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Characterization of a Polymeric Product (AAA) by Asahi Glass

Study director
(Question to:)

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Summary

Asahi Glass conducted a characterization of a polymeric product which substance name is AAA and TRP identification # for NOACK shipment is BBB according to the method described in this report. The result of the characterization is listed below.

Measurement	Units	Results AAA	Method	Comments
Weight % solids	%		Drying	
Mn (Number average molecular weight)	Da		SEC	
Mw (Weight average molecular weight)	Da		SEC	AK-225G/THF Solvent calibrated relative to PMMA
Molality of 8-2 alcohol in product	mol/kg		Calculated	calculated on the basis of specific polymer-recipe
Total organic fluorine (WT)	as percentage (%) as molality mol F/kg polymer as concentration g F/kg polymer		Combustion - ion chromatography	
Total inorganic fluoride	ppm (mg/kg)		ultrafiltration - ion chromatography	
Total carbon	as percentage (%)		Calculated	calculated on the basis of specific polymer-recipe
PFOA, C7F15COOH	ppm (mg/kg) mol/kg		LC/MS	Standard addition method
8-2 alcohol, C8F17C2H4OH				
MW 464.11				
C10H5F17O	ppm (mg/kg) mol/kg		GC	Absolute calibration method
8-2 acrylate, C8F17C2H4OCOCH=CH2				
518.16				
C13H7F17O2	ppm (mg/kg) mol/kg		GC	Absolute calibration method
8-2 ethyl iodide, C8F17C2H4I				
MW 574.01				
C10H4F17I	ppm (mg/kg) mol/kg		GC	Absolute calibration method
8-2 olefine, C8F17CH=CH2				
MW 446.10				
C10H3F17	ppm (mg/kg) mol/kg		GC	Absolute calibration method
C8 iodide, C8F17I				
MW545.95				
C8F17I	ppm (mg/kg) mol/kg		GC	Absolute calibration method
total sum of PFOA and total C8 precursors	mol/kg		Calculated	

1. Substance name and TRP Identification # (for Noack shipment) of the polymeric product

Substance name: AAA Lot. XXXX (TRP Identification #: BBB)

AAA Lot. XXXX was purified for biodegradation test and named AAA purified (TRP Identification #. CCC). The purification process and characterization of AAA purified were detailed in the report¹⁾.

2. Characterization of the polymeric product

2-1 Size exclusion chromatography (SEC)

SEC of the polymeric product for molecular weight analysis was conducted according to OECD guidelines^{2), 3)} and the result was shown in the previously submitted report¹⁾ inclusive of the comparison with the purified polymer. Here the analytical method and result are omitted except for the isolation and preparation of the polymer from the product.

2-1-1 Isolation of the polymer from the product

At first, the polymeric product was shaken well for homogenization. 1 ml of the polymeric product and 5 ml of isopropanol was mixed in a centrifuge tube and shaken well. The precipitated polymer was separated by centrifugation (6,000 rpm, 10 min) and following decantation. The precipitate was then dried in vacuum condition for 20 hours in room temperature. The isolated polymer was dissolved in the mobile phase by 0.75 wt% by shaking for several minutes and stand for overnight. The solubility of the polymer was sufficient: no precipitation or insoluble fraction was observed and the solution looks completely transparent.

2-2 Determination of PFOA in the polymeric product

The method validation and determination in this section was conducted according to the Attachment 1 of this report.

2-2-1 Test and control substances

The test substance, perfluorooctanoic acid (PFOA, 98.9 %, lot. C17001401), and the surrogate standard, 9-hydrohexadecafluorononanoic acid (9H-PFNA, 97.8%, lot. C58002501), were purchased from Daikin Fine Chemical (Osaka, Japan). Distilled water was produced in-house and checked for contaminants by LC/MS before use. Distilled water was filtered through a pre-column, Preclean-ORG (GL Sciences Inc. (Tokyo, Japan)) placed between HPLC pump and auto-sampler. HPLC grade methanol (MeOH), reagent grade ethanol (EtOH) and isopropanol (IPA), and reagent grade ammonium acetate were purchased from Kanto Chemical Co., Inc.

In order to avoid contamination, disposable lab ware (tubes, pipettes, etc) was used. 2 mmol/L ammonium acetate solution was prepared by weighing 154 mg of ammonium acetate and dissolving in 1 L of distilled water.

2-2-2 Preparation of fortification standards

50 µg/ml and 100 µg/ml PFOA solution was prepared using a solvent (2 / 8 (wt) mixture of distilled water / ethanol). 10 mg/ml 8-2 alcohol solution was prepared using isopropanol (IPA) for solvent for the use of latter section (2-3).

2-2-3 Preparation of a surrogate standard

100 ng/ml 9H-PFNA solution was prepared using a solvent (1 / 1 (wt) mixture of distilled water / ethanol).

2-2-4 Preparation of calibration standards

0, 0.1, 0.2, 0.4 ml of the 100 µg/ml PFOA solution was diluted by IPA up to 5 ml. 100 µl of the each solution and 9ml of 100 ng/ml 9H-PFNA solution was mixed in a vial. About 1 ml of each solution was filtered through a 0.2 µm filter, Millex-LG (MILLIPORE, U.S.A), into an auto-sampler vial and injected twice into LC/MS conditioned as follows.

2-2-5 Extraction of PFOA from the polymeric product

Before the sampling of the polymeric product they were shaken well without generating bubbles to homogenize the polymeric product. 1 ml of the polymeric product was put in each of four centrifugation vials. Fortification of PFOA and 8-2 alcohol were conducted as listed in Table 1. Fortification of 8-2 alcohol was conducted for the use of latter section (2-3). IPA was added into all vials until total amount with fortification solution was 5 ml. After putting a lid, each of five vials (with the blank) was shaken vigorously and the precipitation was separated by centrifugation at 6000 rpm for 10 minutes. About 3 ml of each supernatant was dealt out for 8-2 alcohol determination by GC.

100 µl of the each supernatant and 9ml of 100 ng/ml 9H-PFNA solution was mixed in a vial. About 1 ml of each solution was filtered through the 0.2 µm filter into an auto-sampler vial and injected into LC/MS conditioned as follows. These procedures were repeated once again for the verification of the reproducibility.

Table 1 Fortification of C8 precursors and PFOA

Sample	Fortification	
	10 mg/ml 8-2 alcohol	PFOA
A	0 µl	0 µl
B	50 µl	100 µl X 50 µg/ml
C	100 µl	100 µl X 100 µg/ml
D	200 µl	200 µl X 100 µg/ml

2-2-6 LC/MS analysis

LC/MS analysis was conducted with the conditions listed below.

<Instruments>

(1) LC/MS

HPLC

Agilent Technologies, Model 1100

Mass spectrometer

Agilent Technologies, Model 1100MSD (SL)

(2) LC column

Imtakt (Tokyo, Japan), cadenza CD-C18 2 mm (diameter) X 100 mm

(3) PC

Hewlett Packard Kayak PC Workstation OS: MS-Windows NT 4.0

(4) Software

LC/MSD ChemStation, Rev. A. 08. 03

(5) LC/MS vial

2ml vial for auto-sampler, Chromatography-Convenience 400-C80, Tomsic (Tokyo, Japan)

<Analytical conditions>

(1) Column temp.

35 °C

(2) Mobile phase

A: 2 mmol/L ammonium acetate

B: Methanol

(3) Gradient condition

time/min 0 → 2 → 5 → 15 → 15.01 → 25

B/% 57 → 57 → 100 → 100 → 57 → 57

(4) Flow rate

0.3 mL/min

(5) Injection volume

5 µL

(6) Retention time

PFOA (4.3 min), 9H-PFNA (2.5 min)

<MS operating parameters>

(1) Ionization mode

Electrospray (ESI) (negative ion mode)

(2) Fragmentor voltage

100 V

(3) Ion monitored

 $m/z = 413$ ($C_7F_{15}COO^-$), 445 ($CF_2H(CF_2)_7COO^-$)

(4) Desolvation temperature

350 °C

(5) Nebulizer gas

 N_2

(6) Desolvation

 N_2 12 L/min2-2-7 Results

Two calibration curves for standard addition method are plotted and shown in Fig. 1 for the ratio of (peak area of $m/z = 413$) / (peak area of $m/z = 445$) as a vertical axis against the amount of PFOA fortification (μg) as a horizontal axis. The coefficients of correlation are more than 0.9990 for both curves, and the amounts of PFOA determined in the polymeric product are (CBI) ppm and (CBI) ppm (average (CBI) ppm). (CBI) ppm is equivalent to (CBI) mol/kg (specific gravity of AAA is (CBI)).

Two calibration curves for PFOA calibration standards are shown in Fig. 2 for the same axis with Fig. 1. PFOA is not detected (zero count) for 0 μg standard (blank). The coefficients of correlation are more than 0.9995, and the recovery defined as (the slope for the standard addition) / (the slope for the

calibration standards) was 95%. All the linearity of the calibration curve, reproducibility of the result, and recovery satisfied the criteria stipulated in the attachment 1.

(CBI)

(CBI)

Fig. 1 Calibration curves for AAA
by standard addition method

Fig. 2 Calibration curves for PFOA
calibration standards

2-3 Determination of 8-2 alcohol and C8 precursors in the polymeric product

The method validation and determination was conducted according to the Attachment 1 of this report for 8-2 alcohol. C8 precursors other than 8-2 alcohol were determined by absolute calibration method using 4 calibration standards, and not evaluated by standard addition method.

2-3-1 Test and control substances

The test substances used in this section are listed in Table 2. These substances were used without further purification process.

Table 2 The test substances used in 2-3

Standards	Origin	Purity by GC
8-2 alcohol	Reagent grade, purchased from Daikin fine chemical (A-1820 lot. A18202601)	
8-2 acrylate	Received from Seimi Chemical Co., Ltd. (Kanagawa, JAPAN)	99.71 (FID area)%
8-2 olefin	Prepared in-house	99.75 (FID area)%
C8 ethyl iodide	Reagent grade, purchased from Daikin fine chemical (I-1820 lot. I18200Z01)	
C8 iodide	Prepared in-house	89.77 (FID area)%

2-3-2 Preparation of fortification and calibration standards

Mixture solutions of 8-2 alcohol and C8 precursors were prepared using IPA as a solvent as listed in Table 3.

Table 3 Preparation of 8-2 alcohol and C8 precursor standard solutions

Standard	μg/ml IPA solution				
	8-2 alcohol	8-2 acrylate	8-2 olefin	C8 ethyl iodide	C8 iodide
A	10	10	10	10	1
B	50	50	50	50	5
C	500	500	500	500	50
D	3000	3000	3000	3000	300

2-3-3 Extraction of C8 precursors from the polymeric product

Extraction procedures of 8-2 alcohol and C8 precursors are explained in 2-2-5.

2-3-4 GC analysis

GC analysis was conducted with the conditions listed below.

<Instruments>

(1) GC/MS

GC HP 5890 series II with auto-injector

Integrator HP 3396C

(2) GC column (CBI)

(5) Auto-sampler vial 2ml vial for auto-sampler, Chromatography-Convenience 400-C80, Tomsic (Tokyo, Japan)

<Analytical conditions>

(1) Injector temp. 220 °C

(2) Oven temp. 40 °C (2 min) → 10 °C/min → 170 °C (0 min) → 30 °C/min
→ 250 °C (10 min)

(3) Transfer line temp. 250 °C

(4) Column top pressure 15 psi constant

(5) Split flow 50 ml/min

(6) Injection volume 1 µl

(7) Carrier gas He (>99.99%)

(8) Retention time (Rt, min)

Rt: 12.2 min (8-2 alcohol)

Rt: 14.4 min (8-2 acrylate)

Rt: 5.4 min (8-2 olefin)

Rt: 13.0 min (C8 ethyl iodide)

Rt: 7.4 min (C8 iodide)

2-3-5 Results

Calibration curves for determination of 8-2 alcohol in AAA by standard addition method are plotted and shown in Fig. 3. Two curves from different runs, which include the different pretreatment runs, are reproducible. Surrogate standard is not used in this section, therefore, the vertical axis is for GC FID peak area (%) and the horizontal axis is for the amount (µg) of 8-2 alcohol fortified to the 1ml polymeric product.

Three calibration curves for 8-2 alcohol calibration standards are shown in Fig. 4 for the equivalent axis with Fig. 3. That is, the horizontal axis of Fig. 4 shows the amount in 5ml IPA, which is equal to the amount in 1ml polymeric product supposing that the recovery is 100%. In the same way, calibration curves for calibration standards for C8 precursors are shown in Figs. 5-8.

The results are arranged in Table 4. All the reproducibility and recovery satisfied the criteria provided in the Attachment 1.

(CBI)

Fig. 3 Calibration curves of 8-2 alcohol by standard addition method

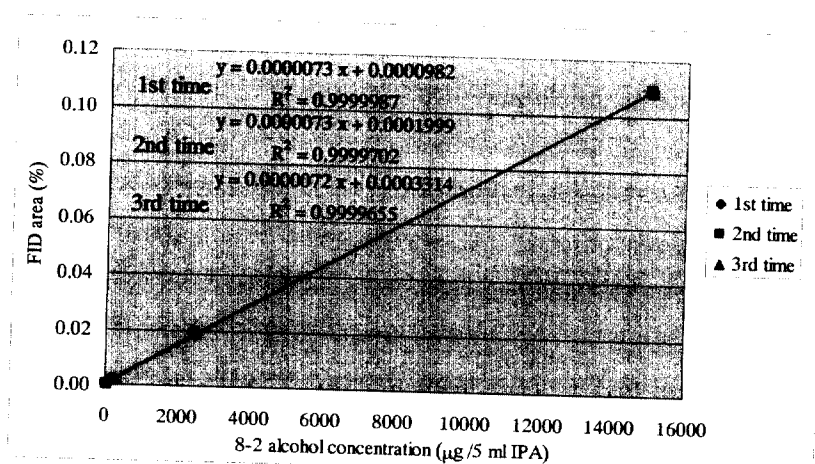


Fig. 4 Calibration curves of 8-2 alcohol calibration standards

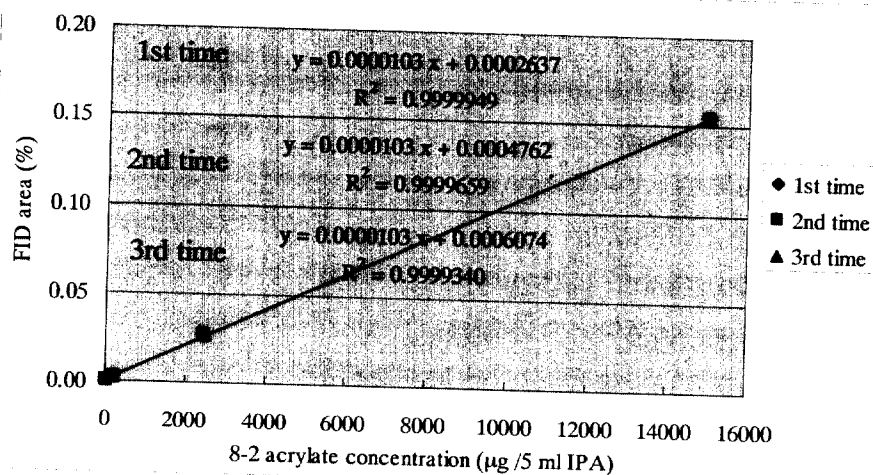


Fig. 5 Calibration curves of 8-2 acrylate calibration standards

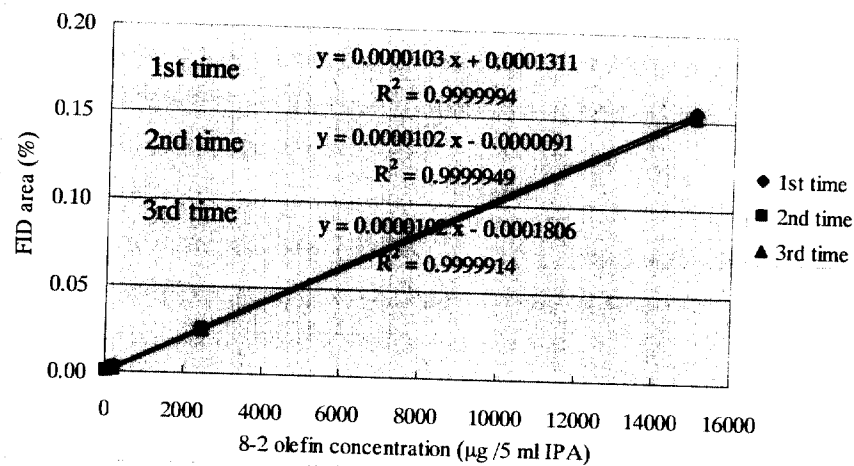


Fig. 6 Calibration curves of 8-2 olefin calibration standards

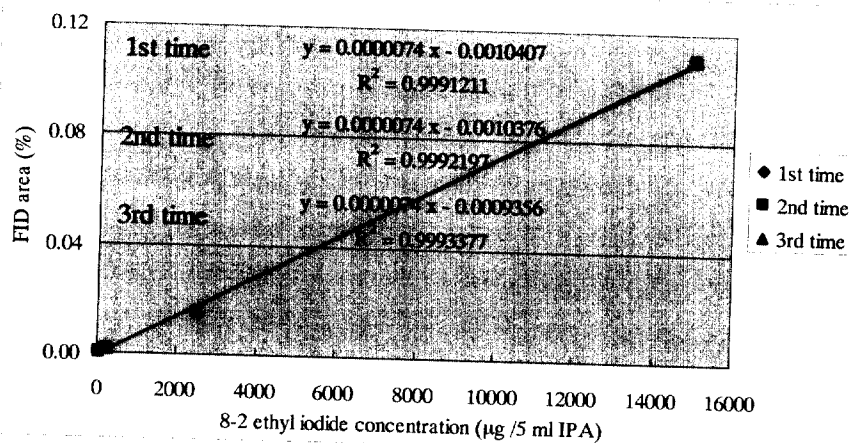


Fig. 7 Calibration curves of 8-2 ethyl iodide calibration standards

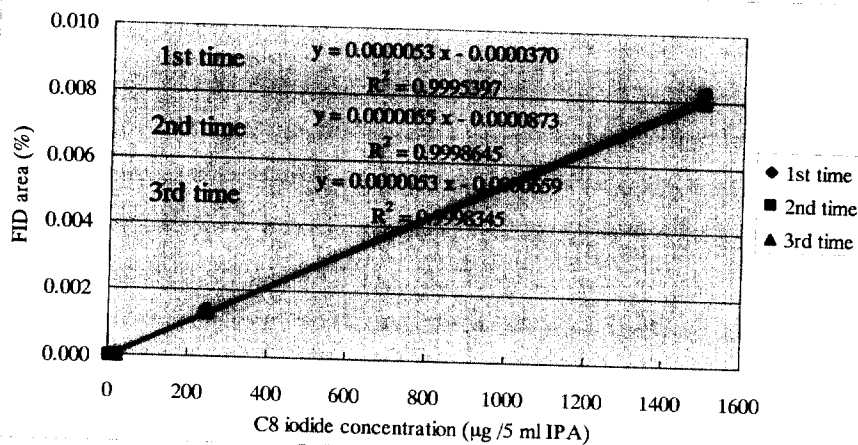


Fig. 8 Calibration curves of C8 iodide calibration standards

Table 4 Result of determination for 8-2 alcohol and C8 precursors

Component	run	8-2 alcohol	8-2 acrylate	8-2 olefin	C8 ethyl iodide	C8 iodide
Retention time (min)						
Molecular weight (g/mol)						
Absolute calibration method (ppm)	1					
average (ppm)	2					
average (mol/kg)						
Standard addition method (ppm)	1					
	2					
Recovery (%)	1					
	2					

2-4 Weight % solids

Before the analysis, weighing bottles were dried in a oven set at 120 °C for more than 30 minutes and left for cooling in a desiccator for 15 minutes. About 1 g of polymeric product was weighed precisely into a weighing bottle after mixing well. This bottle was put in the oven for 4 hours, and after that left in a desiccator for 15 minutes. The weighing bottle was weighed and the solid content was calculated. The result was (CBI)%.

2-5 Determination of total inorganic fluoride

Total inorganic fluoride, the amount of fluoride containing in the polymeric product without such treatment as combustion, is determined by ultrafiltration of the polymeric product and subsequent determination using ion chromatography. At first, 2 ml of the polymeric product was filtered using ultrafiltration membrane. After filtration, 1 ml of the polymeric product (containing practically no polymer) was diluted by 4 ml of distilled water and injected into an ion chromatograph conditioned below.

2-5-1 Apparatus and conditions

<Ultrafiltration>

Membrane	ADVANTEC	Ultra Filter Unit USY-1
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<Ion Chromatography>

Ion chromatograph	Dionex DX-500
Column	Ionpack AG11HC x 2
Mobile phase	KOH aq
Flow rate	1.0 ml/min
Gradient condition	time/min 0 → 5 → 7 → 17 → 20 → 30 B/mM 2 → 2 → 60 → 60 → 2 → 2
Injection volume	50 μ L
Suppressor	ASRS
Detector	Conductive Detector

2-5-2 Procedure of determination

Absolute calibration curve of fluoride was generated for calibration standards consist of potassium fluoride. Fluoride content of the polymeric product was determined using this calibration curve by absolute calibration method.

2-5-3 Result

Fluoride was determined to (CBI) ppm in AAA.

2-6 Determination of total organic fluorine (TOF)

TOF was obtained by combustion-pyrohydrolysis, fluoride trap into aqueous alkaline, followed by determination by ion chromatography. At first, about 20 mg of the polymeric product was heated on a hot plate set at 120 °C for 30 minutes. Then, known amount (2~3 mg) of the polymeric product was introduced into a combustion-F ion analyzer conditioned below.

< Apparatus and conditions >

Instrument (CBI)

Combustion conditions

(CBI)

Ion chromatography conditions

Column	Ionpack AG12+AS12 (Dionex)
Mobile phase	2.7mM Na ₂ CO ₃ + 0.3 mM-NaHCO ₃
Injection volume	10 µL
Suppressor	ASRS
Detector	Conductive Detector

<Procedure of determination>

Calibration curve of fluoride was generated using an ion chromatography for calibration standards consist of potassium fluoride. TOF of standard poly(tetrafluoroethylene) (PTFE, prepared in-house) was obtained and compared with the theoretical value of 76 wt%. TOF of the polymeric product were determined using the calibration curve by absolute calibration method and corrected by the recovery of standard PTFE.

<Result>

TOF of standard PTFE was 71.1%. Therefore the recovery of the combustion was calculated to 93.5%. TOF of AAA was (CBI)% and corrected to (CBI)% using the recovery of standard PTFE. TOF calculated from the composition of the polymeric product (theoretical amount) were (CBI)%. Empirical and theoretical values were in good agreement for the polymeric product.

2-7 Calculation of total carbon

Total carbon in the polymeric product is estimated by calculation based on the sample calculation of Attachment 2. Carbon content is calculated to (CBI) %.

2-8 Calculation of Molality of 8-2 alcohol

Molality of 8-2 alcohol in the polymeric product is estimated by calculation based on the sample calculation of Attachment 3. Molality of 8-2 alcohol is calculated to (CBI) mol/kg.

3. References

- ¹⁾ Purification and characterization of purified Telomer polymer by Asahi Glass, submitted to EPA on May 07, 2004, contains TSCA CBI
- ²⁾ OECD guidelines 118 ("Determination of the Number-Average Molecular Weight and the Molecular Weight Distribution of Polymers using Gel Permeation Chromatography")
- ³⁾ OECD guidelines 119 ("Determination of Low Molecular Weight Content of a Polymer using Gel Permeation Chromatography")
- ⁴⁾ Isemura, T. et. al.; J. Chromatogr., Vol 1026/1-2, pp 109-116 (2004)

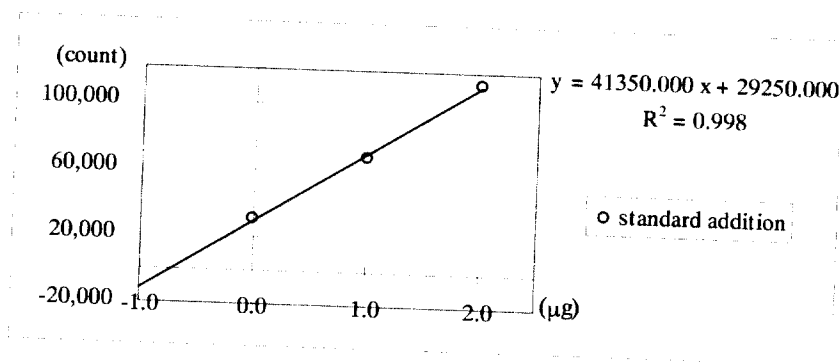
Attachment 1 – Validation Example

A simple validation method to determine PFOA in the purified polymer is proposed. Equivalent method can be employed for the determination of C8 precursors and for the determination of PFOA and C8 precursors in polymer products.

Standard addition method to determine PFOA in the purified polymer

- a. Known amount of PFOA ($p \cdot q$) mg is added to the purified polymer by addition of p ml of q mg/ml PFOA ethanol solution. A zero addition sample and two samples containing varied concentrations should be prepared (three concentrations in all). The amount of the addition should be in the range of 0 - 5 times of expected amount in the purified polymer.
- b. For example, if 1 ppm PFOA is expected in the purified polymer, 0.0, 1.0, 2.0 μ g PFOA is added to the 1 g purified polymer.
- c. PFOA is extracted by ROH (MeOH or EtOH) addition, ultrasonication, and centrifugal separation. Soxhlet extraction by ROH may also be available. Final volumes for all samples must be identical.
- d. Extracted ROH is introduced into the LC/MS(/MS) after the dilution if necessary. Dilution solvent may contain water to prevent band broadening in the HPLC column. Internal standard may be added into the extracted solution for the compensation of the fluctuation of injection volume and MS sensitivity.
- e. The standard addition calibration curve is plotted against the added PFOA weight. The vertical axis is PFOA area (count) or (PFOA area (count)) / (internal standard area (count)).
- f. If the calibration curve ($a \cdot x + b$) satisfied the criteria of $R^2 > 0.99$, it is valid.
- g. PFOA content is obtained from the calibration curve where PFOA content = b/a or y-intercept.
- h. Example calculations are shown below.

PFOA added to the 1g purified polymer	PFOA concentration after extraction and dilution based on 100 % recovery	PFOA area
μg	$\mu\text{g/ml}$	count
0.0	0.00	30,300
1.0	0.02	68,500
2.0	0.04	113,000



$$\text{PFOA content} = 0.71 \mu\text{g/g} = 0.71 \text{ ppm}$$

Reproducibility of the method and homogeneity of the purified polymer

a-g is repeated once more (2 times in all) for subsamples of the same purified polymer.

If the two PFOA values are within the 15% of their average value, both the reproducibility of the method and homogeneity of the purified polymer are sufficient, and the PFOA value is the average value.

Recovery criteria - Calibration curve for the standards

Four concentrations of PFOA solutions containing a solvent blank (not extracted solution but pure standard solutions) are injected into LC/MS. The composition of ROH and water in the solvent should be identical with that injected in the standard addition method (d). Internal standard should be added by similar method. The concentration range should be equivalent to the standard addition range conducted in (a). The PFOA should not be detected or less than 20% of the count of the lowest standard concentration for the solvent blank. The calibration curve for the standards is plotted.

If the calibration curve ($c \cdot x + d$) satisfied the criteria of $R^2 > 0.99$, it is valid.

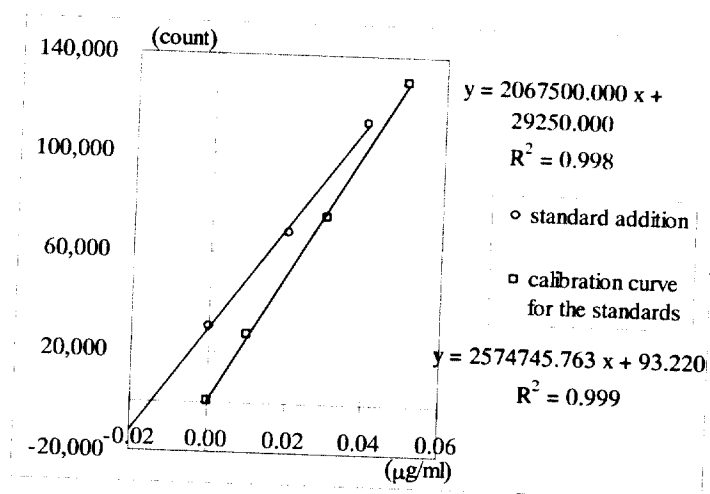
Recovery is defined as (the slope for the standard addition) / (the slope for the standards).

If the recovery satisfied the criteria of 70-120%, it is valid.

Example calculations are shown below.

<Calibration curve for the standards>

PFOA concentration	PFOA area
$\mu\text{g/ml}$	count
0.00	100
0.01	27,000
0.03	75,000
0.05	130,000



$$\text{Recovery: } \frac{2067500}{2574746} = 0.80 = 80\%$$

Recovery is affected by both the matrix effect and extract efficiency.

Recovery does not mean the value (PFOA determined) / (amount of PFOA in the purified polymers), but the value (PFOA recovered) / (PFOA added into the purified polymers). The recovery based on the former definition is practically impossible to obtain because all PFOA in the purified polymers must be extracted. Generally, the recovery is determined based on latter definition.

Example method details

The amount of the purified polymer: 1g

Expected PFOA in the purified polymer: 1ppm

<Standard addition method>

- 1 0.00, 0.10, 0.20 ml of 0.01 mg/ml PFOA EtOH solution is added to the 1 g purified polymer.
- 2 4.80 - 5.00 ml EtOH is added to the each polymer (total 5 ml EtOH)
- 3 PFOA is extracted by ultrasonication and centrifugal separation.
- 4 0.1 ml of extracted ROH is taken out into a vial and 0.9 ml of (EtOH:water = 1:1 (wt)) is added and mixed well.
- 5 The mixture is introduced into the LC/MS(/MS).
- 6 The standard addition calibration curve is plotted against (PFOA weight added) / 1g. The vertical axis is PFOA area (count).

<Calibration curve for the standards>

- 7 0.00, 0.01, 0.03, 0.05 $\mu\text{g/ml}$ PFOA (EtOH:water = 1:1 (wt)) solutions (not extracted solution but pure standard solutions) are injected into LC/MS(/MS).
- 8 The calibration curve is plotted.
- 9 On the same graph, standard addition curve is plotted by PFOA concentration for the extracted and diluted solution as horizontal axis.
- 10 If the "recovery" is 100 %, the slopes of two calibration curves are expected to be identical.

Attachment 2 –Example Calculations of Carbon Content

The example is based on the estimation that the purified polymer is based on e.g. 4 different monomers used in the following weight percent

60%	$\text{RfC}_2\text{H}_4\text{OCOCH}=\text{CH}_2$ (the Rf chain distribution average may be equivalent for C_9F_{19})
35%	$\text{C}_{18}\text{H}_{37}\text{OCOCH}=\text{CH}_2$
2.5%	$\text{HOC}_2\text{H}_4\text{OCOC}(\text{CH}_3)=\text{CH}_2$
2.5%	$\text{HOCH}_2\text{NHCOC}(\text{CH}_3)=\text{CH}_2$

Monomer type	Formula	MW [g/mol]	C-content [%]
$\text{Rf}(=\text{C}_9\text{F}_{19})\text{C}_2\text{H}_4\text{OCOCH}=\text{CH}_2$	$\text{C}_{14}\text{F}_{19}\text{H}_7\text{O}_2$	568,2	29,6
$\text{C}_{18}\text{H}_{37}\text{OCOCH}=\text{CH}_2$	$\text{C}_{21}\text{H}_{40}\text{O}_2$	324,5	77,2
$\text{HOC}_2\text{H}_4\text{OCOC}(\text{CH}_3)=\text{CH}_2$	$\text{C}_6\text{H}_{10}\text{O}_3$	130,1	55,4
$\text{HOCH}_2\text{NHCOC}(\text{CH}_3)=\text{CH}_2$	$\text{C}_5\text{H}_9\text{NO}_2$	115,1	52,2

On that basis the C-content of such a polymer will be

17.76% ($29.6 \times 0,6$) for $\text{RfC}_2\text{H}_4\text{OCOCH}=\text{CH}_2$ (for Rf-average C_9F_{19})

27.02% ($77.2 \times 0,35$) for $\text{C}_{18}\text{H}_{37}\text{OCOCH}=\text{CH}_2$

1.385% ($55.4 \times 0,025$) for $\text{HOC}_2\text{H}_4\text{OCOC}(\text{CH}_3)=\text{CH}_2$

1.305% ($52.2 \times 0,025$) for $\text{HOCH}_2\text{NHCOC}(\text{CH}_3)=\text{CH}_2$

47.47% Sum

The carbon content in such a polymer will be approximately 47.5%.

Attachment 3 – Example Calculations of Molality of 8-2 TB alcohol in polymer

In order to compare the 8-2 TBA content in the different polymer types in addition to a mass based approach (e.g. 8-2 TBA/kg polymer) the content of 8-2 TBA also is needed on a molar basis (moles of 8-2 TBA/kg polymer). The 8-2 TBA content on a molecular basis will also allow a correct interpretation of the test results with respect to the potentially formed transformation products that have different molecular weights in comparison to 8-2 TBA.

In table 1, an example calculation is given for a pure 8-2 acrylate homopolymer.

Table 1.

No.	Description	Values	Remarks
1	8-2 TB Alcohol (MW)	464.11 g/mol	
2	8-2 acrylate (MW)	518.16 g/mol	
3	Repeating group in homopolymer (MW)	518.16 g/mol	= 8-2 acrylate
4	Molality of homopolymer	1.93 mol/Kg	[1000]/518.16 mol/Kg
5	Molality of 8-2 TB Alcohol in homopolymer	1.93 mol/Kg	
6	Concentration of 8-2 TB Alcohol in homopolymer	896 g/Kg	[1]*[5]
7	Mass fraction of 8-2 TB Alcohol in polymer	89.6 % w/w	[6]/10

In the table 2 an example calculation is given for an 8-2 acrylate co-polymer. The co-polymer's repeating group consists in this case of one molecule of 8-2 acrylate and two molecules of Methyl methacrylate.

Table 2.

No.	Description	Calculations	Remarks
1	8-2 TB Alcohol (MW)	464.11 g/mol	CAS No. 678-39-7
2	8-2 acrylate (MW)	518.16 g/mol	CAS No. 27905-45-9
3	Methyl methacrylate (MW)	100.12 g/mol	CAS No. 80-62-6
4	Repeating group in co-polymer (MW)	718.40 g/mol	[2] + 2*[3]
5	Molality of co-polymer	1.39 mol/Kg	[1000]/718.40 mol/Kg
6	Molality of 8-2 TB Alcohol in co-polymer	1.39 mol/Kg	
7	Conc. of 8-2 TB Alcohol in co-polymer	646 g/Kg	[1]*[6]
8	Mass fraction of 8-2 TB Alcohol in polymer	64.6 % w/w	[6]/10