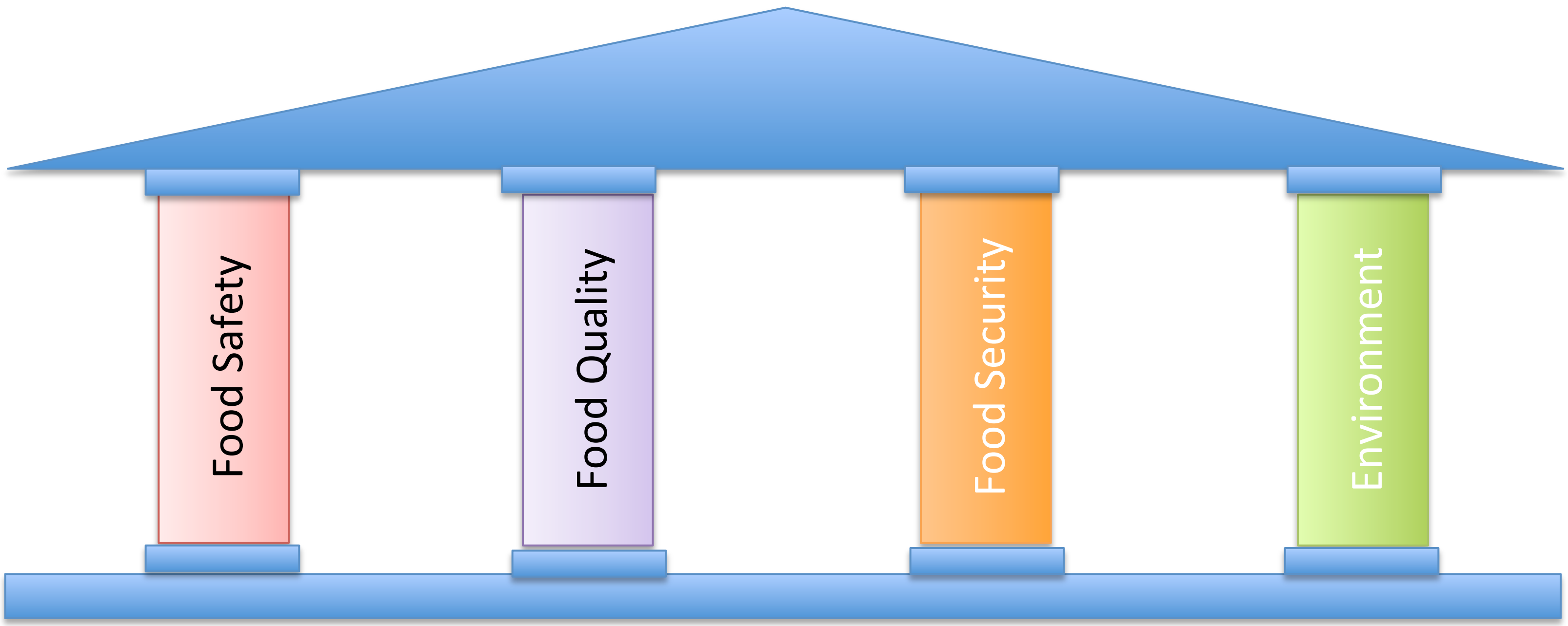
Outline

- Modeling Food Quality and Safety
- Food Modeling Tools
- Case Studies
- Challenges

Outline

- **Modeling Food Quality and Safety**
- Food Modeling Tools
- Case Studies
- Challenges

Food Pilars

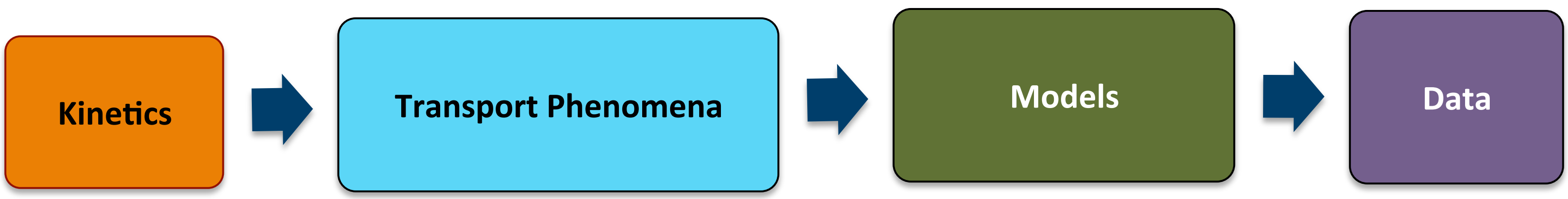


Food Quality

Food production and distribution need to achieve food safety while:

→ nutritious	→ fresh	→ ready-to-eat
→ healthy	→ natural	→ affordable
→ tasty	→ convenient	→ environmentally-friend

Computer simulation



Models

Mathematical description of a real system in the form of a computer program.

- Composed of equations duplicating the functional relationships

- Mechanistic or empirical

  - Empirical are simpler

  - Mechanistic are more complex, requiring more computational effort

- Borderline between mechanistic and empirical models is often not well defined

Models *(cont.)*

- Modeling procedures

  - finite differences; finite elements; finite volumes

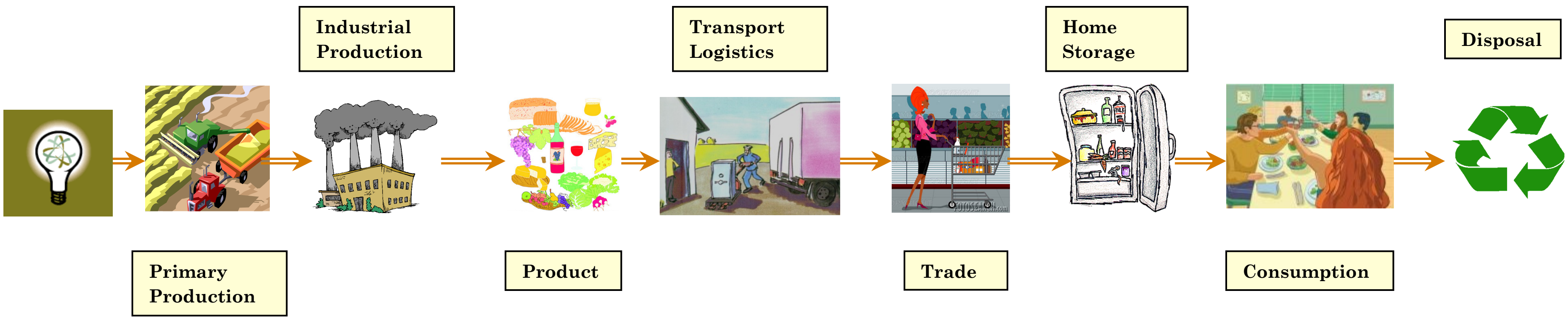
  - computational fluid dynamics (CFD) softwares, artificial neural network, fuzzy modelling, etc

- Response surface optimization

Role of Modeling in Food

- Process design
- Product design
- Process and product optimization
- Prediction of storage and distribution
- Optimization of storage and distribution

Food Supply Chain



Food Suply Chain

Farm-to-table → Holistic approach

Computer models in Food

Characterizing food quality

Process design and optimization

Real-time process monitoring and control

Food Storage

Performance management

Cost Action CA 15118 – Food MC – *WG1*

Outline

- Modeling Food Quality and Safety
- **Food Modeling Tools**
- Case Studies
- Challenges

Predictive Microbiology

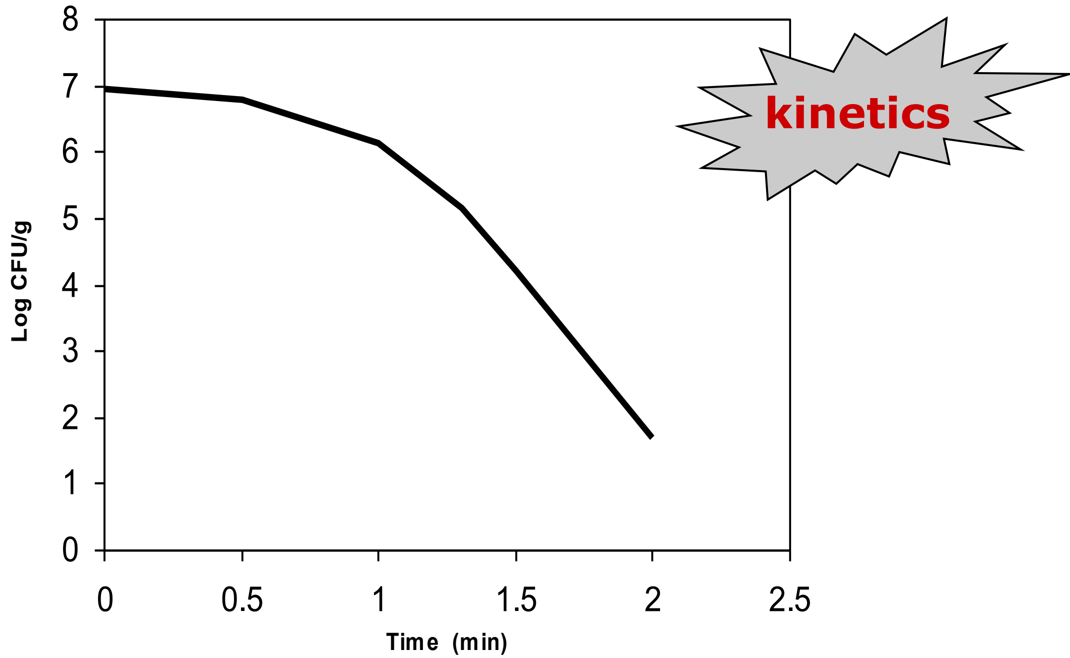
The use of **mathematical models** in the description of **microbial responses** to environmental stressing factors

temperature, pH
&
water activity.

Predictive Microbiology *(cont.)*

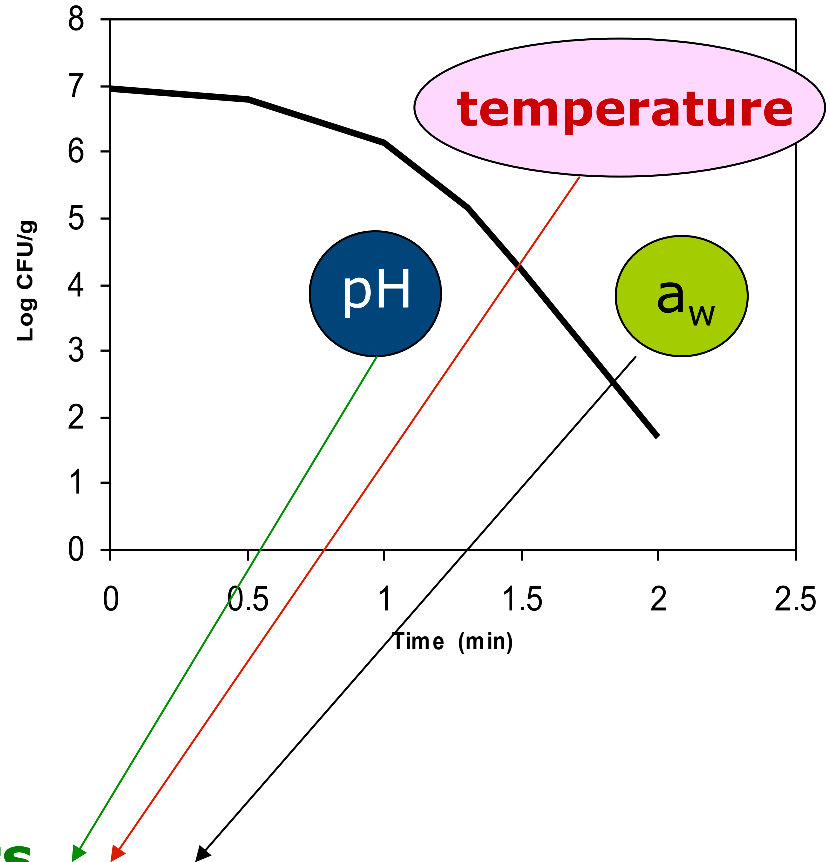
- **primary model**

parameters



Predictive Microbiology *(cont.)*

- primary model

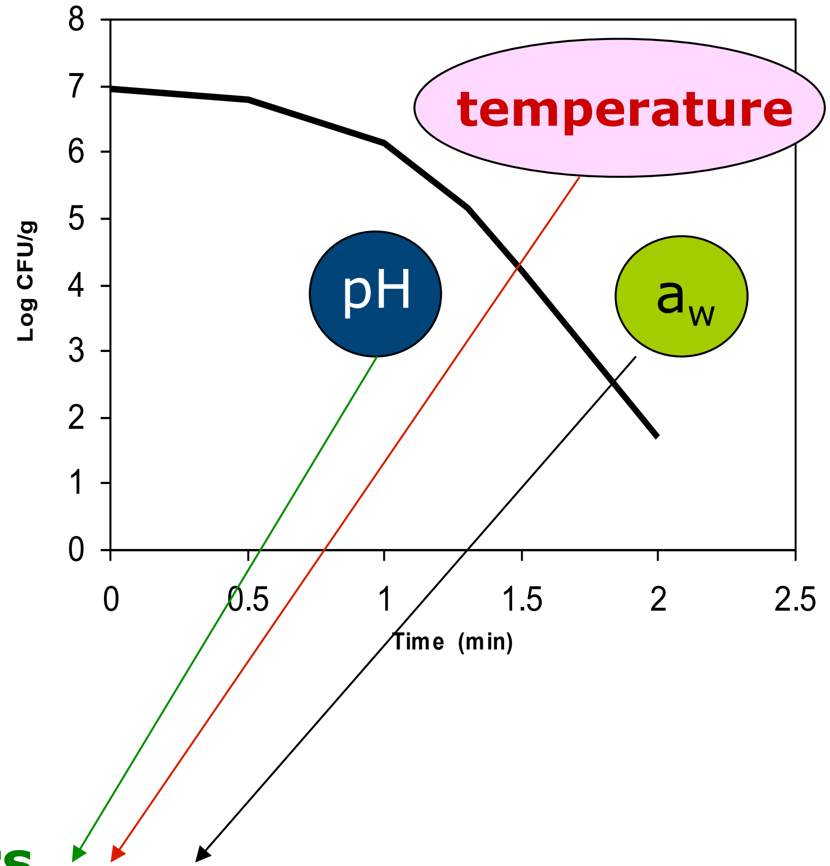


- secondary model

parameters

Predictive Microbiology *(cont.)*

- **primary model**



- **secondary model**

parameters

tertiary - integration of the previous models - **software**

Predictive Microbiology (cont)

Predictive microbiology utilizes mathematical models (built with data from laboratory testing) and computer software to graphically describe these responses.

Transfer of results is compromised

Isothermal

Non-isothermal

→ Design of processing conditions
→ Shelf-life studies

Available for industry:

e.g. Baseline, Combase, etc

Tenenhaus-Aziza & Ellouze, 2015

Predictive Quality

The use of **mathematical models** in the description of **QUALITY responses** to environmental factors

Quality changes kinetics

Historically: → single-response studies

→ static conditions

Quality changes kinetics

Single-response → empirical

Atribute at time t

Initial value

Time

Activation energy

Kinetic Models

Zero order

$$C = C_0 - k_{(T)}t$$

1st order

$$C = C_0\, e^{-k_{(T)}t}$$

Fractionary

$$\frac{C - C_{eq}}{C_0 - C_{eq}} = e^{-kt}$$

Equilibrium value

Reaction rate

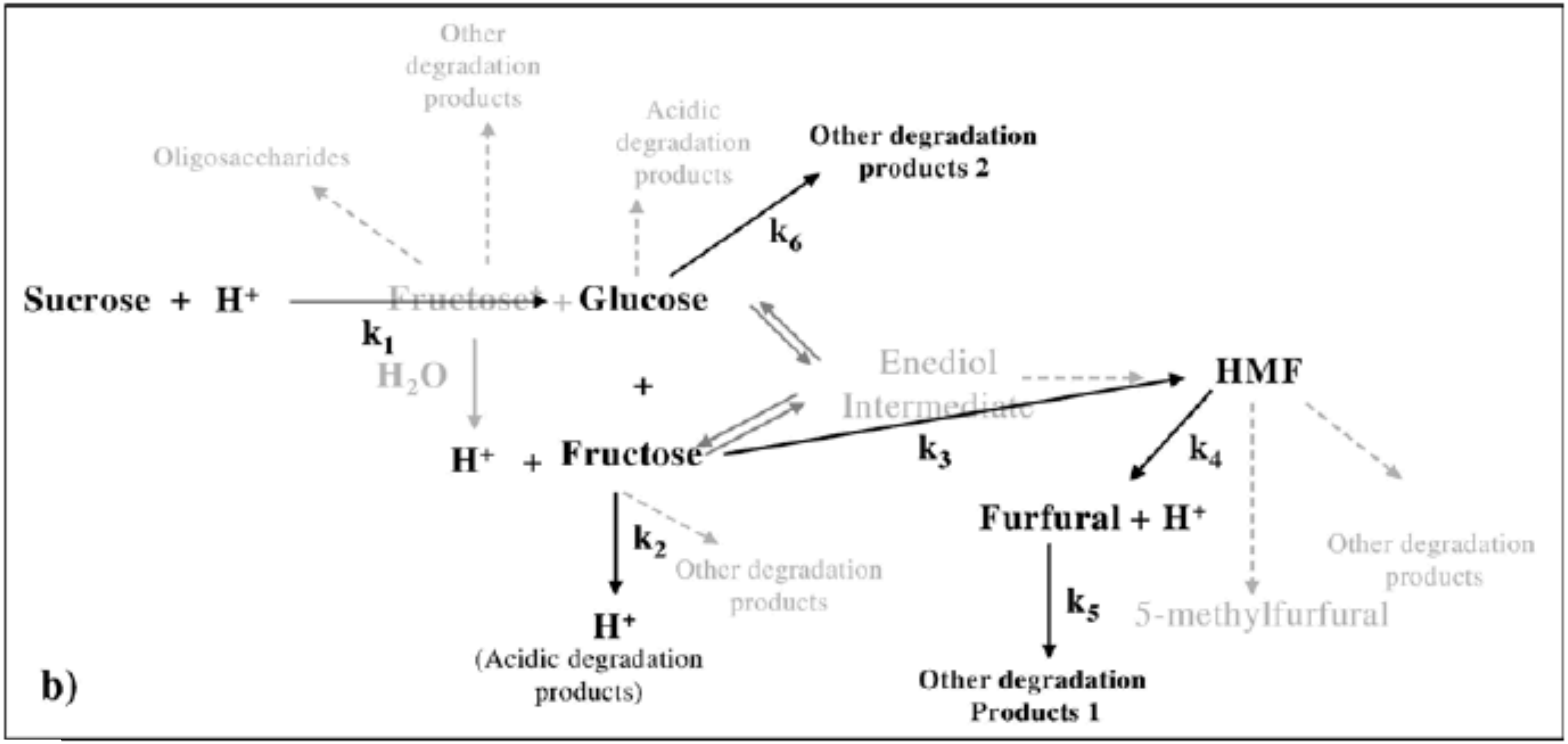
$$k_{(T)} = k_{ref} \exp\left[-\frac{Ea}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right]$$

T effect on k

Arrhenius behaviour

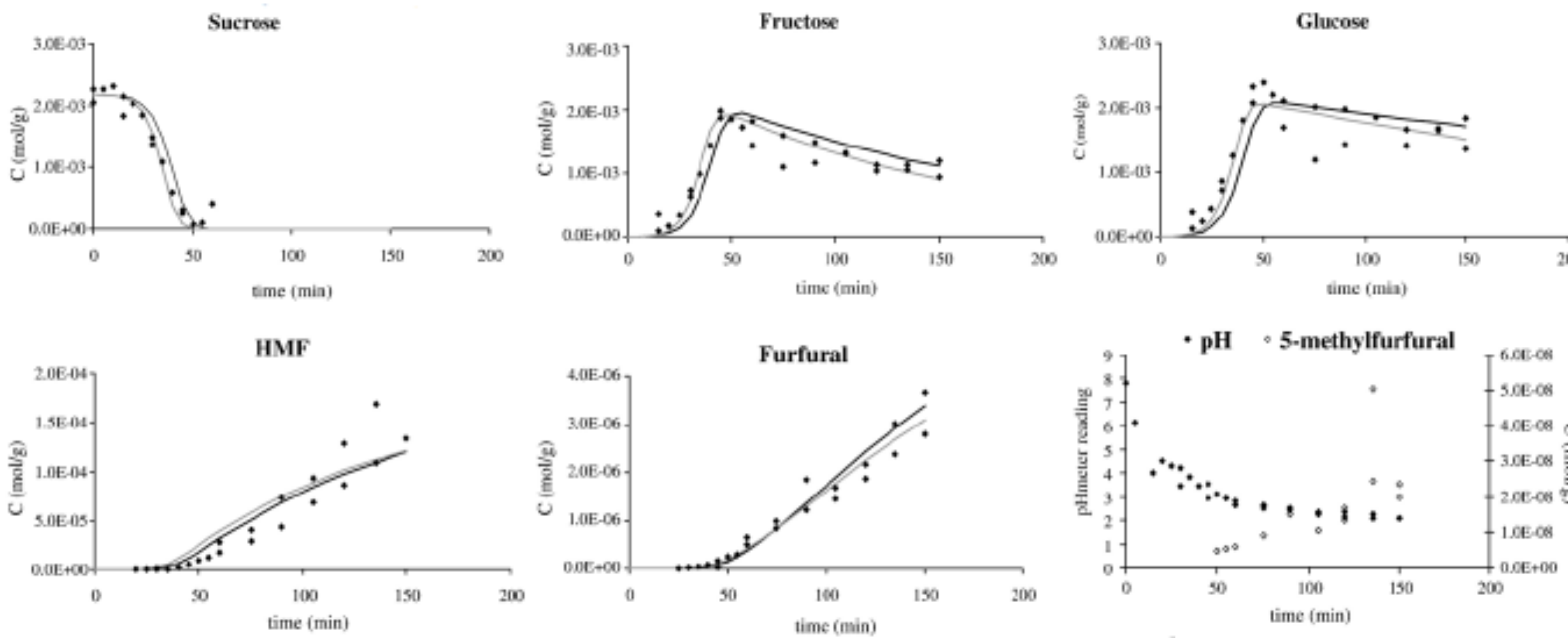
Quality changes kinetics

Multiresponse Modelling → mechanistic



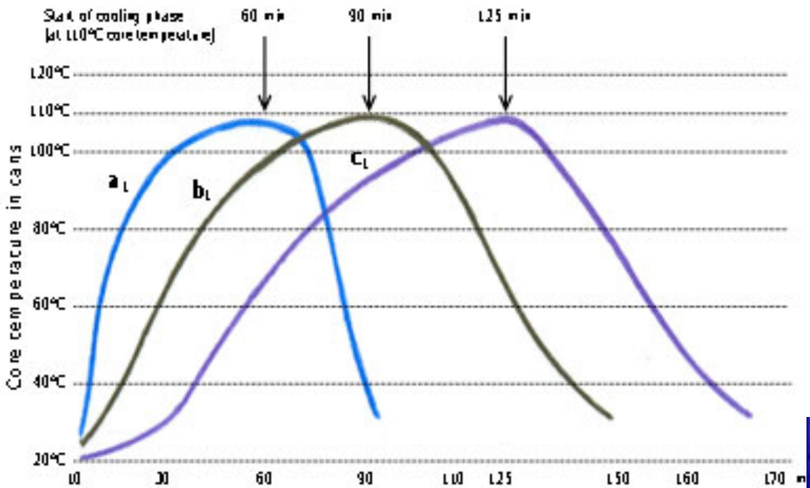
Quintas et al, 2007

Quality changes kinetics

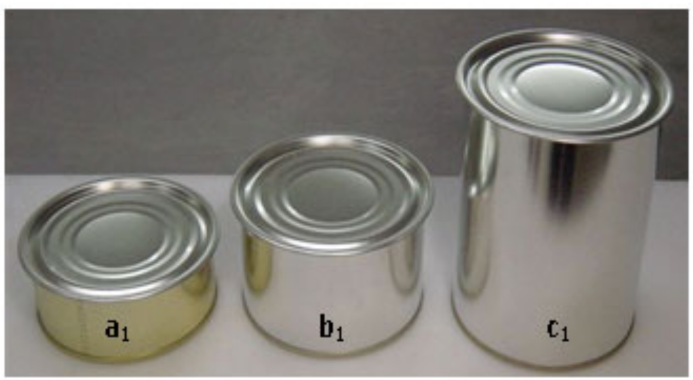


Quintas et al, 2007

Quality changes kinetics



→ **Need to have temperature histories and distributions**



Quality changes kinetics

Isothermal conditions

$$C = C_0 - \left(k_{ref} \exp\left(-\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) t\right)$$

$$C = C_0 \exp\left(-k_{ref} \exp\left(-\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) t\right)$$

$$C = C_{eq} + (C_0 - C_{eq}) \exp\left(-k_{ref} \exp\left(-\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) t\right)$$

Non-Isothermal conditions

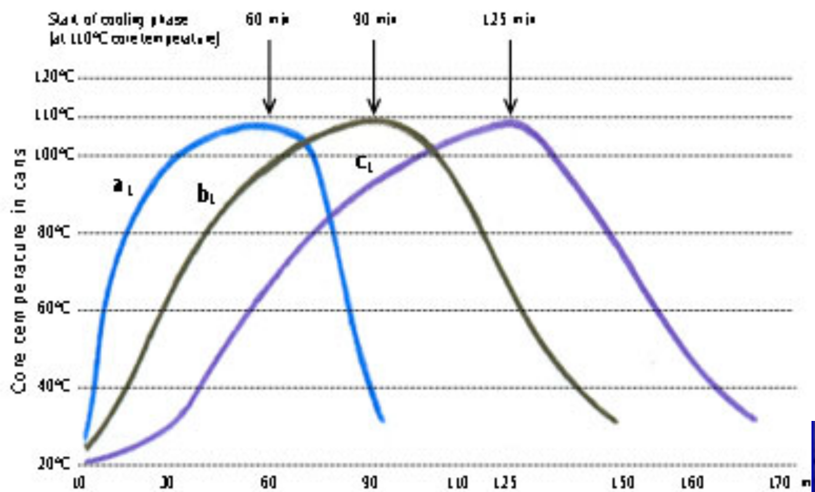
$$C = C_0 - \left[k_{ref} \int_0^t \exp\left[-\frac{E_a}{R}\left(\frac{1}{T(t)} - \frac{1}{T_{ref}}\right)\right] dt\right]$$

$$C = C_0 \exp\left[-k_{ref} \int_0^t \exp\left[-\frac{E_a}{R}\left(\frac{1}{T(t)} - \frac{1}{T_{ref}}\right)\right] dt\right]$$

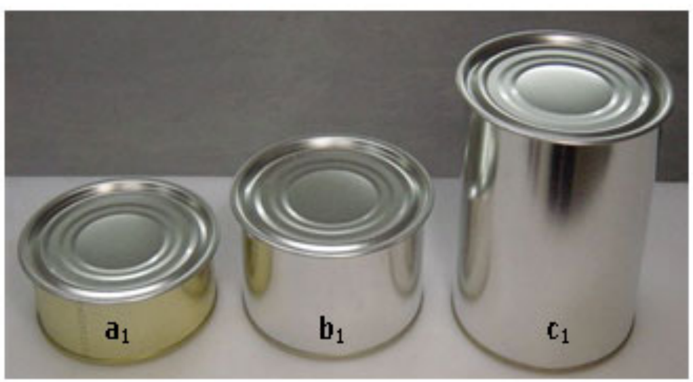
$$C = C_{eq} + (C_0 - C_{eq}) \exp\left[-k_{ref} \int_0^t \exp\left[-\frac{E_a}{R}\left(\frac{1}{T(t)} - \frac{1}{T_{ref}}\right)\right] dt\right]$$

Integration

Quality changes kinetics



→Reverse Engineering
can be an excellent tool



Integrative Predictive Modeling

Combining mathematical **models for safety and quality responses**, considering the whole food chain.

COST Action CA15118 - FoodMC

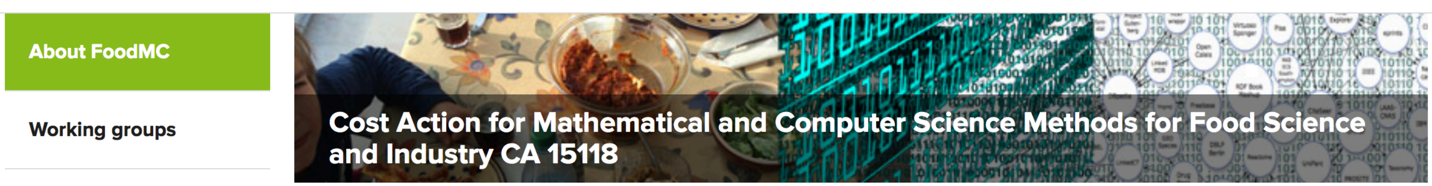
"Support the food sector in facing futures challenges in production and processing, adopting modelling and optimization methods from Maths and Computer Science"

https://www6.inra.fr/foodmc

Chair: **Dr. Alberto TONDA** (FR)

INRA SCIENCE & IMPACT

cost EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY



COST Action CA15118 - FoodMC *(cont.)*

- **Model link food processing - food structure**

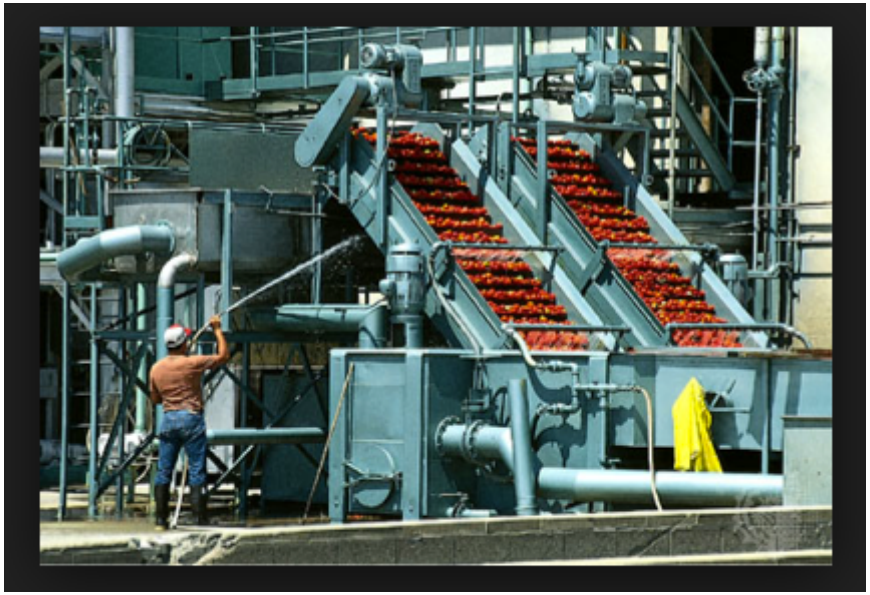
- **Modeling for eco-design of food processes**

- **Software tools for the food industry**

Outline

- Modeling Food Quality and Safety
- Food Modeling Tools
- **Case Studies**
- Challenges

Postharvest treatment



Postharvest treatment

Turning maturity stage (TM)

Tomato
(cv. Zinac)

Pink maturity stage (PM)

Industrial decontamination
(**HIPO:** 150 ppm chlorine, 5 ºC, pH 6.5, 2 min)

Water heat treatment
(**WHT**: 40 ºC / 30 min)

Rising
(water)

Cooling
(5 min, water / ice)

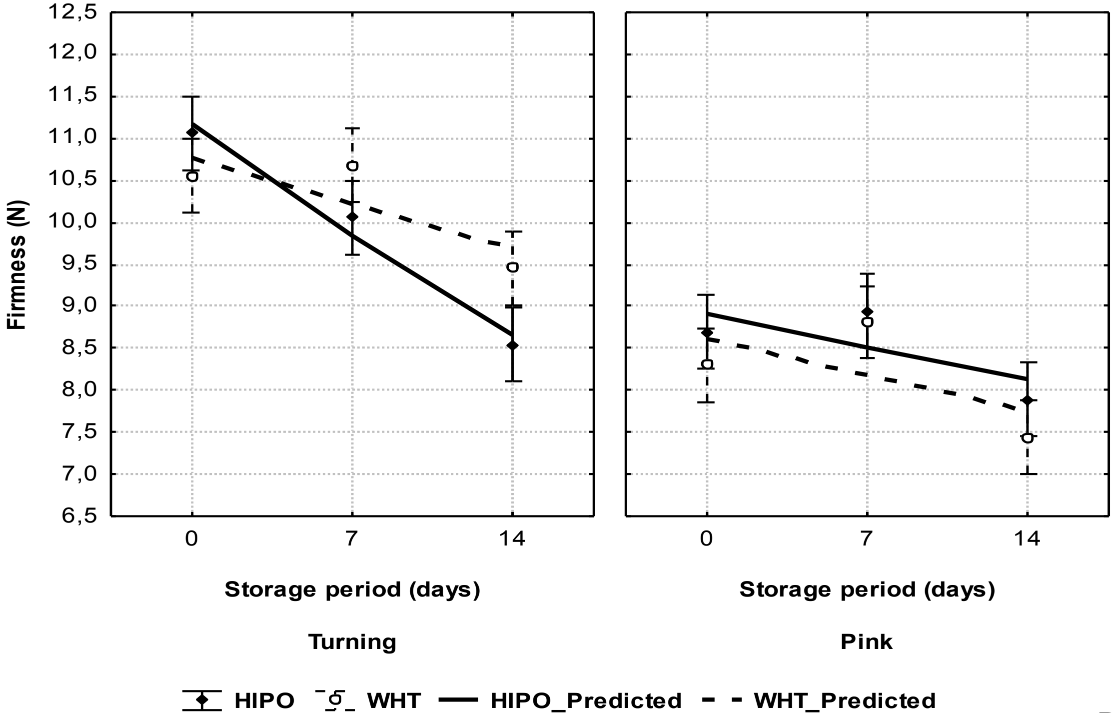
Drying
(Absorbent paper)

Storage
(10 ºC / 14 days)

Pinheiro et al, 2014

Postharvest treatment

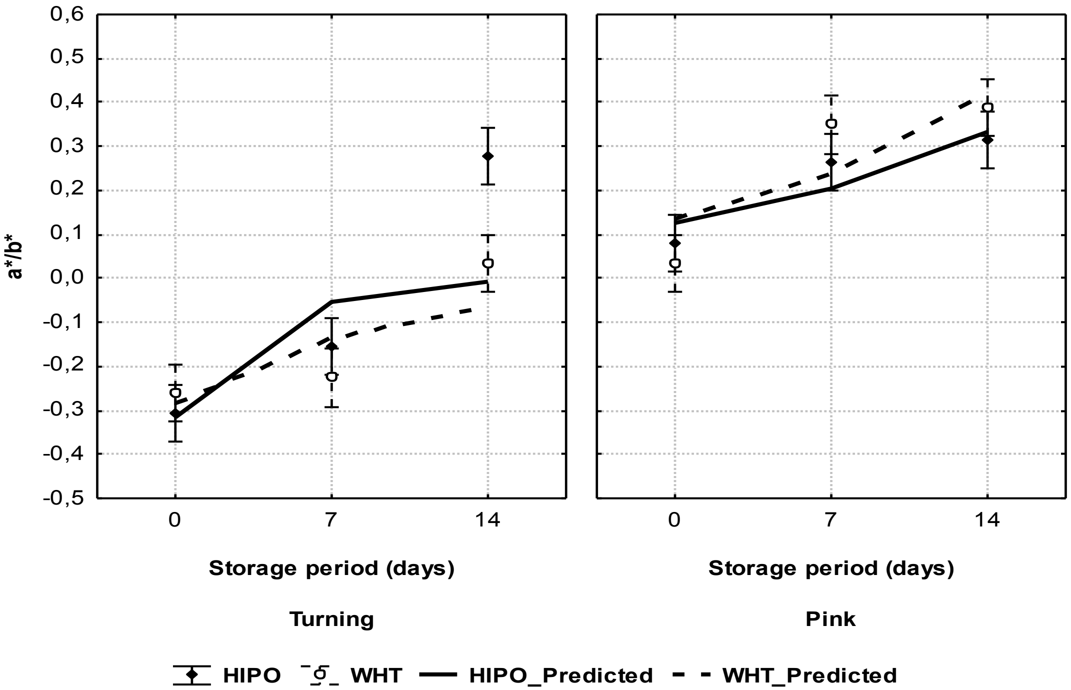
Firmness



Pinheiro et al, 2014

Postharvest treatment

Colour



Pinheiro et al, 2014

Postharvest treatment

$$C = C_0\, e^{-k_{(T)} t}$$

Maturity stages	Treatment	*a*/b**	Firmness (N)
Turning	HIPO	C_0 = - 0.32 ± 0.12 $k_{10ºC}$ (day $^{-1}$) = 0.25 ± 0.32	C_0 = 11.16 ± 0.52 $k_{10ºC}$ (day $^{-1}$) = 0.02 ± 0.006
	WHT	C_0 = - 0.28 ± 0.11 $k_{10ºC}$ (day $^{-1}$) = 0.11 ± 0.10	C_0 = 10.77 ± 0.69 $k_{10ºC}$ (day $^{-1}$) = 0.01 ± 0.01
Pink	HIPO	C_0 = 0.13 ± 0.07 $k_{10ºC}$ (day $^{-1}$) = - 0.07 ± 0.05	C_0 = 8.90 ± 0.43 $k_{10ºC}$ (day $^{-1}$) = 0.01 ± 0.01
	WHT	C_0 = 0.13 ± 0.07 $k_{10ºC}$ (day $^{-1}$) = - 0.08 ± 0.04	C_0 = 8.60 ± 0.72 $k_{10ºC}$ (day $^{-1}$) = 0.01 ± 0.01

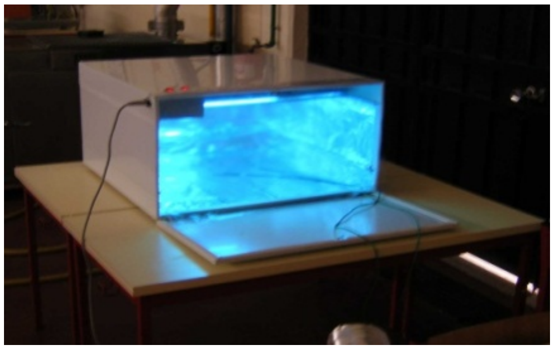
→ Results provide strong evidence that postharvest water **heat treatment (40 ºC - 30 min)** for tomato fruits (cv. 'Zinac') at <u>turning maturity stage</u> guarantees the overall quality at 10 ºC, **twice as long of fruits washed with chlorinated water**.

Pinheiro et al, 2014

Non-thermal technologies for *Alicyclobacillus acidoterrestris* inactivation in apple juice

UV-C radiation

(13.44 W/m^2 for 8 min)



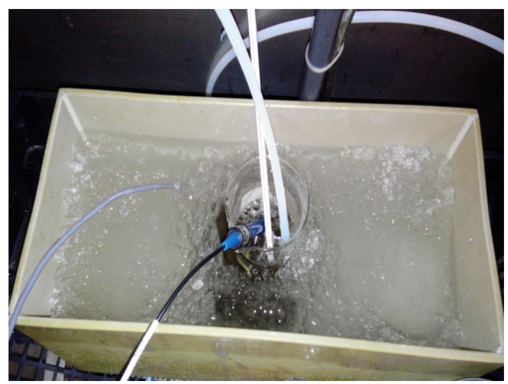
Ultrasound (US)

(35 kHz frequency and

120-480 W power for 30 min)

Ozone

(500 mV for 60 min)



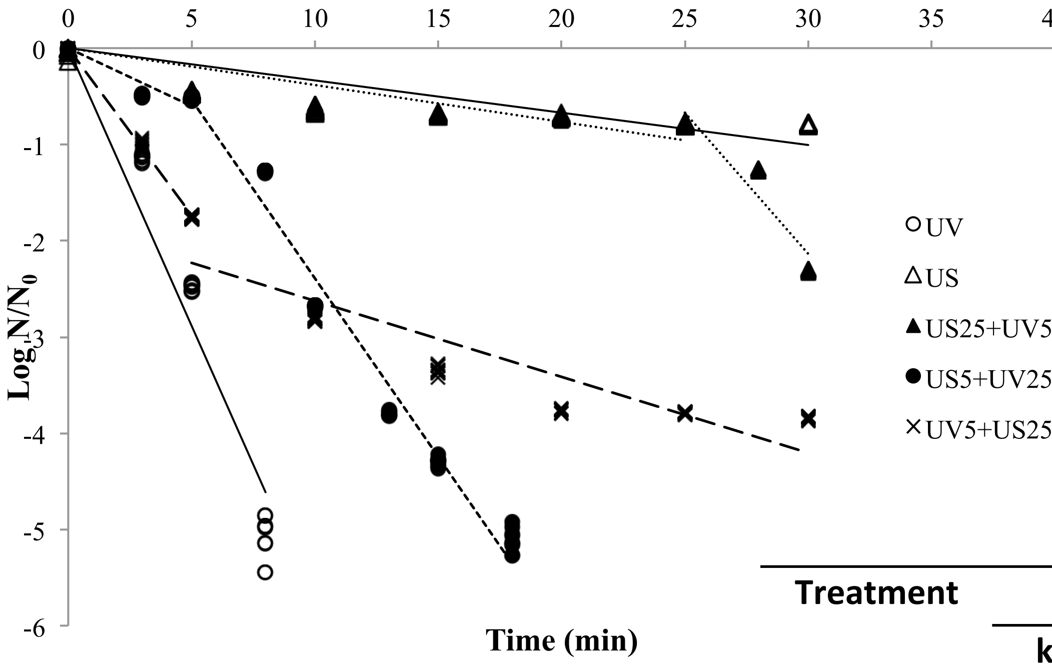
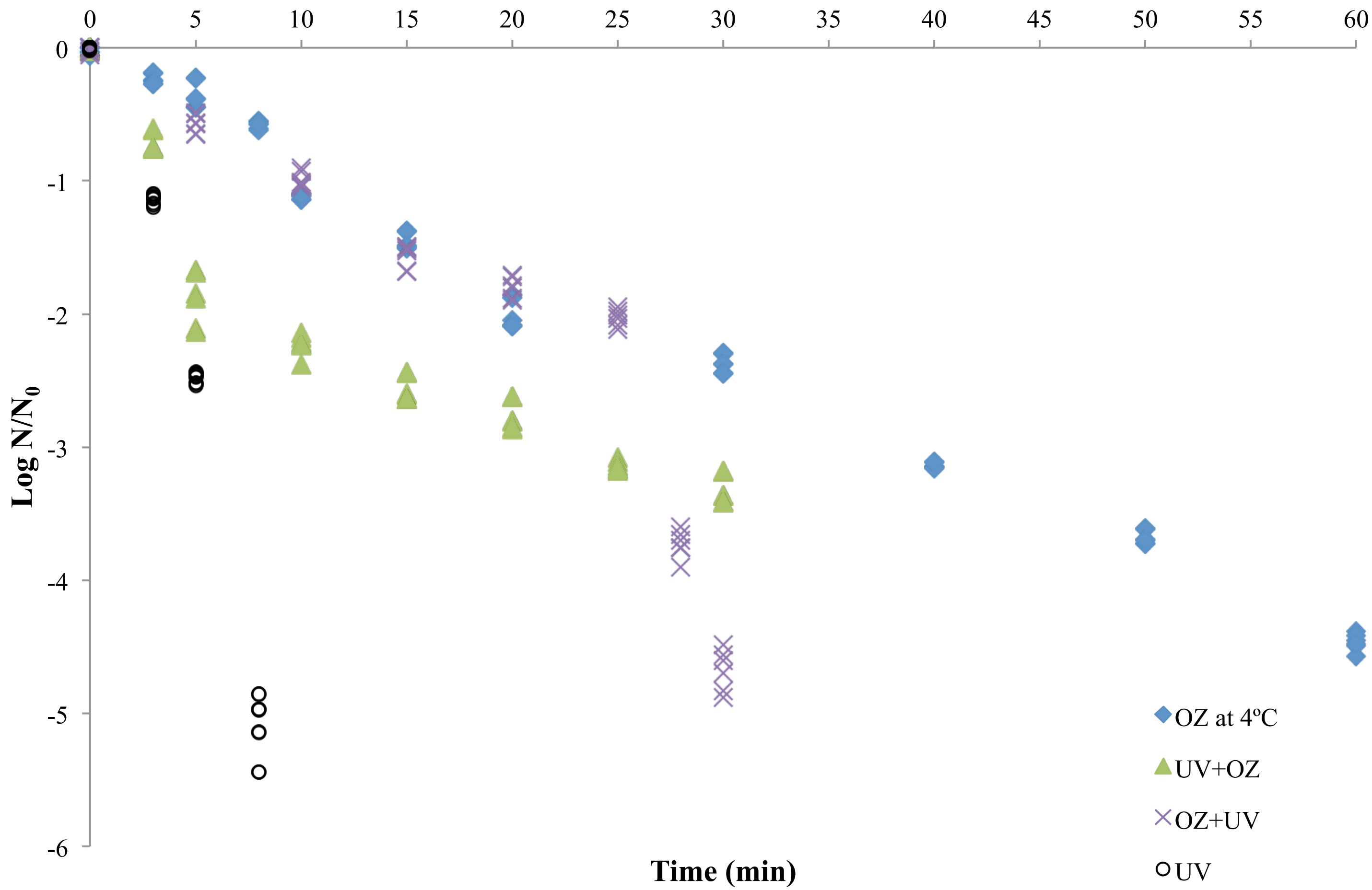


Figure 1. *A. acidoterrestris* inactivation in apple juice applying different treatments:

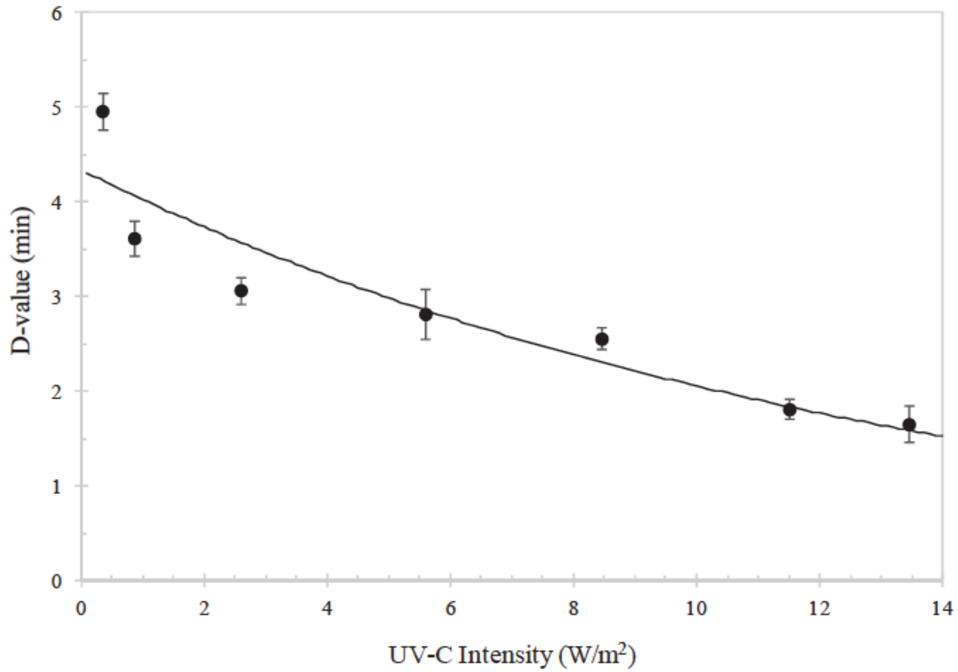
Table 1. Inactivation rates of *A. acidoterrestris* spores in apple juices; confidence intervals at 95% ($CI_{95\%}$) and correlation coefficients (R) are included.

Treatment	First treatment		Second treatment	
	k(min^{-1}) ± $CI_{95\%}/2$	|R|	**k**(min^{-1}) ± $CI_{95\%}/2$	|R|
UV-C	0.576±0.031	0.97	-	-
US	0.033±0.003	0.61	-	-
TS	0.259±0.011	0.98	-	-
UV5+US25	0.346±0.004	0.99	0.079±0.011	0.90
US5+UV25	0.120±0.011	0.92	0.369±0.012	0.98
US25+UV5	0.038±0.003	0.76	0.293±0.041	0.95

Tremarin et al, 2017



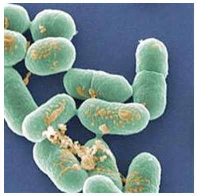
Tremarin et al, 2017



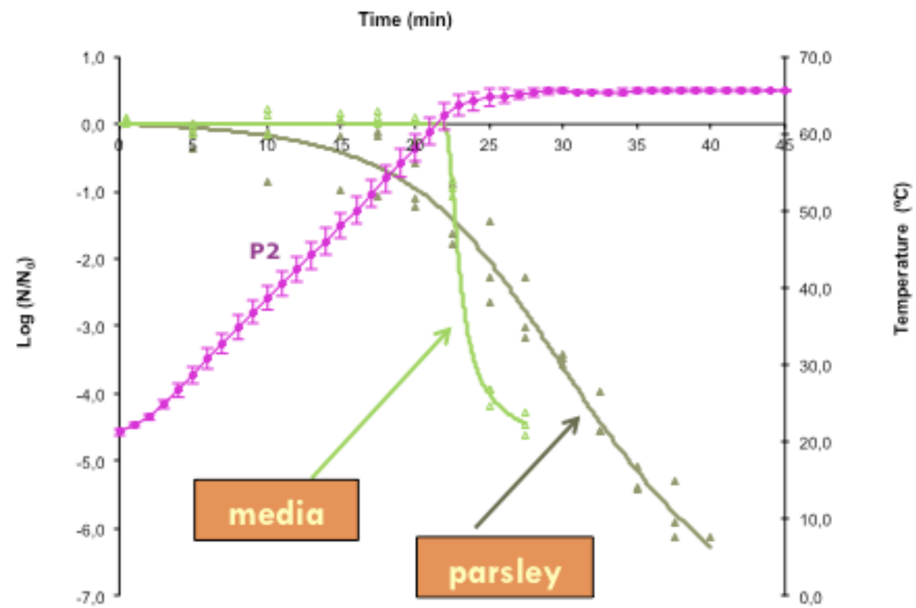
$$\log\left(\frac{N}{N_0}\right) = -\frac{1}{D}t$$

$$D = D_{ref}10^{\left(\frac{I_{ref}-I}{z}\right)}$$

Tremarin et al, 2017

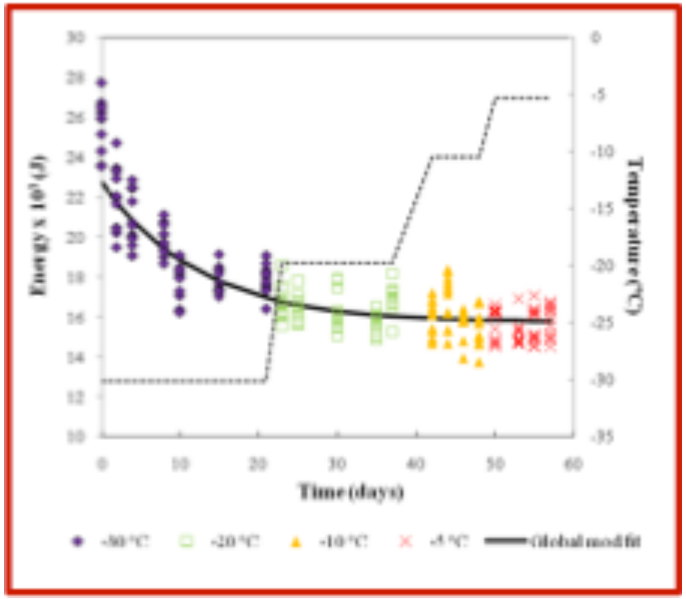


Thermal inactivation of *Listeria* in culture media and foods



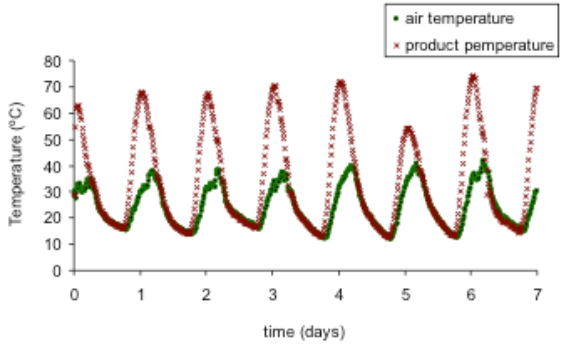
Gil et al, 2016

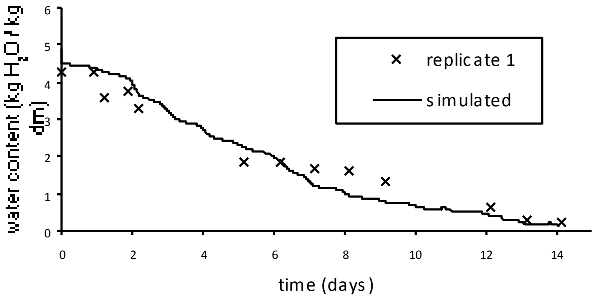
Frozen storage of vegetables



Gonçalves et al, 2011

Solar drying of grapes





Ramos et al, 2015

Outline

- Modeling Food Quality and Safety
- Food Modeling Tools
- Case Studies
- **Challenges**

Challenges

- ✓ Development of ***Integrative models***, considering the whole food chain.
- ✓ Food quality kinetic studies under dynamic conditions.
- ✓ Use of reverse engineering.
- ✓ Multiresponse models – mechanistic.
- ✓ Development of a so called ***Predictive Quality*** – open access to database of kinetic studies.

Thank you!