



HAL
open science

Industrial validation of a predictive model of the nutritional quality of tomato-based products during processes

Mélodie Gil, Claire Dufour, Xuan Mi Meyer, Cédric Brandam, Marie Roland, Magali Wagner, Stéphanie Georgé

► To cite this version:

Mélodie Gil, Claire Dufour, Xuan Mi Meyer, Cédric Brandam, Marie Roland, et al.. Industrial validation of a predictive model of the nutritional quality of tomato-based products during processes. *Acta Horticulturae*, 2015, 1081, pp.267-274. 10.17660/ActaHortic.2015.1081.34 . hal-02134883

HAL Id: hal-02134883

<https://hal.science/hal-02134883>

Submitted on 20 May 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Open Archive Toulouse Archive Ouverte (OATAO)

OATAO is an open access repository that collects the work of some Toulouse researchers and makes it freely available over the web where possible.

This is an author's version published in: <http://oatao.univ-toulouse.fr/20600>

Official URL: <https://doi.org/10.17660/ActaHortic.2015.1081.34>

To cite this version:

Gil, Mélodie and Dufour, Claire and Meyer, Xuân-Mi and Brandam, Cédric and Roland, M. and Wagner, Magali and Georgé, Stéphanie Industrial validation of a predictive model of the nutritional quality of tomato-based products during processes. (2015) Acta Horticulturae, 1081. 267-274. ISSN 0567-7572

Any correspondence concerning this service should be sent to the repository administrator:

tech-oatao@listes-diff.inp-toulouse.fr

Industrial Validation of a Predictive Model of the Nutritional Quality of Tomato-Based Products during Processes

M. Gil^{1,2}, C. Dufour^{1,2}, X. Meyer^{3,4}, C. Brandam^{3,4}, M. Roland³, M. Wagner⁵ and S. Georgé⁵

¹ INRA, UMR408, Sécurité et Qualité des Produits d'Origine Végétale, France

² Université d'Avignon, UMR408, Sécurité et Qualité des Produits d'Origine Végétale, France

³ Université de Toulouse, INPT, UPS, Laboratoire de Génie Chimique, France

⁴ CNRS, UMR 5503, Laboratoire de Génie Chimique, France

⁵ CTCPA, France

Keywords: tomato, food processing, modelling, prediction, tool

Abstract

Opti'Tom aims to develop and confirm, at pilot and industrial scale, stoichiokinetic models describing changes in micronutrients contents in tomato-based products during processing. Two kinds of processes were studied such as production of tomato paste from fresh tomatoes and sauces from tomato paste. Several pilot trials were conducted and the data (amounts of microconstituents, schedules of the processes) were exploited to develop a software in order to optimize the current manufacturing processes.

INTRODUCTION

Food companies want to improve the quality of their products ensuring complex organoleptic properties and high nutritional value. The development of such foods and the reassessment of existing products and processes require controlling the interaction between structure and chemical reactivity of the food in relation with applied treatments. The study and at last the control of these reactions are an important challenge of progress for food industry.

During a previous project (Chanforan, C. – PhD thesis 2010, Université d'Avignon), a partial model of tomato sauce process, using kinetic laws, was obtained in model systems. The aim of this project is to develop and validate at pilot and industrial scale stoichiokinetic models describing the evolution of tomato compounds of interest during transformation. A tool will enable to improve existing processes and predict the final nutritional quality avoiding many uncertain and expensive preindustrial trials. It was built for companies in the sector of tomato-based products.

MATERIALS AND METHODS

Compounds Targeted

(E)-lycopene, (E)- β -carotene, chlorogenic acid, rutin, naringenin, naringenin chalcone, ascorbic acid and α -tocopherol were chosen as nutritional markers of tomato and analyzed at each step of processes.

Pilot Plan Trials

Two types of products were targeted such as tomato paste (directly processed from tomato) and tomato sauce (processed from tomato paste). These trials were conducted on 35 L-instrumented pilot equipment to collect technological data during processes such as temperatures or flow rates. Experiments have been designed to collect data providing a maximum of information in order:

- to develop and validate the stoichiokinetic models
- to reduce model parameters uncertainty.

With this approach, the resulting experiments presented atypical temperature profiles compared to classical industrial practices.

1. Fresh Tomato to Tomato Paste. In the industry, two types of processes are usually used like Hot Break (HB) or Cold Break (CB). This study focused on the CB process.

The different steps of the CB process are: receiving fresh product, washing, crushing, sieving, preheating, concentration, pasteurization in retort. The study of the evolution of compounds was conducted at different conditions and different steps:

1. Before sieving at 25, 30 and 35°C during 3 h.
2. Cold break at 50, 60, 70 and 80°C during 2 h and at 60 and 80°C during 2 h but packed in pouches without oxygen.
3. Scheduled process at 95°C during 25 and 60 min, at 105°C during 15, 25 and 60 min and at 125°C during 25 and 60 min.

2. Tomato Paste to Tomato Sauce. The different steps were the recipe (water 69%, tomato paste 25%, sugar 1.5%, salt 1.5%, starch 1.5% and sunflower oil 1.5%), the re-heat and the scheduled process. The study of the compound evolution was conducted at different conditions at different steps:

1. Re-heat at 50, 60, 70, 80 and 95°C during 2 h and at 50, 70 and 95°C during 2 h but packed in pouches without oxygen.
2. Scheduled process at 125°C during 30, 60 and 90 min.

Model, Identification of Kinetic Parameters and Software

The dynamic model basis was elaborated with a first qualitative analysis more than 2000 independent data resulting from the various experiments. Reactions to be taken into account were established and a kinetic law for each reaction was proposed. Kinetic parameters like reaction rate constants and activation energies were identified with Matlab toolbox. The model was able to calculate the concentration of the considered compounds for a temperature profile applied.

This stoichio-kinetic model was implemented in Matlab with a friendly-user interface. This computer tool named SiMiNuT⁷ is directly usable by industrials and able to simulate effects of temperature profile and oxygen transfer on considered compounds. It can predict the final nutritional quality from a given raw material.

RESULTS AND DISCUSSION

Fresh Tomato to Tomato Paste Processing Model

The degradation rates of the compounds were significantly different even inside the same compound family (carotenoids or phenolic compounds).

No degradation was observed for lycopene, rutin, naringenin and α -tocopherol, whatever the temperature was between 25 and 125°C (Table 1). Conversion of E- β -carotene into Z- β -carotene occurred only when the temperature was higher than 50°C. Beyond this temperature, the kinetic of the degradation showed a good adequacy with a first order Arrhenius type kinetic law.

For ascorbic acid, experimental results (Table 2) highlighted two degradation pathways: oxidation until 80°C and thermal degradation at higher temperatures. For both pathways, first order Arrhenius type kinetic laws fitted with good agreement to experimental measurements. The oxygen transfer between 50 and 95°C was modelled through a temperature dependent mass transfer (k_{la}) coefficient. Above 95°C it was assumed that the liquid phase was free from oxygen.

Chlorogenic acid degradation was shown to be significant only at 50°C, when dissolved oxygen was not a limiting factor. At 25 and 35°C as well as between 60 and 125°C when oxygen was consumed by acid ascorbic oxidation, no degradation was observed (Table 2). A first order kinetic law regarding each reactant was assumed for the degradation of this component depending on chlorogenic acid and dissolved oxygen contents.

Table 3 summarizes the kinetic parameters values for fresh tomato to tomato paste processing.

Tomato Paste to Tomato Sauce Processing Model

The behavior was quite different for processing tomato paste into tomato sauce.

Ascorbic acid was the main affected compound. Under a reheating step, its concentration decreased by 90% after half an hour, and totally disappeared after one hour at any temperature tested (Table 4). Under a reheating under nitrogen, the decrease is lower at any temperature.

No degradation was observed for rutin, chlorogenic acid and naringenin, whatever the temperature was (50-95°C). But for beta-carotene and lycopene, we observe a low decrease linked to the temperature (50 < 60 < 70 < 80 < 95°C) (Table 5).

Table 6 summarizes the kinetic parameters values for tomato paste to tomato sauce processing.

Simulation Tool

The model described formerly and identified from experimental data was implemented into Matlab and a user-friendly interface was developed to make it directly usable by industrials (Fig. 1). The interface includes the initial concentrations of the compounds of interest and the process thermal profile. This profile can be provided manually or charged from an Excel file when available.

Figure 2 gives an example of the outcome of the tool. Each calculated component content profile is plotted versus time (continuous line). The temperature profile is reminded on all graphs (dotted lines). A pasteurization value is proposed. Finally, the results can be exported into an Excel file upon request.

Industrial Validation

An industrial validation will be performed by sampling tomato products directly on the process line. These samples will be analysed to quantify the compound targeted and the process data will be recovered.

This phase will ultimately characterize the model from a statistical standpoint (robustness, reliability...) and ensure its reliability regarding industrial requirements.

CONCLUSION

Opti'Tom has permitted to develop a prediction software. This operational tool will allow companies to optimize their processes to offer consumers products with better nutritional quality and thus enhance the value of their commercial products, save time testing during the development of new products or new recipes and to be more responsive in the development of new products, particularly in response to tenders of supermarkets.

ACKNOWLEDGEMENT

This project was funded by the French "Ministère de l'agriculture, de l'alimentation, de la pêche, de la ruralité et de l'aménagement du territoire" with the contract n° CP13 PACA 05 12-1.

Literature Cited

- Abushita, A.A., Daood, H.G. and Biacs, P.A. 2000. Change in carotenoids and antioxidant vitamins in tomato as a function of varietal technological factors. *J. Agric. Food Chem.* 48:2075-2081.
- Bosch, V., Cilla, A., García-Llatas, G., Gilabert, V., Boix, R. and Alegría, A. 2013. Kinetics of ascorbic acid degradation in fruit-based infant foods during storage. *Journal of Food Engineering* 116:298-303.
- Capanoğlu, E., Beekwilder, J., Boyacıoğlu, D., Hall, R. and De Vos, R. 2008. Changes in antioxidant and metabolite profiles during production of tomato paste. *J. Agric. Food Chem.* 56:964-973
- Chanforan, C. 2010. Stabilité de microconstituants de la tomate (composés phénoliques, caroténoïdes, vitamines C et E) au cours des procédés de transformation: études en systèmes modèles, mise au point d'un modèle stoechio-cinétique et validation pour

- l'étape unitaire de préparation de sauce tomate. Thèse de Docteur en Sciences, Université d'Avignon et des Pays de Vaucluse
- Chanforan, C., Loonis, M., Mora, N., Caris-Veyrat, C. and Dufour, C. 2012. The impact of industrial processing on health-beneficial tomato microconstituents. *Food Chem.* 134:1786-1795.
- Dhuique-Mayer, C. 2007. Thermal degradation of antioxydant micronutrients in citrus Juice: kinetics and newly formed compounds. *J. Agric. Food Chem.* 55:4209-4216.
- Penicaud, C., Achir, N., Dhuique-Mayer, C., Dornier, M. and Bohuon, P. 2011. Degradation of β -carotene during fruit and vegetable processing or storage: reaction mechanisms and kinetic aspects: a review. *Fruits* 66(6):417-440.
- Re, R., Bramley, P.M. and Rice-Evans, C. 2002. Effects of food processing on flavonoids and lycopene status in a Mediterranean tomato variety. *Free Radical Res.* 36(7):803-810.

Tables

Table 1. Concentration expressed in mg/100 g of dry matter.

		Process step													
		Before sieving			Cold break				Pasteurisation						
		25°C	30°C	35°C	50°C	60°C	70°C	80°C	95°C 25 min	95°C 60 min	105°C 15 min	105°C 25 min	105°C 60 min	125°C 25 min	125°C 60 min
A-tocopherol	Before process	11,0 <i>0,8</i>	11,6 <i>1,0</i>	12,3 <i>0,3</i>	13,1 <i>0,5</i>	n.t.	12,3 <i>1,5</i>	n.t.	13,4 <i>1,0</i>	13,4 <i>1,0</i>	12,0 <i>0,9</i>	13,6 <i>0,2</i>	13,6 <i>0,2</i>	11,9 <i>1,1</i>	12,5 <i>1,0</i>
	After process	11,5 <i>0,3</i>	13,2 <i>0,2</i>	11,9 <i>0,8</i>	12,6 <i>0,2</i>	n.t.	12,4 <i>0,9</i>	n.t.	14,1 <i>0,7</i>	14,0 <i>0,8</i>	14,1 <i>0,9</i>	15,0 <i>0,7</i>	14,6 <i>1,0</i>	14,2 <i>0,8</i>	15,4 <i>0,7</i>
Rutin	Before process	6,8 <i>0,5</i>	7,3 <i>0,6</i>	7,5 <i>0,2</i>	7,6 <i>0,4</i>	n.t.	8,0 <i>0,5</i>	n.t.	6,8 <i>0,4</i>	6,8 <i>0,4</i>	7,6 <i>0,3</i>	7,4 <i>0,3</i>	7,6 <i>0,3</i>	9,4 <i>2,4</i>	8,7 <i>1,6</i>
	After process	7,5 <i>0,4</i>	8,3 <i>0,4</i>	7,8 <i>0,4</i>	7,4 <i>0,3</i>	n.t.	8,2 <i>0,1</i>	n.t.	6,4 <i>0,4</i>	6,9 <i>0,2</i>	7,9 <i>0,4</i>	7,8 <i>0,2</i>	8,6 <i>0,3</i>	10,1 <i>0,2</i>	11,6 <i>0,5</i>
Naringenin	Before process	0,2 <i>0,0</i>	0,2 <i>0,0</i>	0,2 <i>0,0</i>	0,3 <i>0,1</i>	n.t.	0,3 <i>0,0</i>	n.t.	0,2 <i>0,0</i>	0,2 <i>0,0</i>	0,4 <i>0,0</i>	0,4 <i>0,0</i>	0,4 <i>0,0</i>	0,5 <i>0,2</i>	0,5 <i>0,1</i>
	After process	0,2 <i>0,0</i>	0,2 <i>0,0</i>	0,1 <i>0,0</i>	0,1 <i>0,0</i>	n.t.	0,6 <i>0,0</i>	n.t.	0,3 <i>0,0</i>	0,4 <i>0,0</i>	1,6 <i>0,0</i>	1,7 <i>0,0</i>	2,0 <i>0,1</i>	2,5 <i>0,0</i>	2,8 <i>0,1</i>
β-carotene	Before process	3,6 <i>0,5</i>	4,1 <i>0,2</i>	3,9 <i>0,1</i>	4,0 <i>0,1</i>	9,6 <i>0,6</i>	4,5 <i>0,1</i>	9,2 <i>0,6</i>	4,0 <i>0,1</i>	4,0 <i>0,1</i>	4,6 <i>0,1</i>	4,8 <i>0,0</i>	4,6 <i>0,1</i>	4,8 <i>0,0</i>	4,8 <i>0,1</i>
	After process	3,9 <i>0,1</i>	4,6 <i>0,2</i>	4,1 <i>0,2</i>	3,6 <i>0,0</i>	8,1 <i>0,1</i>	3,5 <i>0,0</i>	7,4 <i>0,1</i>	3,3 <i>0,1</i>	2,9 <i>0,0</i>	3,8 <i>0,0</i>	3,7 <i>0,1</i>	3,3 <i>0,2</i>	2,7 <i>0,1</i>	2,5 <i>0,1</i>
Lycopene	Before process	101,3 <i>2,5</i>	102,7 <i>4,4</i>	91,0 <i>3,4</i>	122,3 <i>5,9</i>	37,9 <i>2,8</i>	123,4 <i>4,7</i>	39,7 <i>4,0</i>	105,9 <i>3,5</i>	105,9 <i>3,5</i>	152,8 <i>7,7</i>	155,5 <i>3,2</i>	152,8 <i>7,7</i>	134,7 <i>5,0</i>	137,6 <i>3,0</i>
	After process	108,6 <i>11,2</i>	124,3 <i>12,1</i>	115,1 <i>3,5</i>	109,7 <i>7,8</i>	33,2 <i>0,9</i>	124,6 <i>6,3</i>	38,0 <i>1,3</i>	110,9 <i>7,3</i>	111,0 <i>4,7</i>	159,2 <i>5,9</i>	155,5 <i>8,1</i>	160,5 <i>8,0</i>	132,8 <i>3,7</i>	138,2 <i>1,9</i>

In bold the average and in italic the standard deviation of 4 repetitions (2 analytic and 2 pilot repetitions). n.t. = not tested.

Table 2. Concentration expressed in mg/100 g of dry matter.

Process step	Temperature (°C)	Ascorbic acid				Chlorogenic acid			
		Before process		After process		Before process		After process	
Before sieving	25	308,3	<i>11,4</i>	184,7	<i>7,8</i>	7,8	<i>0,3</i>	8,5	<i>0,1</i>
	30	320,2	<i>10,3</i>	210,1	<i>7,8</i>	8,2	<i>0,8</i>	8,1	<i>0,4</i>
	35	321,2	<i>18,2</i>	175,0	<i>5,2</i>	7,3	<i>0,2</i>	7,1	<i>0,5</i>
Cold break	50	281,7	<i>6,6</i>	149,6	<i>2,1</i>	8,4	<i>0,3</i>	2,1	<i>0,6</i>
	60	279,4	<i>8,0</i>	161,3	<i>12,4</i>	21,6	<i>1,6</i>	22,4	<i>1,1</i>
	70	329,2	<i>9,5</i>	52,4	<i>6,6</i>	9,3	<i>0,4</i>	9,3	<i>0,4</i>
	80	263,5	<i>7,2</i>	3,9	<i>0,1</i>	14,6	<i>0,4</i>	15,6	<i>1,0</i>
Pasteurisation	95°C - 25 min	272,9	<i>1,5</i>	247,0	<i>1,9</i>	7,0	<i>0,5</i>	6,4	<i>0,5</i>
	95°C - 60 min	n.t.	-	n.t.	-	7,0	<i>0,5</i>	6,8	<i>0,3</i>
	105°C - 15 min	224,2	<i>4,4</i>	201,5	<i>9,3</i>	8,9	<i>0,4</i>	8,8	<i>0,6</i>
	105°C - 25 min	189,1	<i>5,6</i>	163,1	<i>4,3</i>	9,1	<i>0,2</i>	9,4	<i>0,4</i>
	105°C - 60 min	238,8	<i>3,8</i>	202,1	<i>17,7</i>	8,9	<i>0,4</i>	8,7	<i>0,4</i>
	125°C - 25 min	222,0	<i>6,2</i>	163,7	<i>2,1</i>	6,9	<i>0,3</i>	7,6	<i>0,2</i>
	125°C - 60 min	227,6	<i>5,1</i>	112,1	<i>4,0</i>	6,9	<i>0,5</i>	7,0	<i>0,8</i>
Cold break under N2	60	217,8	<i>3,9</i>	130,3	<i>16,6</i>	9,7	<i>0,4</i>	10,5	<i>0,9</i>
	80	177,2	<i>7,6</i>	63,0	<i>3,5</i>	8,4	<i>0,9</i>	8,7	<i>0,4</i>

In bold the average and in italic the standard deviation of 4 repetitions (2 analytic and 2 pilot repetitions). n.t. = not tested.

Table 3. Parameter kinetic values and temperature range validity for all micronutrients.

Component	kinetic	parameter values	validity
Chlorogenic acid	First-Order	$k_{ACHL}(50\text{ °C}) = 1,10 \cdot 10^{-2} \text{ min}^{-1}$	50 °C
	No degradation		[25-35 °C] ; [60-125 °C]
Ascorbic acid	First-order / Arrhenius	$k_{AASC}^{\infty} = 16,01 \text{ min}^{-1}$ $E_a = 21,3 \text{ kJ} \cdot \text{mol}^{-1}$	[25-80 °C]
	Thermal degradation, first-order, Arrhenius-like law $k_T = k_T^{\infty} \exp(-A/T)$ (T en K)	$k_T^{\infty} = 3,17 \cdot 10^6 \text{ min}^{-1}$ $A = 7,70 \cdot 10^3 \text{ K}$	[95-125 °C]
β -Carotene	No degradation		[25-80 °C]
	First-order / Arrhenius	$k_{CARO}^{\infty} = 2,23 \cdot 10^3 \text{ min}^{-1}$ $E_a = 38,8 \text{ kJ} \cdot \text{mol}^{-1}$	[95-125 °C]
Lycopene	No degradation		[25-125 °C]
Rutin/Naringenin			
α -Tocopherol			
O ₂ transfer	Transfer / Arrhenius type $r = kla([O_2]_{sat} - [O_2])$ $kla = kla^{\infty} \exp(-A/T)$ (T en K)	$kla^{\infty} = 1,73 \cdot 10^6 \text{ min}^{-1}$ $A = 7,08 \cdot 10^3 \text{ K}$	[50-80 °C]

Table 4. Concentration expressed in mg/100 g of dry matter.

	Process step	Process step							
		Re-heating					Re-heating under N2		
		50°C	60°C	70°C	80°C	95°C	50°C	70°C	95°C
Ascorbic acid	Before process	88,0	104,9	114,3	191,5	183,3	112,2	106,6	106,1
		<i>1,0</i>	<i>7,7</i>	<i>2,1</i>	<i>2,5</i>	<i>5,8</i>	<i>0,8</i>	<i>1,6</i>	<i>2,1</i>
	After process	2,0	1,8	0,4	0,0	7,6	91,8	90,6	83,6
		<i>1,3</i>	<i>0,2</i>	<i>0,0</i>	-	<i>0,3</i>	<i>1,3</i>	<i>0,3</i>	<i>0,5</i>

In bold the average and in italic the standard deviation of 4 repetitions (2 analytic and 2 pilot repetitions).

Table 5. Concentration expressed in mg/100 of dry matter.

		Process step								
		Re-heating					Re-heating under N2			
		50°C	60°C	70°C	80°C	95°C	50°C	70°C	95°C	
Rutin	Before process	14,8 <i>0,1</i>	n.t. -	14,6 <i>0,4</i>	26,2 <i>0,5</i>	21,2 <i>0,9</i>	n.t. -	n.t. -	n.t. -	
	After process	15,2 <i>0,3</i>	n.t. -	14,5 <i>0,6</i>	23,5 <i>2,1</i>	22,6 <i>1,9</i>	n.t. -	n.t. -	n.t. -	
Chlorogenic acid	Before process	5,5 <i>0,1</i>	n.t. -	5,2 <i>0,1</i>	13,6 <i>0,7</i>	16,8 <i>0,9</i>	n.t. -	n.t. -	n.t. -	
	After process	5,3 <i>0,1</i>	n.t. -	4,9 <i>0,1</i>	12,7 <i>0,7</i>	17,8 <i>1,3</i>	n.t. -	n.t. -	n.t. -	
Naringenin	Before process	1,4 <i>0,0</i>	n.t. -	1,4 <i>0,0</i>	7,1 <i>0,1</i>	6,1 <i>0,3</i>	n.t. -	n.t. -	n.t. -	
	After process	1,4 <i>0,1</i>	n.t. -	1,3 <i>0,0</i>	5,4 <i>0,5</i>	5,4 <i>0,5</i>	n.t. -	n.t. -	n.t. -	
β-carotene	Before process	3,7 <i>0,1</i>	3,4 <i>0,1</i>	3,7 <i>0,1</i>	5,3 <i>0,1</i>	6,0 <i>0,3</i>	3,7 <i>0,1</i>	3,5 <i>0,0</i>	3,5 <i>0,1</i>	
	After process	3,4 <i>0,1</i>	3,2 <i>0,1</i>	3,0 <i>0,1</i>	4,1 <i>0,1</i>	3,7 <i>0,2</i>	3,6 <i>0,2</i>	3,5 <i>0,1</i>	3,1 <i>0,2</i>	
Lycopene	Before process	102,9 <i>3,6</i>	100,2 <i>0,7</i>	97,8 <i>1,9</i>	149,2 <i>44,4</i>	91,2 <i>7,8</i>	94,3 <i>3,7</i>	96,1 <i>5,3</i>	92,5 <i>0,0</i>	
	After process	96,4 <i>2,3</i>	84,2 <i>10,1</i>	70,9 <i>4,4</i>	77,0 <i>6,6</i>	69,8 <i>10,4</i>	94,6 <i>1,9</i>	91,6 <i>2,6</i>	70,6 <i>11,6</i>	

In bold the average and in italic the standard deviation of 4 repetitions (2 analytic and 2 pilot repetitions).
n.t. = not tested.

Table 6. Parameter kinetic values and temperature range validity for all micronutrients.

Component	Kinetic	Parameter values	Validity
Chlorogenic acid	No degradation		[50-95 °C]
Ascorbic acid	First-order / Arrhenius	$k_{AASC}^{\infty} = 247,0 \text{ min}^{-1}$ $E_a = 22,5 \text{ kJ.mol}^{-1}$	[50-95 °C]
β-Carotene	First-order / Arrhenius	$k_{Caro}^{\infty} = 13,3 \text{ min}^{-1}$ $E_a = 27,7 \text{ kJ.mol}^{-1}$	[50-95 °C]
Lycopene	First-order / Arrhenius	$k_{Lyco}^{\infty} = 2,7 \cdot 10^{12} \text{ min}^{-1}$ $E_a = 97,6 \text{ kJ.mol}^{-1}$	[50-95 °C]
Rutin	No degradation		[50-95 °C]
Naringenine	First-order / Arrhenius	$k_{Nar}^{\infty} = 1,98 \cdot 10^6 \text{ min}^{-1}$ $E_a = 63,9 \text{ kJ.mol}^{-1}$	[80-95 °C]
	No degradation		[50-70 °C]
α-Tocopherol	No degradation		[50-95 °C]

Figures

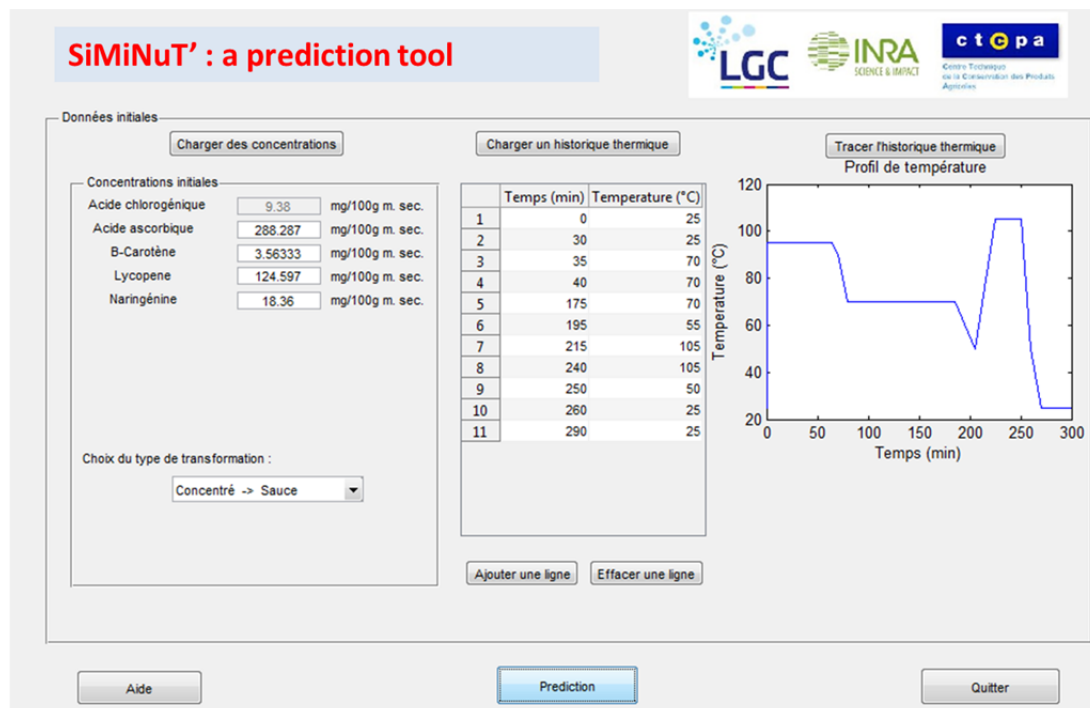


Fig. 1. User-friendly interface of the SiMiNuT tool.

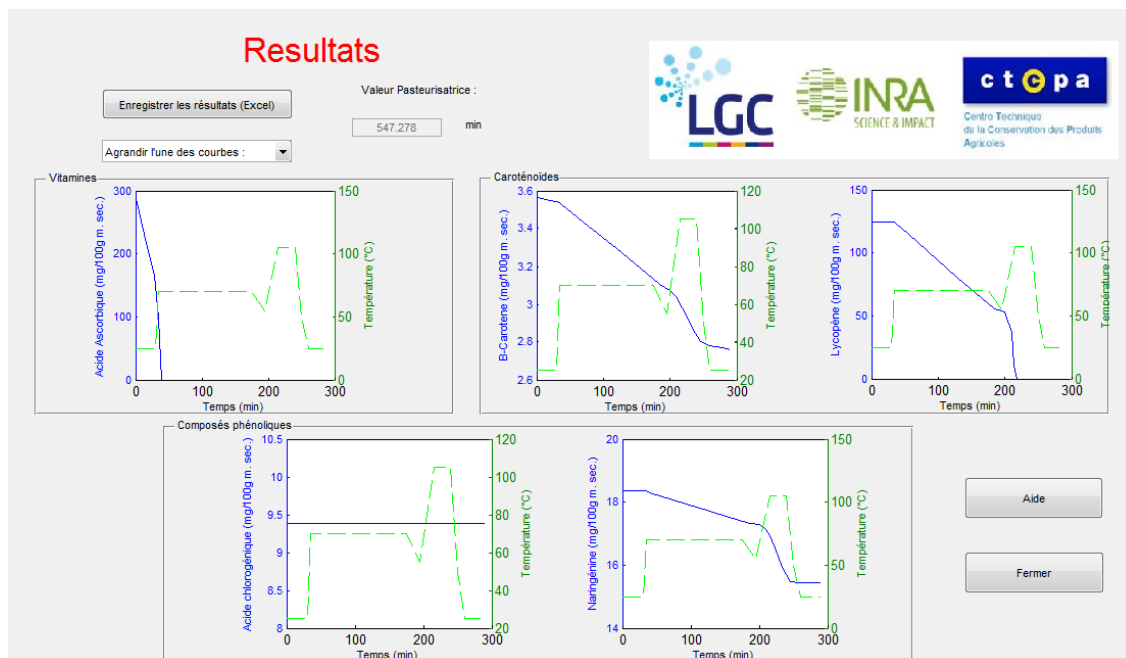


Fig. 2. Example of outcome from the simulation tool.