PET Flake Injection

Novel Technology Development

Data Monitoring Report

report required by Article 13 of Regulation (EU) 2022/1616

10 October 2023

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Introduction

The novel technology PET Flake Injection was notified as required under Articles 10(2) and 10(3) of Commission Regulation (EU) 2022/1616 on 17th March 2023.

Article 13 of Commission Regulation (EU) 2022/1616 States the following:

"*a recycler operating a decontamination installation in accordance with Article 11* of the regulation *shall monitor the average contaminant level on the basis of a robust sampling strategy which samples the plastic input batches and the corresponding plastic output batches".*

The enclosed report provides a summary of the data forthcoming from the monitoring, based on the latest information from all installations using the novel technology received in accordance with paragraph 3 along with the information required by Article 13(5) of the Regulation.

a) Brief description of the novel technology

The Flake Injection process has the capability to combine depolymerised recycled Polyethylene Terephthalate (rPET) with virgin material at different stages of a conventional PET production process for subsequent food contact use. The input material of the Flake Injection process is previously processed PET as detailed in Table 2 of ANNEX I of COMMISSION REGULATION (EU) 2022/1616 and is deliberately depolymerized (preprocessed) before it enters the high surface area decontamination polymerisation reactor. Referring to the flow scheme Appendix I: Flake Injection – PET Production Process; previously processed PET may be introduced directly to injection point 1. or partially depolymerised with ethylene glycol, in either a stir-tank reactor or an extruder, to a defined degree of polymerisation to correspond with that of the polymer in the PET production process at the injection points labelled 2 to 6 in the flow scheme *or any points in-between*. This initial depolymerisation process of the previously processed PET allows for filtration of the intermediate polymer to remove solid contaminants before the introduction of the recycled material into a PET production process at a blend rate of up to 100% recycled content. The high surface area decontamination polymerisation technology increases the Intrinsic Viscosity (IV) of the PET polymer and removes polymerisation by-products under high vacuum of less than 20mbar, with a high temperature greater than 260°C and with a residence time greater than 30 minutes. This high surface area polymerisation technology also serves as a Decontamination Technology to efficiently remove vapourised contaminants that may have been introduced into the process further upstream by the addition of previously processed PET. Following the high surface area polymerisation and decontamination, the polymer melt is filtered for either direct use, or granulation, in the manufacture of food contact materials or articles or for introduction into a Solid State Polycondensation (SSP) process or a Conditioning Silo should further processing be needed to meet the material parameters required for its end use.

b) Summary of the reasoning on the capability of the novel technology and the recycling process(es) to manufacture recycled plastic materials and articles that meet the requirements of Article 3 of Regulation (EC) No 1935/2004 and that are microbiologically safe.

Flake To Resin (FTR)

Ref. ANNEX II Table 1 (1) Decontamination efficiency of a new post-consumer poly(ethylene terephthalate) (PET) recycling concept. FRANK WELLE. Fraunhofer Institute for Process Engineering and Packaging (IVV), Giggenhauser Straße 35, 85354 Freising, Germany.

Table VI. Concentrations (determined using the HFIP extraction method) of the surrogates in the investigated PET samples of Trial 2 (cocktail A at 10 ml min^{-1}, 50% PCR flakes).

	Concentration (ppm)						
	Toluene	Chloroform	Chlorobenzene	Phenyl cyclohexane	Methyl salicylate	Benzophenone	Lindane
Calculated contamination concentration	3295	5194	1255	327	1004	885	775
Before deep-cleansing	1999 ± 28	3075 ± 47	655 ± 9	163 ± 2	<1.0	345 ± 1	133 ± 1
After deep-cleansing (final product)	<2.7	<0.8	<0.9	<0.2	<1.0	<0.2	<0.8

The cleaning efficiencies for the applied surrogates are above or far above 99.9%. The high cleaning efficiencies are due to the high diffusion rates of compounds in the molten PET.

Based on EFSA's criteria for safety evaluation of PET recycling processes - if a recycling process is able to reduce an input reference contamination of 3 mg/kg PET to a Cres (Residual Concentration) not higher than a Cmod (Modelled Concentration) corresponding to the relevant migration criterion, the potential dietary exposure cannot be higher than 0.0025 µg/kg bw/day and recycled PET manufactured with such recycling process is not considered of safety concern.

Ref. ANNEX II Table 1 (2) Fraunhofer_Dossier-FTR_20061109.pdf

Reversed Approach

Based on Safety Evaluation of Polyethylene Terephthalate Chemical Re-cycling Processes. Frank Welle. 'Reversed Approach'.

Ref. ANNEX II Table 1 (3) !chemical_recycling_submitted.pdf

FTR: Calculated maximum concentration (Reference Contamination – the level of contamination that the process can remove, i.e. Cmod:Cres =1) corresponding to a migration of 0.1 µg/l after storage for 365 d at 25 °C (EU cube, AP = 3.1, tau 1577 K, bottle wall thickness 200 µm, density of PET 1.4 g/cm^3). Decontamination Efficiency of 99.9%.

mm Hg (25°C)	°C	$g.mol^{-1}$	FTR	Reference Contamination	Decontamination Efficiency	*Cres*	*Cmod*	
Vapour Pressure	BP	Mw	Surrogate	mg/kg	%	mg/kg	mg/kg	Cmod:Cres
28.4	110.6	92.1	Toluene	**90**	99.9%	0.09	0.09	1.0
197	61.1	119.4	Chloroform	**100**	99.9%	0.10	0.10	1.0
12	131.7	112.6	Chlorobenzene	**90**	99.9%	0.09	0.09	1.0
0.0343	222.9	152.2	Methyl Salicylate	**130**	99.9%	0.13	0.13	1.0
0.04	240.1	160.3	Phenyl Cyclohexane	**140**	99.9%	0.14	0.14	1.0
0.00193	305.4	182.2	Benzophenone	**160**	99.9%	0.16	0.16	1.0
9.40E-06	311.0	290.8	Lindane	**310**	99.9%	0.31	0.31	1.0

Artenius.

EFSA-Q-2011-00969 - EFSA refused to evaluate as out of the scope of Regulation (EC) 282/2008.

Ref. ANNEX II Table 1 (7) EFSA_Letter Related to Artenius Unique Process.pdf

Ref. ANNEX II Table 1 (8) Fraunhofer Institute. Challenge Test.pdf

US FDA Guidance

Use of Recycled Plastics in Food Packaging (Chemistry Considerations): Guidance for Industry.

U.S. Department of Health and Human Services Food and Drug Administration Center for Food Safety and Applied Nutrition July 2021

VIII. Elimination of Data Recommendations for 3° Recycling Processes for PET and PEN

Based on a comprehensive review of all surrogate testing data submitted over the past decade for 3° recycling processes for PET and polyethylene naphthalate (PEN), FDA concludes that 3° recycling of PET or PEN by methanolysis or glycolysis results in the production of monomers or oligomers that are readily purified to produce a finished polymer that is suitable for food-contact use. Both 3° processes will clean the polyester sufficiently to allow it to be considered of suitable purity, even assuming 100% migration of residual surrogate to food. This is a significant difference from the surrogate testing of 2° recycling processes. Secondary recycling processes often produce PET that is insufficiently cleaned to withstand 100% migration calculations for the residual surrogates. Under these circumstances, FDA recommends additional migration tests to demonstrate that the finished PET meets the 1.5 µg/person/day EDI limit.

Based on a determination that 3° recycling processes produce PET or PEN of suitable purity for foodcontact use, FDA no longer recommends that such recyclers submit data for agency evaluation. Because 3° processes for polymers other than PET and PEN were not the subject of FDA reviews, recyclers who wish to engage in 3° recycling of polymers other than PET and PEN are encouraged to submit data for evaluation.

Ref. ANNEX II Table 1 (9) Recycled-Plastics-Food-Packaging-Chemistry-ConsiderationsGuidance-04112022-1321.pdf

c) List a list of all substances with a molecular weight below 1000 Dalton found in the plastic inputs and recycled plastic output

As developer of the Novel Technology, PET-Europe has coordinated with the recyclers regarding the selection of the sampling strategy, the analysis to be performed and the selection of a third-party laboratory. The choice of the laboratory was based on its experience and expertise in analysing PET samples, the relevance of its analytical equipment and validated methods as well as the capability to identify and to risk assess non-intentionally added substances (NIAS) taking into account the particularity of this specific technology.

The results of the Targeted analysis of inorganic substances by ICP-MS are not included due to an issue with metal contamination of samples during the milling phase used for sample preparation rendering the ICP-MS results unreliable, The laboratory is in the process of rectifying and repeating the analysis but with the large amount of samples to test this will inevitably be delayed. Therefore, the outcome of the analysis will be added to the report as soon as they become available.

Volatiles

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE1	1-Propanol, 2-(2-hydroxypropoxy)-	$C_6H_{14}O_3$	106-62-7	8565.71	2170.85	74.7
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5	8315.69	2958.10	64.4
	1-Propanol, 2,2'oxybis-	$C_6H_{14}O_3$	108-61-2	7452.90	2525.77	66.1
	Ethanol, 2-(dodecyloxy)-	$C_{14}H_{30}O_2$	4536-30-5	4499.72		100.0
	Undecane, 2,3dimethyl-	$C_{13}H_{28}$	17312-77-5	628.75		100.0
	1-Dodecanol	$C_{12}H_{26}O$	112-53-8	524.63		100.0
	Octanoic acid	$C_8H_{16}O_2$	124-07-2	421.32		100.0
	1-Heptanol, 2-propyl-	$C_{10}H_{22}O$	10042-59-8	303.55		100.0
	1-Eicosanol	$C_{20}H_{42}O$	629-96-9	230.29		100.0
	Decanal	$C_{10}H_{20}O$	112-31-2	177.07		100.0
	D-Limonene	$C_{10}H_{16}$	5989-27-5	144.01		100.0
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	82304-66-3	51.68		100.0
	2,5-di-tert-Butyl-1,4benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	23.35		100.0
	2,5-di-tert-Butyl-1,4benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	21.40		100.0
	2,5-di-tert-Butyl-1,4benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	14.86		100.0
	Nonanal	$C_9H_{18}O$	124-19-6		102.06	-

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 2	Ethanol, 2-(dodecyloxy)-	$C_{14}H_{30}O_2$	4536-30-5	1368.96		100.0
	Dodecanal	$C_{12}H_{24}O$	112-54-9	605.10	87.58	-
	1-Hexanol, 2-ethyl-	$C_8H_{18}O$	104-76-7	305.85		100.0
	Nonanal	$C_9H_{18}O$	124-19-6	285.43		100.0
	α-Terpineol	$C_{10}H_{18}O$	98-55-5	79.40		100.0
	Toluene	C_7H_8	108-88-3	17.42		100.0
	m-Xylene (Benzene, 1,3-dimethyl)	C_8H_{10}	108-38-3	12.93		100.0
	Chloroxylenol	C_8H_9ClO	88-04-0	10.84		100.0
	Mesitylene (Benzene, 1,3,5-trimethy)	C_9H_{12}	108-67-8	10.24		100.0
	Ethylbenzene	C_8H_{10}	100-41-4	8.46		100.0
	p-Xylene (Benzene, 1,4-dimethyl-)	C_8H_{10}	106-42-3	5.74		100.0
	Benzene, 1-ethyl-2methyl-	C_9H_{12}	611-14-3	4.35		100.0
	Benzene, 1-ethyl-3methyl-	C_9H_{12}	620-14-4	3.89		100.0
	Benzene, 1-ethyl-4methyl-	C_9H_{12}	622-96-8	3.85		100.0
	1,3-Dioxolane, 2-methyl-	$C_4H_8O_2$	497-26-7		1997.90	-
	Octanoic acid, ethyl ester	$C_{10}H_{20}O_2$	106-32-1		44.69	-
	1-Undecanol	$C_{11}H_{24}O$	112-42-5		238.63	-
	Tetradecane	$C_{14}H_{30}$	629-59-4		46.90	-

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 3	Acetic acid, methoxy-	$C_3H_6O_3$	625-45-6	99547.49		100.0
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5	10661.55		100.0
	1-Propanol, 2-(2-hydroxypropoxy)-	$C_6H_{14}O_3$	106-62-7	9984.90		100.0
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5	9587.44		100.0
	Ethanol, 2-(dodecyloxy)-	$C_{14}H_{30}O_2$	4536-30-5	3735.35	47.00	98.7
	Nonanal	$C_9H_{18}O$	124-19-6	801.21		100.0
	Phthalic acid, diisobutyl ester	$C_{16}H_{22}O_4$	84-69-5	225.12		100.0
	2-Decenal, (E)-	$C_{10}H_{18}O$	3913-81-3	168.56		100.0
	1-Octadecanol	$C_{18}H_{38}O$	112-92-5	146.82		100.0
	Decanal	$C_{10}H_{20}O$	112-31-2	129.62		100.0
	Dodecanal	$C_{12}H_{24}O$	112-54-9	77.10		100.0
	Tetradecane	$C_{14}H_{30}$	629-59-4	51.20	87.84	-71.6
	Nonanoic acid	$C_9H_{18}O_2$	112-05-0	38.81		100.0
	2,5-di-tert-Butyl-1,4-benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	27.88		100.0
	2,5-di-tert-Butyl-1,4-benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	25.55	6.14	76.0
	2,5-di-tert-Butyl-1,4-benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	15.41		100.0
	p-Xylene	C_8H_{10}	106-42-3	5.77		100.0
	2-Propanol, 1,1'oxybis-	$C_6H_{14}O_3$	110-98-5		2423.53	-
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5		1528.43	-
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5		2166.73	-
	7,9-Di-tert-butyl-oxaspiro(4,5)deca6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	82304-66-3		25.03	-
	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	57-10-3		<10	-

Volatiles (contd)

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 4	p-Cymene	C10H14	99-87-6	5860.05		100.0
	6-Methyl-1-octanol	C9H20O	110453-78-6	4008.33		100.0
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5	3296.64		100.0
	Phthalic acid, butyl tetradecyl ester	$C_{26}H_{42}O_4$	-	202.28		100.0
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5	181.62		100.0
	Phthalic acid, butyl tetradecyl ester	$C_{26}H_{42}O_4$	-	114.34		100.0
	1-Undecanol	C11H24O	112-42-5	79.20	53.40	32.6
	2,5-di-tert-Butyl-1,4-benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	64.81	64.81	0.0
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	82304-66-3	53.50		100.0
	1,4-benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	53.50		100.0
	D-Limonene	C10H16	5989-27-5	32.07		100.0
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	82304-66-3	14.46	4.82	66.7
	Dodecanal	$C_{12}H_{24}O$	112-54-9	9.33		100.0
	1-Hexadecanol, 2-methyl-	C 17H36O	2490-48-4	3.84		100.0
	Dipropylene glycol	C6H14O3	110-98-5		1732.47	-
	Dipropylene glycol	C6H14O3	110-98-5		1199.75	-
	Dipropylene glycol	C6H14O3	110-98-5		1703.76	-
	p-Benzoquinone, 2,6-di-tert-butyl-	C 14H20O2	719-22-2		69.11	-
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5		5.43	-

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 5	Ethanol, 2-(dodecyloxy)	C14H30O2	4536-30-5	53.68	63.86	-19.0
	Dodecanal	C12H24O	112-54-9	53.60		100.0
	2,5-di-tert-Butyl-1,4-benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	11.11	13.26	-19.4
	2,5-di-tert-Butyl-1,4-benzoquinone	$C_{14}H_{20}O_2$	2460-77-7	9.76	9.82	-0.6
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	82304-66-3	4.00		100.0
	Diisobutyl phthalate	$C_{16}H_{22}O_4$	84-69-5	1.63	1.92	-17.8
	2-Propanol, 1,1'oxybis-	$C_6H_{14}O_3$	110-98-5		8833.31	-
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5		5489.31	-
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5		6351.70	-

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 6	Nonanal	$C_9H_{18}O$	124-19-6	2924.22	1145.84	60.8
	Decanal	$C_{10}H_{20}O$	112-31-2	1541.90		100.0
	Nonanoic acid	$C_9H_{18}O_2$	112-05-0	483.84		100.0
	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-	$C_{10}H_{18}O$	619-01-2	348.10		100.0
	Acetic acid	$C_2H_4O_2$	64-19-7	129.14		100.0
	p-Xylene	C_8H_{10}	106-42-3	61.16		100.0
	Benzene, 1,2,4-trimethyl-	C_9H_{12}	95-63-6	35.80		100.0
	Toluene	C_7H_8	108-88-3	21.63		100.0
	2-Butenal	C_4H_6O	123-73-9		5155.20	-

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 7	1-Butanol, 3-methoxy	C5H12O2	2517-43-3	4499.63	0.00	100.0
	Ethanol, 2-(dodecyloxy)	C14H30O2	4536-30-5	964.38	0.00	100.0
	Dodecanal	C12H24O	112-54-9	721.23	101.51	85.9
	Nonanal	C9H18O	124-19-6	434.37		100.0
	Undecanal	C11H22O	112-44-7	110.88		100.0
	D-Limonene	C10H16	5989-27-5	24.90		100.0
	Dipropylene glycol	C6H14O3	110-98-5		770.38	-
	Dipropylene glycol	C6H14O3	110-98-5		291.53	-
	Dipropylene glycol	C6H14O3	110-98-5		366.56	-
	Linalool	C10H18O	78-70-6		20.72	-
	α-Terpineol	C10H18O	98-55-5		37.32	-
	Benzenesulfonamide N-butyl-	C10H15NO2S	3622-84-2		<1	-

Volatiles (contd)

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 8	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5	7239.35	0.00	100.0
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5	4267.60		100.0
	1-Propanol, 2-(2-hydroxypropoxy)-	$C_6H_{14}O_3$	106-62-7	3991.76		100.0
	Nonanal	$C_9H_{18}O$	124-19-6	538.40	116.08	78.4
	1-Undecanol	$C_{11}H_{24}O$	112-42-5	126.28		100.0
	1-Hexadecanol, 2methyl-	$C_{17}H_{36}O$	2490-48-4	85.52		100.0
	D-Limonene	$C_{10}H_{16}$	5989-27-5	25.64		100.0
	L-α-Terpineol	$C_{10}H_{18}O$	10482-56-1	15.64		100.0
	Diphenyl ether	$C_{12}H_{10}O$	101-84-8	3.96		100.0
	Naphthalene, 2ethenyl-	$C_{12}H_{10}$	827-54-3	3.04		100.0
	Benzene	C_6H_6	71-43-2	1.89	0.00	100.0
	Benzyl alcohol	C_7H_8O	100-51-6		7.14	-
	Decanal	$C_{10}H_{20}O$	112-31-2		78.40	-
	Ethanol, phenoxy-	$C_8H_{10}O_2$	122-99-6		24.60	-
	Nonanoic acid	$C_9H_{18}O_2$	112-05-0			-
	Biphenyl	$C_{12}H_{10}$	92-52-4		4.03	-
	Diphenyl ether	$C_{12}H_{10}O$	101-84-8		8.13	-
	2,4-Di-ertbutylphenol	$C_{14}H_{22}O$	96-76-4		13.32	-
	Isopropyl myristate	$C_{17}H_{34}O_2$	110-27-0		53.54	-
	Benzenesulfonamide N-butyl-	C10H15NO2S	3622-84-2		<1	-

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 9	Dodecanal	$C_{12}H_{24}O$	112-54-9	586.00	83.17	85.8
	Nonanal	$C_9H_{18}O$	124-19-6	237.86	71.19	70.1
	1-Undecanol	$C_{11}H_{24}O$	112-42-5	129.59	129.59	0.0
	Mesitylene	C_9H_{12}	108-67-8	10.24		100.0
	Benzene, 1,3dimethyl-	C_8H_{10}	108-38-3	5.74		100.0
	Benzene, 1ethyl-3-methyl-	C_9H_{12}	620-14-4	3.89		100.0

	Name	Formula	CAS	Input µg/kg PET	Outputµg /kg PET	Cleaning efficiency, %
SAMPLE 10	1-Heptanol, 2propyl-	$C_{10}H_{22}O$	10042-59-8	1024.59		100.0
	1-Heptanol, 2propyl-	$C_{10}H_{22}O$	10042-59-8	805.48		100.0
	Nonanal	$C_9H_{18}O$	124-19-6	471.70		100.0
	1-Dodecanol	$C_{12}H_{26}O$	112-53-8	402.82		100.0
	D-Limonene	$C_{10}H_{16}$	5989-27-5	132.19		100.0
	Ethanol, 2-(2butoxyethoxy)-	$C_8H_{18}O_3$	112-34-5	84.37		100.0
	Cyclohexanol, 2-(1,1-dimethylethyl)-, acetate	$C_{12}H_{22}O_2$	20298-69-5	38.57		100.0
	2-Butenal, (Z)-	C_4H_6O	15798-64-8		1033.58	-
	2,4-Hexadiene, 2,5dimethyl-	C_8H_{14}	764-13-6		671.97	-
	2,4-Hexadiene, 3,4dimethyl-,	C_8H_{14}	2417-88-1		789.95	-
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5		4765.67	-
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5		3062.13	-
	Dipropylene glycol	$C_6H_{14}O_3$	110-98-5		3609.89	-
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	82304-66-3		18.55	-
	2,5-di-tert-Butyl-1,4-benzoquinone	$C_{14}H_{20}O_2$	2460-77-7		7.94	-

Non Volatiles

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE I	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	210	164	21.9
	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	187	281	-50.3
	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	88	65.6	25.5
	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	39.9	40.6	-1.8
	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	24.5	30.7	-25.3
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	21.3	16.6	22.1
	6.85	835.1853	Cyclic (TPA4-EG3DEG)	C42H36O17	17.4	20.5	-17.8
	6.11	577.1339/	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	14.3	13.8	3.5
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	12	21.2	-76.7

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 2	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	273	117	57.1
	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	268	359	-34.0
	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	129	186	-44.2
	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	40.5		100.0
	6.82	469.1854	Cyclic NPG-TPA-NPG-TPA	C26H28O8	40	25.7	35.8
	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	34.3	49.2	-43.4
	6.11	577.1339	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	26.2		100.0
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	25.6		100.0
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	21.3		100.0

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 3	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	355	405	-14.1
	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	254	255	-0.4
	6.11	577.1339	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	139	124	10.8
	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	104	120	-15.4
	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	39	51.5	-32.1
	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	28.4	31.1	-9.5
	6.82	469.1854	Cyclic NPG-TPA-NPG-TPA	C26H28O8	23.6	25.3	-7.2
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	22.7	0	100.0
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	16.3	17.6	-8.0

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 4	5.84	429.1187	Cíclico TPA2-EG-DEG	C22H20O9	215	230	-7.0
	6.71	577.1345	Cíclico (TPA-EG)3	C30H24O12	184	166	9.8
	6.57	621.1603	Cíclico (TPA3-EG2DEG)	C32H28O13	93.6	92.7	1.0
	5.77	473.1453	Cíclico (TPA-DEG)2	C24H24O10	48.8	65.3	-33.8
	6.85	835.1853	Cyclic (TPA4-EG3DEG)	C42H36O17	22.1	14	36.7
	6.31	385.0922	Cíclico (TPA-EG)2	C20H16O8	21.4	11.8	44.9
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	19.5	11.6	40.5
	6.11	577.1339/	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	14.9		100.0
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	13	9.8	24.6

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 5	5.84	429.1187	Cíclico TPA2-EG-DEG	C22H20O9	237	231	2.5
	6.71	577.1345	Cíclico (TPA-EG)3	C30H24O12	144	141	2.1
	6.57	621.1603	Cíclico (TPA3-EG2DEG)	C32H28O13	83.2	90.4	-8.7
	5.77	473.1453	Cíclico (TPA-DEG)2	C24H24O10	42.8	63.2	-47.7
	6.31	385.0922	Cíclico (TPA-EG)2	C20H16O8	24.3	27.8	-14.4
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	21.4	16.8	21.5
	6.85	835.1853	Cyclic (TPA4-EG3DEG)	C42H36O17	18	17.3	3.9
	6.11	577.1339	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	14.8	8.9	39.9
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	12.8	17.5	-36.7

Non Volatiles (contd)

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 6	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	341	342	-0.3
	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	282	655	-132.3
	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	126	223	-77.0
	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	50.6	114	-125.3
	6.85	835.1853	Cyclic (TPA4-EG3DEG)	C42H36O17	42.8	60.3	-40.9
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	39	73.2	-87.7
	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	37.5	23.7	36.8
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	31	61.5	-98.4
	6.11	577.1339/	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	30.9	34.3	-11.0

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 7	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	541	425	21.4
	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	377	303	19.6
	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	252	190	24.6
	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	155	130	16.1
	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	61.9	52	16.0
	6.82	469.1854	Cyclic NPG-TPA-NPG-TPA	C26H28O8	40	25.7	35.8
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	29.2		100.0
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	27.1	20.4	24.7
	6.11	577.1339	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	25.8		100.0

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 8	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	391	497	-27.1
	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	340	327	3.8
	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	149	166	-11.4
	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	58.6	67.7	-15.5
	6.85	835.1853	Cyclic NPG-TPA-NPG-TPA	C42H36O17	52.6	48.4	8.0
	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	45.2	37.5	17.0
	6.11	577.1339	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	44.7	19.6	56.2
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	38.3	36.7	4.2
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	34.7	36	-3.7

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 9	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	251	211	15.9
	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	173	174	-0.6
	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	83.9	44.4	47.1
	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	59.2	107	-80.7
	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	25.8	25.9	-0.4
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	19.3	22.9	-18.7

	RT	Mass	Candidate	Formula	Input µg/kg PET	Output µg/kg PET	Cleaning efficiency, %
SAMPLE 10	6.71	577.1345	Cyclic (TPA-EG)3	C30H24O12	242	274	-13.2
	5.84	429.1187	Cyclic TPA2-EG-DEG	C22H20O9	220	272	-23.6
	6.57	621.1603	Cyclic (TPA3-EG2-DEG)	C32H28O13	99.2	114	-14.9
	6.31	385.0922	Cyclic (TPA-EG)2	C20H16O8	37.2	0	100.0
	5.77	473.1453	Cyclic (TPA-DEG)2	C24H24O10	34.4	42.4	-23.3
	5.31	385.0915	(TPA-DEG)2+H2O	Fragment of 425.0843 m/z C20H18O9	21.9	12.9	41.1
	6.11	577.1339	(TPA-EG)3+H2O	Fragment of 617.1263 m/z C30H26O1	18.2	10.8	40.7
	5.98	661.1533	TPA3-EG2-DEG+H2O	C32H30O14	14.9	9.06	39.2
	6.82	469.1854	Cyclic NPG-TPA- NPG-TPA	C26H28O8		512	-

Inorganic Substances - To be completed on receipt of the delayed analysis report

Primary Aromatic Amines

Primary Aromatic Amines were not detected in the Input or Output samples.

No	Analyte	Name	CAS	LOQ (µg/Kg PET)	Sample pellets
1	p-PDA	*p*-Fenilendiamina	106-50-3	79.8	<LOQ
2	m-PDA	*m*- Fenilendiamina	108-45-2	79.8	<LOQ
3	2,6-TDA	2,6-Toluendiamina	823-40-5	14.6	<LOQ
4	4-M-m-PDA	4-Methoxy-*m*-phenylenediamine	615-05-4	14.6	<LOQ
5	2,4-TDA	2,4-Toluendiamina	95-80-7	14.6	<LOQ
6	1,5-DAN	1,5-Diaminonaftaleno	2243-62-1	16.5	<LOQ
7	ANL	Anilina	62-53-3	11.3	<LOQ
8	BNZ	Bencidina	92-87-5	41.3	<LOQ
9	o-ASD	*o*-Anisidina	90-04-0	99	<LOQ
10	4,4-DPE	4,4-Oxidianilina	101-80-4	20.1	<LOQ
11	o-T	o-Toluidina	95-53-4	33	<LOQ
12	4-CA	4-Cloroanilina	106-47-8	33	<LOQ
13	4,4-MDA	4,4-Metilenodianilina	101-77-9	21.5	<LOQ
14	o-diASD	*o*-Dianisidina	119-90-4	3	<LOQ
15	2-M-5-MA	2-Metoxi-5-m-toluidina	120-71-8	41.3	<LOQ
16	3,3-DMB	3,3-Dimetilbencidina	119-93-7	17.9	<LOQ
17	2,4-DMA	2,4-Dimetilanilina	87-62-7	3	<LOQ
18	4,4’-thioANL	4,4’-Tiodianilina	139-65-1	71.5	<LOQ
19	2,6-DMA	2,6-Dimetilanilina	95-68-1	3	<LOQ
20	2-NA	2-Naftilamina	91-59-8	7.7	<LOQ
21	4,4-MDoT	4,4-Metilenodi-*o*-toluidina	838-88-0	85.3	<LOQ
22	4-ABP	4-Aminobifenilo	92-67-1	41.3	<LOQ
23	4-AAB	4-Aminoazobenceno	60-09-3	17.3	<LOQ
24	5-N-o-T	5-Nitro-o-toluidina	99-55-8	5.8	<LOQ
25	1,4,5-TMA	2,4,5-Trimetilanilina	137-17-7	22	<LOQ
26	4-CT	4-Cloro-o-toluidina	95-69-2	63.3	<LOQ
27	AAT	o-Aminoazotolueno	97-56-3	5	<LOQ
28	3,3-DCB	3,3-Diclorobencidina	91-94-1	129.3	<LOQ
29	4,4-MCA	4,4-Metileno-bis-(2-cloroanilina)	101-14-4	4.4	<LOQ

Plastics Additives

Plastics Additives Indicated in the following table were not detected in the Input or Output Samples

Additives	CAS	LOD (µg/Kg PET)	Results Input & Output
Irgafos 168	31570-04-4	LOD=110	<LOQ
TopanolCA	1843-03-4	LOD=2750	<LOQ
Chimassorb 81	1843-05-6	LOD=113	<LOQ
Cyasorb UV 1084	14516-71-3	LOD=850	<LOQ
Tinuvin 326	05/11/3896	LOD=157	<LOQ
Irganox1010	6683-19-8	LOD=83	<LOQ
Tinuvin 327	01/09/3864	LOD=270	<LOQ
Irgafos 38	145650-60-8	LOD=570	<LOQ
Irganox 1076	2082-79-3	LOD=725	<LOQ
Tinuvin P	2440-22-4	LOD=2700	<LOQ
9,9-bis(methoxymethyl)fluorene	182121-12-6	LOD=75	<LOQ
N,N-Bis(2-hydroxyethyl)alkylamines (C12)	942-293-6	LOD=50	<LOQ
Erucamide	112-84-5	LOD=193	<LOQ
Bis(2-ethylhexyl) adipate	103-23-1	LOD=82	<LOQ
Tributylcitrate	77-94-1	LOD=105	<LOQ
Trybutyl o-acetylcitrate	77-90-7	LOD=75	<LOQ
TXIB (2,2,4- Trimethyl-1,3-pentanedioldiisobutyrate)	6846-50-0	LOD=2600	<LOQ
Bis(2-ethylhexyl) sebacate	122-62-3	LOD=52	<LOQ
NX8000	882073-43-0	LOD=1650	<LOQ

d) List of contaminating materials regularly present in the plastic input

Table 1 lists the contaminating materials regularly present in the plastic input.

Typical Residuals		
Property	Maximum	Units
PVC	50	mg/kg
Polyolefin (caps/labels)	20	mg/kg
Other Polymers	100	mg/kg
Metal	10	mg/kg
Other Inert Materials	30	mg/kg

Table 1. Contaminating materials regularly present in the plastic input.

e) Analysis of the most likely origin of the identified contaminants referred to in points (c) and (d).

Input material

Depending on the collection and sorting process, post-consumer PET waste can contain a limited amount of other polymers and materials such as polyolefins, polyvinyl Chloride (PVC), polyamide (PA), ethylene vinyl alcohol (EVOH), polystyrene (PS) and fillers. These polymers and materials originate from the following sources:

- Polyolefins like polyethylene (PE) and polypropylene (PP) are used to manufacture bottle closures and are present in a wide range of other plastic products.
- PVC is used in the manufacturing of certain labels and sleeves for bottles.
- PS is used in disposable cups and other packaging materials.
- EVOH is used as oxygen barrier in food packaging.
- PA is often used as barrier layer in flexible packaging films.
- Fillers are used in plastic packaging materials to modify their properties and enhance their performance.

The likely origin of the substances detected in the input material is as follows:

- Limonene: since a large fraction of PET bottles is used to pack flavoured beverages, the flavouring substance limonene is found in nearly all post-consumer PET waste streams (Franz *et al.*, 2004).
- Acetaldehyde: PET degradation product formed during injection moulding.

Output material

- Oligomers are generated during the PET Polymerisation Process.
- Acetaldehyde: PET degradation product formed during injection moulding

f) Measurement or estimation of the migration levels to food of contaminants present in the recycled plastic materials and articles.

Potential migration

Assuming worse case 100% of migration to food and considering that the average weight of PET of one litre PET bottle is 27.2g, the potential migration would be:

	Name	Formula	CAS	Output µg/kg PET	Potential Migration ug/Kg in food
SAMPLE 1	1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3	106-62-7	2170.85	59.05
	Dipropylene glycol	C6H14O3	110-98-5	2958.10	80.46
	1-Propanol, 2,2'oxybis-	C6H14O3	108-61-2	2525.77	68.70
	Nonanal	C9H18O	124-19-6	102.06	2.78
SAMPLE 2					
	Dodecanal	$C_{12}H_{24}O$	112-54-9	87.58	2.38
	1,3-Dioxolane, 2-methyl-	C4H8O2	497-26-7	1997.90	54.34
	Octanoic acid, ethyl ester	C10H20O2	106-32-1	44.69	1.22
	1-Undecanol	C11H24O	112-42-5	238.63	6.49
	Tetradecane	C14H30	629-59-4	46.90	1.28
SAMPLE 3	Ethanol, 2-(dodecyloxy)-	C14H30O2	4536-30-5	47.00	1.28
	Tetradecane	C14H30	629-59-4	87.84	2.39
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	6.14	0.17
	2-Propanol, 1,1'oxybis-	C6H14O3	110-98-5	2423.53	65.92
	Dipropylene glycol	C6H14O3	110-98-5	1528.43	41.57
	Dipropylene glycol	C6H14O3	110-98-5	2166.73	58.94
	7,9-Di-tert-butyl-oxaspiro(4,5)deca6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	82304-66-3	25.03	0.68
	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	57-10-3	10.00	0.27
SAMPLE 4	Dipropylene glycol	C6H14O3	110-98-5	1732.47	47.12
	Dipropylene glycol	C6H14O3	110-98-5	1199.75	32.63
	Dipropylene glycol	C6H14O3	110-98-5	1703.76	46.34
	1-Undecanol	C11H24O	112-42-5	53.40	1.45
	p-Benzoquinone, 2,6-di-tert-butyl-	C 14H20O2	719-22-2	69.11	1.88
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	64.81	1.76
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	C17H24O3	82304-66-3	4.82	0.13
	Dipropylene glycol	C6H14O3	110-98-5	5.43	0.15
SAMPLE 5	2-Propanol, 1,1'oxybis-	C6H14O3	110-98-5	8833.31	240.27
	Dipropylene glycol	C6H14O3	110-98-5	5489.31	149.31
	Dipropylene glycol	C6H14O3	110-98-5	6351.70	172.77
	Ethanol, 2-(dodecyloxy)	C14H30O2	4536-30-5	63.86	1.74
	Diisobutyl phthalate	C16H22O4	84-69-5	1.92	0.05
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	9.82	0.27
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	13.26	0.36

Migration levels continued

	Name	Formula	CAS	Output µg/kg PET	Potential Migration ug/Kg in food
SAMPLE 6	2-Butenal	C_4H_6O	123-73-9	5155.20	140.22
	Nonanal	$C_9H_{18}O$	124-19-6	1145.84	31.17
SAMPLE 7	Dodecanal	C12H24O	112-54-9	101.51	2.76
	Dipropylene glycol	C6H14O3	110-98-5	770.38	20.95
	Dipropylene glycol	C6H14O3	110-98-5	291.53	7.93
	Dipropylene glycol	C6H14O3	110-98-5	366.56	9.97
	Linalool	C10H18O	78-70-6	20.72	0.56
	α-Terpineol	C10H18O	98-55-5	37.32	1.02
	Benzenesulfonamide N-butyl-	C10H15NO2S	3622-84-2	1.00	0.03
SAMPLE 8	Benzyl alcohol	C_7H_8O	100-51-6	7.14	0.19
	Nonanal	C9H18O	124-19-6	116.08	3.16
	Decanal	C10H20O	112-31-2	78.40	2.13
	Ethanol, phenoxy-	C8H10O2	122-99-6	24.60	0.67
	Biphenyl	C12H10	92-52-4	4.03	0.11
	Diphenyl ether	C12H10O	101-84-8	8.13	0.22
	2,4-Di-ertbutylphenol	C14H22O	96-76-4	13.32	0.36
	Isopropyl myristate	C17H34O2	110-27-0	53.54	1.46
SAMPLE 9	Nonanal	C9H18O	124-19-6	71.19	1.94
	1-Undecanol	C11H24O	112-42-5	129.59	3.52
	Dodecanal	C12H24O	112-54-9	83.17	2.26
SAMPLE 10	2-Butenal, (Z)-	C_4H_6O	15798-64-8	1033.58	28.11
	2,4-Hexadiene, 2,5dimethyl-	C8H14	764-13-6	671.97	18.28
	2,4-Hexadiene, 3,4dimethyl-,	C8H14	2417-88-1	789.95	21.49
	Dipropylene glycol	C6H14O3	110-98-5	4765.67	129.63
	Dipropylene glycol	C6H14O3	110-98-5	3062.13	83.29
	Dipropylene glycol	C6H14O3	110-98-5	3609.89	98.19
	7,9-Di-tert-butyl-1oxaspiro(4,5)deca6,9-diene-2,8-dione	C17H24O3	82304-66-3	18.55	0.50
	2,5-di-tert-Butyl-1,4-benzoquinone	C14H20O2	2460-77-7	7.94	0.22

g) Description of the applied sampling strategy

Samples of input batches and their resultant output batches were collected. Samples were analysed for the following substances:

- Volatile substances,
- Semi-volatile substances,
- Non-volatile substances,
- Inorganic substances,
- Primary aromatic amines.

The analysis was carried out by an independent third-party analytical laboratory.

The Laboratory was chosen based on its experience and expertise in analysing PET samples and its relevant analytical equipment and validated methods.

h) Description of the analytical procedures and methods used.

Samples of PET input batches and corresponding output batches were labelled for traceability purposes and shipped in clear and hermetically sealed containers.

The analytical procedures and method used for the analysis of the samples as well as their limits of detection and quantification are summarised in Table 2.

Table 1. Applied analytical procedures and methods including their limits of detection and quantification.

	Analytical method	**Sample Preparation**	**LOD**	**LOQ**
Untargeted screening of volatile substances	HS-SPME-GC-MS 3min@80°C [a]			
Untargeted screening of semi-volatile substances	HS-SPME-GC-MS 3min@80°C [a]	Dissolution with HFIP		
untargeted screening of non-volatile substances	UPLC-MS-QTOF pos + neg mode [c]	Dissolution with HFIP		
Targeted analysis of primary aromatic amines	UPLC-MS-MS[d]	Extraction with 3% acetic acid		See table
Targeted analysis of inorganic substances (Annex II of EU 10/2011)	ICP-MS [e]	Pressure digestion		See table

GC: Gas chromatography; MS: Mass spectroscopy; QToF: Quadrupole- time-of-flight; FID: Flame Ionisation Detector; LC: liquid chromatography; UPLC: *ultrahigh performance LC;* ICP: Inductively Coupled Plasma

Analysis of organic substances is done through a non-targeted screening of volatile, semi-volatile and non-volatile substances with different methods (Table 2).

For volatile substances, a solid phase microextraction in headspace mode connected to GC-MS method (HS-SPME-GC-MS) is used which is a versatile technique employed in a wide range of industries and research areas to identify, quantify, and characterize volatile and semi-volatile compounds in plastic/polymer samples. The concentration of the volatile and semi volatile compounds on the SPME microfibre increases a lot the sensitivity of the method in such a way that a few ppbs (1-50 depends on the compound) can be detected for most of the volatile substances. The adsorption conditions for SPME of 3 mins@80°C specifically allow the exhaustive extraction of volatile substances present in PET without degrading the sample. The detection is done by MS and the mass spectra were compared with a mass spectra library (NIST or WYLEY).

For semi-volatile and non-volatile substance, the samples were first extracted. The solvent and extraction conditions have been chosen to swell the polymer, without generating new substances (Nerin *et al.*, 2022). The extracts were analysed using GC/MS and LC/MS-QToF for semi-volatile and non-volatile substances, respectively. High-resolution MS detectors like the QToF provide accurate masses isotopic patterns and intensities, which can lead to theoretical information about composition of fragments (Peters *et al*. 2019). This allows for the identification of unknown NIAS.

The application ranges of the above used non-targeted screening methods overlap but the sensitivity of the methods is different. In case the same substance was detected by different methods, the highest concentration of both analyses was reported in paragraph 4.

For the screening for primary aromatic amines a dedicated method was used as the concentration level of interest is so low that general non-target screening methods cannot detect them (Nerin *et al*., 2022).

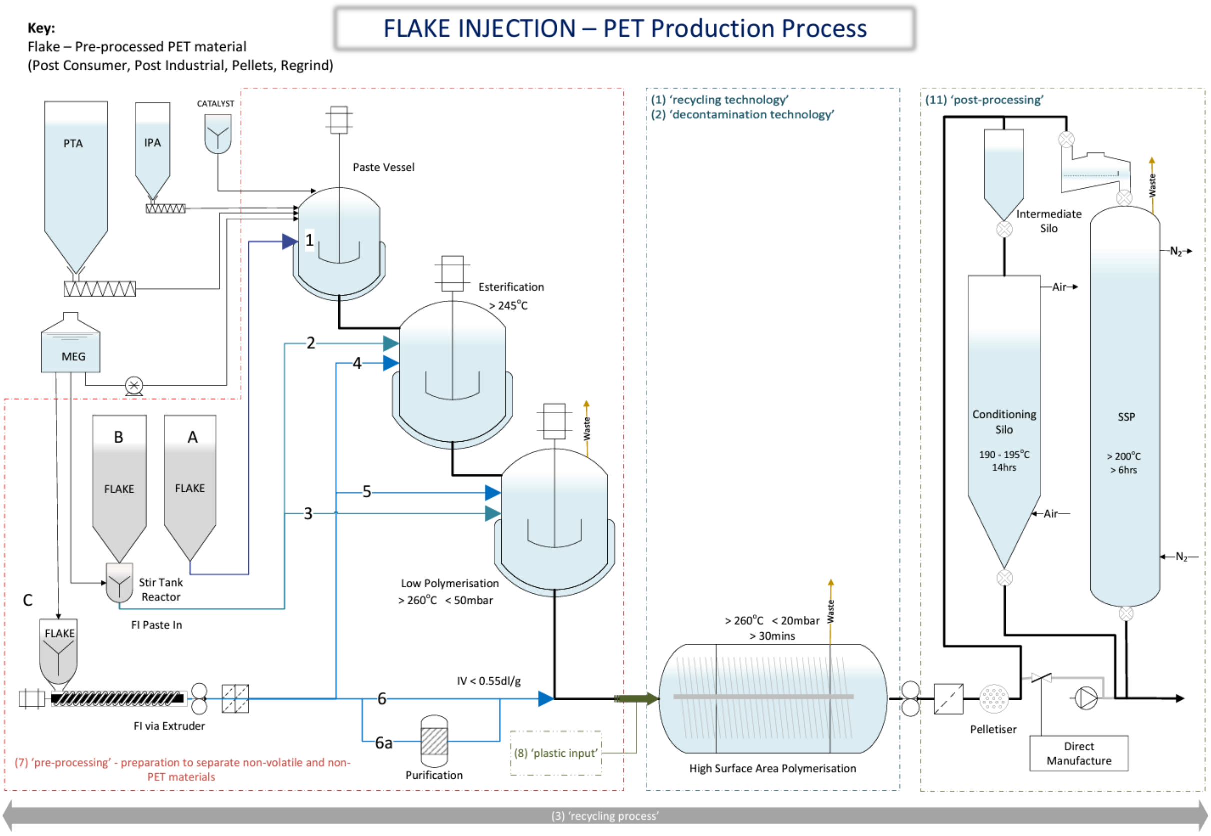
Inorganic substances were analysed using ICP-MS which is a sensitive elemental analysis technique that detects trace metals and non-metals at ultralow concentrations.

The Independent third-party laboratory follows ISO17025 quality control measures and all analytical methods are validated.

i) Analysis and explanation of any discrepancies observed between contaminant levels expected and decontamination efficiency.

No discrepancies have been observed between contaminant levels expected.

Appendix I –.



FLAKE INJECTION – PET Production Process
Key:
Flake – Pre-processed PET material
(Post Consumer, Post Industrial, Pellets, Regrind)
PTA
IPA
CATALYST
MEG
Paste Vessel
Esterification
> 245°C
Low Polymerisation
> 260°C < 50mbar
Waste
B
A
FLAKE
FLAKE
Stir Tank Reactor
FI Paste In
C
FLAKE
FI via Extruder
1
2
3
4
5
6
6a
IV < 0.55dl/g
Purification
(7) 'pre-processing' - preparation to separate non-volatile and non-PET materials
(8) 'plastic input'
(1) 'recycling technology'
(2) 'decontamination technology'
> 260°C < 20mbar
> 30mins
High Surface Area Polymerisation
(11) 'post-processing'
Intermediate Silo
Conditioning Silo
190 - 195°C
14hrs
Air
SSP
> 200°C
> 6hrs
N2
Pelletiser
Direct Manufacture
(3) 'recycling process'

Glossary of Terms

Cmod	Modelled concentration
DEG	diethylene glycol
EG	ethylene glycol
GC	gas chromatography
HPLC	high performance liquid chromatography
ICP-MS	Inductively Coupled Plasma Mass Spectrometry
ICP-AES	Inductively Coupled Plasma Atomic Emission Spectroscopy
IPA	isophthalic acid
MHET	mono(2-hydroxyethyl)terephthalate
MS	Mass Spectrometry
NIAS	non-intentionally added substances
PE	polyethylene
PET	polyethylene terephthalate
PP	polypropylene
PVC	polyvinyl chloride
TPA	terephthalic acid
TTC	Threshold of Toxicological Concern
XRF	X-ray fluorescence spectroscopy

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