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SOIL ADSORPTION

TEST SUBSTANCE

Identity: Perfluorooctanesulfonate; may also be referred to as PFOS or FC-95. (1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, potassium salt, CAS # 2795-39-3)

Remarks: The test substance is a white powder. Sample was re-crystalized from a production lot of FC-95. Purity determined to be 97.9% by LC/MS, ^{1}H-HMR, ^{19}F-NMR and elemental analyses techniques.

METHOD

Method: Based on OECD 106
GLP (Y/N): Yes
Year completed: 2001
Statistical methods: Statistical analysis and plotting of the data was done according to OECD Method 106 using Microsoft Excel.
Temperature: Room Temperature (19-30°C)
Stock and test solution preparation: The test concentrations and conditions were determined in a Preliminary experiment. For the definitive experiment, test solutions were made by diluting a stock solution of un-radiolabeled Perfluorooctanesulfonate to a final test substance concentration of approximately 0.5 mg/L in aqueous 0.01 M $CaCl_2$.

Soil Characteristics:

Soil Class	Clay	Loam	Clay Loam	Sandy Loam	River Sediment	Domestic Sludge
Source	Agvise Laboratories, Northwood, ND	Agvise Laboratories, Northwood, ND	Agvise Laboratories, Northwood, ND	Agvise Laboratories, Northwood, ND	Agvise Laboratories, Northwood, ND	NIST, from Denver, CO POTW
Lot Number	00-2407	00-2404	00-2405	99-2564	00-2046	2781
Physical Description	1.00 mm air-dried, 0-6" deep	1.00 mm air-dried, 0-6" deep	1.00 mm air-dried, 0-6" deep	1.00 mm air-dried, 0-6" deep	1.00 mm air-dried, 0-6" deep	200 mesh, oven-dried, sterilized
% Organic Carbon	2.6%	4.9%	2.6%	2.8%	1.3%	Not analyzed
% Sand	16%	39%	21%	58%	39%	Not analyzed
% Silt	22%	50%	46%	22%	42%	Not analyzed
% Clay	62%	11%	33%	20%	19%	Not analyzed
CEC (meq/100g)	54.5	23.9	24.7	23.3	17.5	Not analyzed
pH in 0.01 M $CaCl_2$	7.2	7.4	6.0	7.8[1]	7.7	Not analyzed

[1] Value is for pH in water not pH in 0.1M $CaCl_2$

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Test Conditions:

Adsorption Kinetics: Replicate study samples containing the soils (or sediments or sludges) were equilibrated by shaking for at least 12 hours at room temperature with 0.01 M $CaCl_2$. Study samples were dosed with the test substance at approximately 0.5 mg/L and placed on an orbital shaker. Replicate sets of these study samples were removed at designated time points throughout a 48 hour time period. Study samples were then prepared and analyzed for the target analyte. The adsorption kinetics were determined using this data. The last set of study samples (48 hour) were saved and used for the desorption kinetics portion of the method.

Desorption Kinetics (One concentration): After the adsorption kinetics experiment, the 48 hour study samples were centrifuged and the aqueous phase removed. The volume of solution removed was replaced by an equal volume of 0.01 M $CaCl_2$ without test substance. The new mixture was agitated until the desorption equilibrium was reached. During a 48-hour period, at defined time intervals, small aliquots of the aqueous phase were removed and analyzed for the target analyte. The desorption kinetics were determined using this data.

RESULTS

Adsorption Kinetics of PFOS, 1:5 Soil:Solution Ratio,
48 Hour Time Point

Soil Type	Average Distribution coefficient, K_d, L/g	Percentage of Organic Carbon in Soil	Average Organic Carbon normalized Adsorption Coefficient, K_{oc}, L/g
Clay	0.0183	2.6	70.4
Clay Loam	0.00972	2.6	37.4
Sandy Loam	0.0353	2.8	126
River Sediment	0.00742	1.3	57.1
Domestic Sludge	< 0.120	Not available	Not calculable

All matrices adsorbed the test substance strongly. The sludge demonstrated very strong adsorption (>96%) and PFOS was not detected in the extracts. The data indicate that adsorption occurred within the first few hours of exposure and the test substance concentration did not vary significantly after 16 hours.

Apparent Desorption Kinetics of PFOS, 1:5 Soil:Solution Ratio,
48 hour Time Point

Soil Type	Desorption Coefficient, K_{des}, L/g
Barnes Loam	0.0000471
Clay Loam	0.0000158
Clay	0.0000349
River Sediment	0.0000100
Domestic Sludge	< 0.000237

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The test substance was poorly desorbed from the soil/sediment/sludge matrices during the 48-hour study period. The river sediment displayed the most desorption at 39% after 48 hours. The sludge samples did not desorb a detectable amount of test substance. Desorption that did occur was accomplished rather quickly; after the 8 hour time point the test substance concentration did not vary significantly.

Adsorption Isotherms

Soil type	Log K^{ads}_F	K^{ads}_F (1)	Regression constant, 1/n	Regression Constant, n
Clay	-1.2515	0.0560	0.884	1.13
Clay Loam	-1.3762	0.0421	0.841	1.19
Sandy Loam	-1.0369	0.0919	0.829	1.21
River Sediment	-2.0261	0.0094	0.989	1.01
Domestic Sludge	-1.246	0.0568	1.2581	0.795

(1) Freundlich adsorption coefficient

. Desorption Isotherms

Soil Type	Log K^{des}_F	K^{des}_F (1)	Regression Constant, 1/n	Regression Constant, n
Clay	-0.653	0.222	0.935	1.07
Clay Loam	-1.084	0.082	0.954	1.05
Sandy Loam	-0.981	0.104	1.01	0.988
River Sediment	-1.41	0.039	1.02	0.984
Domestic Sludge	1.47	29.5	0.327	3.06

(1) Freundlich desorption coefficient

Freundlich adsorption isotherms relate the amount of test substance adsorbed on the soil to the amount present in the aqueous solution at equilibrium. The values calculated for the regression constant indicate that the data obtained for the test substance over two orders of magnitude is slightly non-linear.

CONCLUSIONS

Perfluorooctanesulfonate (PFOS) appeared to adsorb strongly to all of the soil/sediment/sludge matrices tested. PFOS would not be considered to be qualitatively mobile as per OECD Guideline106 (1/21/00) as the K_d values are > 1 mL/g. The test substance, once adsorbed, does not desorb readily, even when extracted with an organic solvent. In either case, adsorption or desorption, an equilibrium is achieved in less than 24 hours, with substantial adsorption (>50%) occurring in some of the time 0 samples after approximately 1-minute of contact. The test substance exhibited low mobility in all of the adsorbants tested.

The shape of the PFOS adsorption isotherm (H-type) indicates a very strong chemical/adsorbent interaction. Because PFOS is a strong acid, it likely forms strong bonds with soils, sludge and sediment via the mechanism of chemisorption.

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DATA QUALITY

Reliability: Klimisch ranking 1.

REFERENCES

3M Technical Report "Soil Adsorption/Desorption Study of Potassium Perfluorooctanesulfonate (PFOS)". Mark E. Ellefson, Project Number E00-1311, Final Report Completion Date June 4, 2001.

OTHER

Last Changed: June 27, 2001