

Transport between environmental compartments
(fugacity modeling) included in letter from Don Mackay
on the air/water partitioning coefficient calculations

TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY)

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-heptafluoro-, potassium salt, CAS # 2795-39-3)

Remarks: NA

METHOD

Test (test type): Fugacity Modeling

Method: Level I, II, and III EQC Computer Modeling

Year completed: 1999

Remarks field for Test Conditions: Modeling conducted by Don Mackay of D. Mackay Environmental Research Limited in Peterborough, Ontario Canada. The following parameters were used:

$$K_{aw} = 0^*$$

Soil/water partition coefficient (L/kg) = 2.4

Sediment/water partition coefficient (L/kg) = 4.8

Fish/water partition coefficient (dimensionless) = 1000

Degradation half life = 10 years

* See Air/Water Partition Coefficient Robust Summary

RESULTS

Level I results indicate the test substance, if released to water, has a tendency to remain in water (typically 80% would remain in water and 20% would partition to soil).

Level II results indicate the same conclusion as for Level I. Advection in water is predicted to be the dominant process for removal from the environment with degradation being very slow. The persistence in a region is estimated to be controlled by the water residence time.

Level III results indicate:

- 1) Discharges to air will result in rapid deposition to soil (90%) and water (10%)

- 2) Discharges to soil will tend to remain in the soil. Its low sorption tendency indicates the major removal pathway will be from run-off to water.
- 3) Discharges to water will tend to remain in the water and the dominant removal process (90%) will be through advective flow with little sorption to sediments.

CONCLUSIONS

Don Mackay writes:

"In summary, 'this substance' behaves much as one would expect of a strongly ionic compound."

"I believe it is important to measure real partition coefficients for inclusion in the model and perhaps refine the half lives."

These studies are considered a "small first step".

Submitter: 3M Company, Environmental Laboratory, P.O. Box 33331, St. Paul, Minnesota, 55133

DATA QUALITY

Reliability: Klimisch ranking 3. These studies are preliminary only. Further characterization of the necessary input values is needed before more definitive modeling can be conducted.

REFERENCES

Study summary letter from Don Mackay, D. Mackay Environmental Research Limited, 1664 Champlain Drive, Peterborough, Ontario, Canada K9L1N6

OTHER

Last changed: 4/30/00

DMER

D. Mackay Environmental Research Limited

1664 Champlain Drive
Peterborough, Ontario
Canada K9L 1N6
Tel (705) 740-2911
GST Reg. #R-101420263

3M991

To: Dr. Rich Purdy, 3M
Dr. Joyce Smith Cooper, Battelle

Dear Rich and Joyce:

I received the "Fluorochemical Fugacity Modeling Requirements" statement. It is generally in agreement with our expectations and we will do our best to satisfy your needs. The principal problem will, I suspect, be gathering the input data. We can keep in close contact with you regarding the model development.

We obtained from you the PFOS air-water partitioning data. As I interpret the lab results they established an initial concentration of 50 mg/L in 200 mL water then distilled off 10 mL aliquots and analysed the residue. They then calculated the percentage of the original PFOS present which remained in the beaker unevaporated. These "percent recoveries" ranged from 136 to 105 with no real trend. I conclude that the PFOS did not evaporate to any measurable extent. This is a very sensitive method of measuring low air-water partition coefficients. It can be shown that if water and the solute evaporate equally (i.e. the contents do not change in composition as would occur with an azeotrope) then K_{AW} or H is identical for water and the solute. For water H is approximately 2400 Pa (approximately 20°C) divided by 55000 mol/m³ or 0.044 Pa m³/mol or a K_{AW} of about 2×10^{-5} . PFOS must thus have a K_{AW} considerably less than this, i.e. less than 2×10^{-6} . It is thus essentially non-volatile from aqueous solution. This is probably because of its ionic nature. The simple expedient is to assign it a K_{AW} of zero, i.e. it is a type 2 involatile chemical in our nomenclature.

We did sample EQC model runs using a K_{AW} of zero, and partition coefficients L/kg for soil-water of 2.4, sediment-water of 4.8 and fish-water (dimensionless) of 1000. The dimensionless partition coefficients are higher by a factor corresponding to the density. The degradation half lives were all set at 10 years. I attach the Level I, II and III results.

The Level I results show that PFOS has a strong tendency to remain in water, i.e. typically 80% with 20% in soil.

The Level II results show an identical distribution. The major loss is by advection in water with

only very slow degradation. The overall persistence in a region is controlled by the water residence time.

The Level III results show that:-

If discharged to air it will rapidly deposit to soil (90%) and water (10%).

If discharged to soil it tends to remain there with the major loss being run-off to water because of its low sorption tendency.

If discharged to water it tends to remain in solution and is subject to removal by advective flow (90%).

There is little sorption to sediments.

In summary, it behaves much as one would expect of strongly ionic compound.

I believe it is important to measure real partition coefficients for inclusion in the model and perhaps refine the half lives. In the present regulatory climate a substance which is so persistent is going to come under very close scrutiny. I wonder if it is possible to build a degradation weakness into the molecule?

In conclusion, we are ready and willing to do modeling at your request. Please regard this as just a small first step.

Yours truly

A handwritten signature in dark ink, appearing to read 'Don', enclosed within a circular scribble.

Don Mackay

DM/mm