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Design of experiments to study the risk of sous vide cooking for possible migration of hazardous compounds from the packaging to the food. Analysis by DI-SPME-GC-MS and UPLC-IMS-QTOF

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Introduction

Sous Vide cooking is a fashionable technique in today's gastronomy, widely used by top chefs in some of the world's best restaurants for industrial food processing and can be adapted to home cooking (Baldwin 2012). However, since the cooking technique involves the use of plastic material intended to come into direct contact with the food, it is necessary to consider not only the preservation of the organoleptic and nutritional properties of the food, but also the risk of possible hazardous compounds that may migrate from the packaging to the food (Vera et al. 2023; Su et al. 2021; Cherif Lahimer et al. 2017; Arvanitoyannis, Bosnea 2004).

Regulation (EC) No 1935/2004 of the European Parliament and of the Council makes it clear that the basic rules apply to all food contact materials. One of the main criteria is that this material must be sufficiently inert so as not to transfer, through migration processes, high-risk substances that could affect the health of the consumer and/or alter organoleptic properties.
Novel techniques such as DI-SPME-GC-MS and UPLC-IMS-QTOF have been used to identify the compounds. For the migration tests, three simulants have been used under the conditions of the legislation.

Aims

Using design of experiments (DoE) and response surface methodology, the influence of Sous Vide cooking time and temperature conditions on the migration of volatile and non-volatile hazardous compounds into the food was studied. Migration has been studied in HDPE-PA and PP-PA and in three simulants, analysing the compounds of interest by DI-SPME-GC-MS and UPLC-IMS-QTOF.

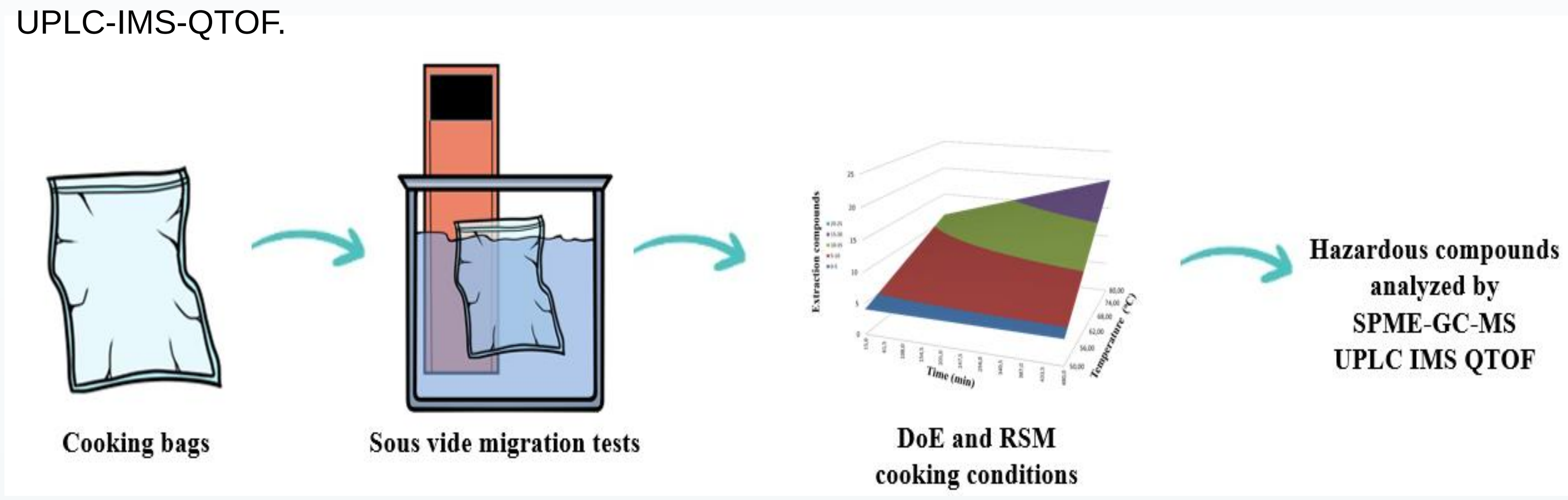

Figure 1: Methodology flowchart

Methodology

The methodology of the migration study, as well as the analyses carried out, are presented in the form of a flow chart in Figure 1. The experimental conditions carried out, including the variables of the factorial design (v1 and v2), are presented in Table 1.

Experiment Nomenclature	Time (v1)		Temperature (v2)	
	min	Norm.	ºC	Norm.
E1	15	-1	50	-1
E2	15	-1	80	1
E3	247,5	0	65	0
E4	480	1	50	-1
E5	480	1	80	1

Table 2: Volatile and semi-volatile compounds identified for PP bags in ethanol 10% by SPME-GC-MS

RT (min)	Compound	CAS	Formula	Classification
6.33	p-Xylene	106-42-3	C_8H_{10}	NIAS
6.79	Styrene	100-42-5	C_8H_8	NIAS
7.48	Oxime-, methoxy-phenyl-_	1000222-86-6	$C_8H_9NO_2$	NIAS
16.35	2,4-Di-tert-butylphenol	96-76-4	$C_{14}H_{22}O$	Antioxidant/ UV
17.37	Diethyl Phthalate	84-66-2	$C_{12}H_{14}O_4$	Plasticizer
17.80	p-Octylacetophenone	10541-56-7	$C_{16}H_{24}O$	NIAS
19.35	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	$C_{15}H_{22}O_2$	NIAS
20.37	Phthalic acid, isobutyl octyl ester	1010309-04-5	$C_{20}H_{30}O_4$	Plasticizer
20.41	2,5-di-tert-Butyl-1,4-benzoquinone	2460-77-7	$C_{14}H_{20}O_2$	NIAS
20.91	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	$C_{17}H_{24}O_3$	Antioxidant (NIAS)
21.03	Diphenyl sulphone	127-63-9	$C_{12}H_{10}O_2S$	Thermosetting
21.11	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	6386-38-5	$C_{18}H_{28}O_3$	Antioxidant
21.21	n-Hexadecanoic acid	57-10-3	$C_{16}H_{32}O_2$	NIAS
21.30	Dibutyl phthalate	84-74-2	$C_{16}H_{22}O_4$	Plasticizer
21.60	3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid	20170-32-5	$C_{17}H_{26}O_3$	Additive (Fenozan)
21.89	9-Acetylphenanthrene	2039-77-2	$C_{16}H_{12}O$	NIAS
23.09	Octadecanoic acid	057-11-4	$C_{18}H_{36}O_2$	Additive
23.29	9-Octadecenamide, (Z)	301-02-0	$C_{18}H_{35}NO$	Additive (Resistence)
25.13	Diisooctyl adipate	1330-86-5	$C_{22}H_{42}O_4$	Plasticizer
26.02	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	23470-00-0	$C_{19}H_{38}O_4$	NIAS
27.61	Octadecanoic acid, 2,3-dihydroxypropyl ester	123-94-4	$C_{21}H_{42}O_4$	Additive
28.04	13-Docosenamide, (Z)-	112-84-5	$C_{22}H_{43}NO$	Slip additive

Results

In this study, different volatile and semi volatile compounds, including IAS and NIAS, have been identified in two plastic bags (i) bioriented polyamide and polypropylene (PP + PA) and (ii) bioriented polyamide and high-density polyethylene (HDPE + PA). Compounds of interest have been found in all simulants.

As the example in Figure 2 shows, temperature (v2) has a higher effect than time (v1) or the interaction between time and temperature (v12). Table 2 shows the list of the volatile and non-volatile compounds identified.

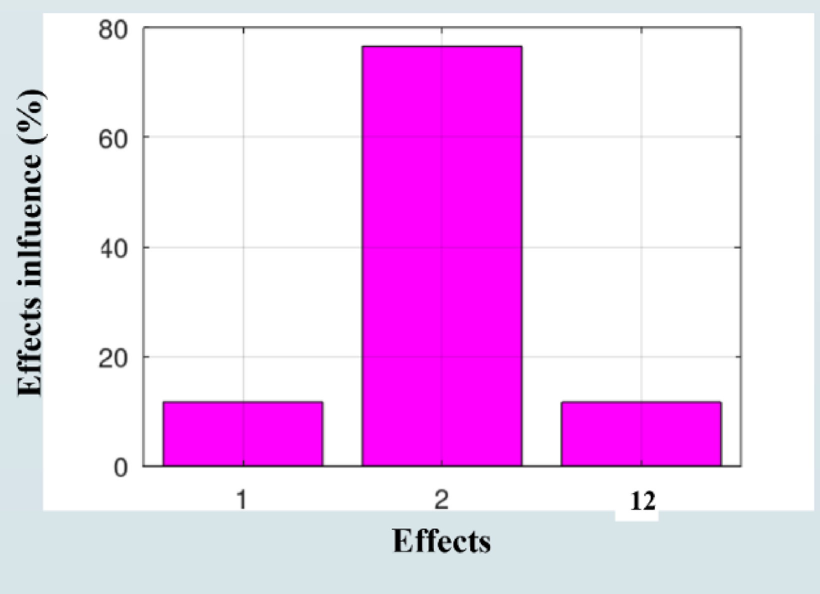

Figure 2: Variable effect diagram (1: time, 2: temperatura and 12: interaction time-temperature)

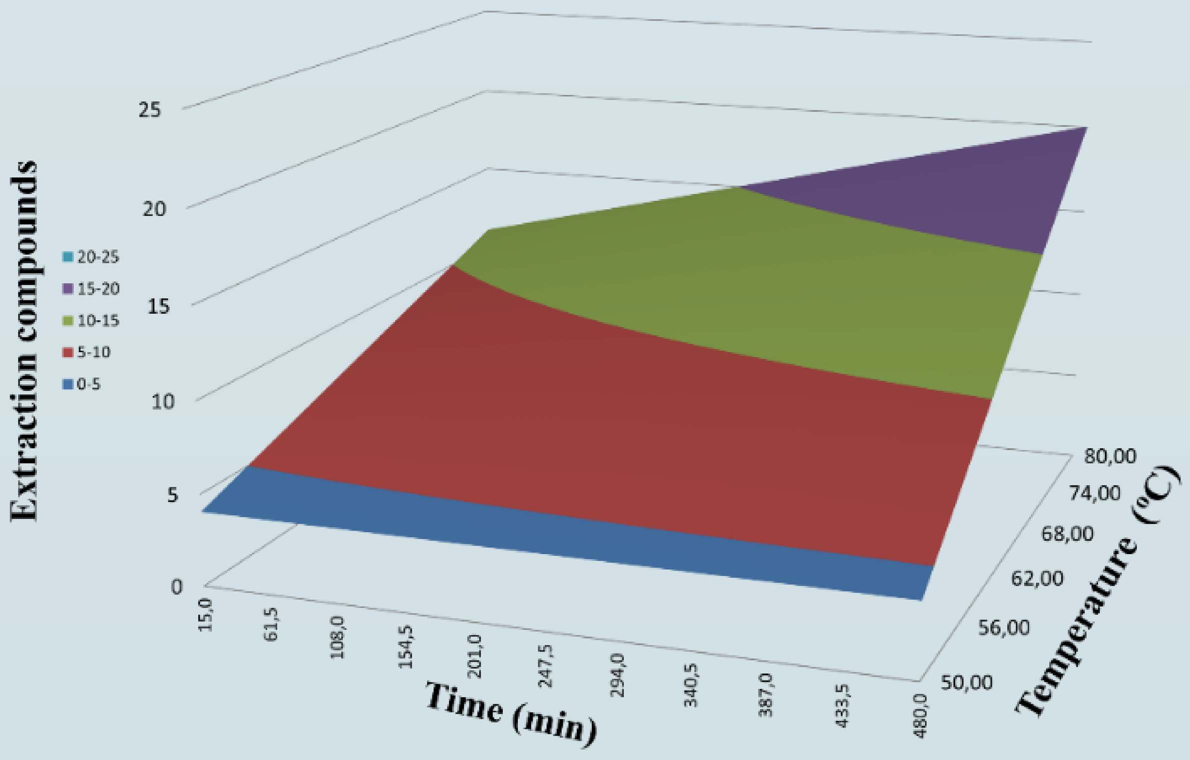

Figure 3: Surface response for PP + PA bags in ethanol 10%

Conclusions

Temperature has been shown to be the key factor in the number of compounds migrating to 10% ethanol in PP+PA plastic bags, as suggested in figure 3. In fact, the maximum migration conditions start after 250 minutes and with the temperature above 68ºC.

A part of the compounds is intentionally added substances (IAS) and used as plasticizers (phthalates and adipates), antioxidants (2,4-Di-tert-butylphenol) and additives to improve the mechanical properties of the plastic (13-Docosenamide, (Z)-; Diphenyl sulfone).

The rest of the compounds found are non-intentionally added substances (NIAS) which may originate from side reactions, contamination (p-xylene) or decomposition products (7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione: degradation product of antioxidants).

Quantification of these compounds should be carried out to fully asses the risk to human helth.

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