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VALIDATION OF TOXFATE, A CONTAMINANT FATE MODEL  
FOR A LARGE LAKE SYSTEM (LAKE ONTARIO)

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Executive Summary

A toxic contaminant FATE model, TOXFATE, has been used to predict the fate of four chlorobenzenes which have entered Lake Ontario from the Niagara River since 1909, they are: 1,2,4-trichlorobenzene (1,2,4-TCB), 1,2,3,4-tetrachlorobenzene (1,2,3,4-TeCB), penta- (QCB) and hexachlorobenzene (HCB). TOXFATE predicts concentrations in the water column and bottom sediments as well as volatilization, burial and transport rates. The mathematical model has been validated by comparing computed compartment masses of contaminants and process losses to those estimated from field data. Computed sedimentation, volatilization and transport rates to the St. Lawrence River agree with field estimated within a few percentage points. Simulation show that on average about 67% of HCB loadings and 73 to 89% of the other three chlorobenzenes are lost from the lake through volatilization; the model predicts that only 3% of the 1,2,4-TCB loadings remain in the bottom sediments while 13 to 29% of the other congeners do. Despite total chemical inputs to the lake of 15000 to 310000 kg, the water fraction in 1983 contains only a minute proportion, namely 60 to 800 kg for each chemical over the whole lake, resulting in very low water concentrations on the order of 0.1 ng/L or 0.1 ppt. The amount in fish is much lower, 6 kg for HCB and as little as 0.14 kg for 1,2,4-TCB in the whole lake.

# VALIDATION DU MODÈLE TOXFATE, QUI PERMET DE DÉTERMINER CE QU'IL ADVIENT DES CONTAMINANTS DANS UN GRAND SYSTÈME LACUSTRE (LAC ONTARIO)

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## Résumé administratif

On s'est servi du modèle TOXFATE, qui permet de déterminer la destination ultime des contaminants toxiques, pour prévoir celle de quatre chlorobenzènes que la rivière Niagara déverse dans le lac Ontario depuis 1909 : le 1,2,4-trichlorobenzène (1,2,4-TCB), le 1,2,3,4-tétrachlorobenzène (1,2,3,4-TeCB), le pentachlorobenzène (QCB) et l'hexachlorobenzène (HCB). À l'aide du modèle TOXFATE, on peut prévoir les concentrations d'un contaminant dans la colonne d'eau et dans les dépôts de fond, de même que les taux de volatilisation, d'enfouissement et de transport. Le modèle mathématique a été validé en comparant les masses de contaminants modélisées et les pertes attribuables à différents processus avec les valeurs estimées à partir de données réelles. Les taux modélisés de sédimentation, de volatilisation et de déversement dans le fleuve Saint-Laurent concordent avec les valeurs estimatives réelles à quelques points de pourcentage près. D'après les simulations, il semble qu'en moyenne, environ 67 p. 100 des charges de HCB et entre 73 p. 100 et 89 p. 100 des trois autres chlorobenzènes se dispersent par volatilisation. Le modèle prévoit également que seulement 3 p. 100 de la charge de 1,2,4-TCB se dépose dans les sédiments du fond tandis que la proportion des autres chlorobenzènes se situe entre 13 p. 100 et 29 p. 100. Malgré un apport total de contaminants toxiques de l'ordre de 15 000 à 310 000 kg, on n'a trouvé, en 1983, qu'une faible proportion de chaque produit chimique pour l'ensemble du lac, soit entre 60 et 800 kg. Par conséquent, les concentrations dans l'eau se sont révélées très faibles, soit 0,1 ng/L ou 0,1 ppm. Les quantités décelées dans les poissons étaient encore moindres, soit 6 kg de HCB et seulement 0,14 kg de 1,2,4-TCB pour l'ensemble du lac.

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## ABSTRACT

A TOXic contaminants FATE model, TOXFATE, has been used to predict the fate of four chlorobenzenes which have entered Lake Ontario from the Niagara River since 1909, they are: 1,2,4-trichlorobenzene (1,2,4-TCB), 1,2,3,4-tetrachlorobenzene (1,2,3,4-TeCB), penta- (QCB) and hexachlorobenzene (HCB). TOXFATE predicts concentrations in the water column and bottom sediments as well as volatilization, burial and transport rates. The mathematical model has been validated by comparing computed compartment masses of contaminants and process losses to those estimated from field data. Computed sedimentation, volatilization and transport rates to the St. Lawrence River agree with field estimates within a few percentage points. Simulations show that on average about 67% of HCB loadings and 73 to 89% of the other three chlorobenzenes are lost from the lake through volatilization; the model predicts that only 3% of 1,2,4-TCB loadings remain in the bottom sediments while 13 to 29% of the other congeners do. Despite total chemical inputs to the lake of 15000 to 310000 kg, the water fraction in 1983 contains only a minute proportion, namely 60 to 800 kg for each chemical over the whole lake, resulting in very low water concentrations on the order of 0.1 ng/L or 0.1 ppt. The amount in fish is much lower, 6 kg for HCB and as little as 0.14 kg for 1,2,4-TCB in the whole lake.

## INTRODUCTION

Lake Ontario, one of the Great Lakes of North America, receives large amounts of toxic contaminants from inflowing rivers and from the atmosphere (1). The problem of toxic contaminants is of particular concern since Lake Ontario is a source of freshwater to many towns along its shores, Kingston, Toronto, Hamilton, Rochester and Oswego, in addition to being a potentially rich source for commercial fishing. Unfortunately, the continuous inputs of various chemicals has lead to significant residue levels in fish (2).

Fate models have been proposed as tools to predict the fate of toxic contaminants. The spatial scales involved - the lake is 300 km long with a volume of  $10^{12}$  m<sup>3</sup> and wind driven currents transport a water mass ten times greater than the Niagara River flow ( $6000$  m<sup>3</sup>/s) (3) - make any modelling effort difficult; the physical transport plays an important role in determining the spatial distribution, fate and persistence. The contaminants may undergo a number of chemical transformations and changes of phases: they may be biodegraded, oxidized or photolyzed, they can move to the atmosphere by volatilization or be buried in the bottom sediments, they can leave the lake via the St. Lawrence River or bioaccumulate in the food chain. A mathematical model must take all these factors into consideration to produce an integrated and reliable prediction of a contaminant's fate.

TOXFATE, an organic TOXic contaminants FATE model, was developed (4) in 1983 for the specific purpose of modeling the fate of toxic contaminants in large lakes after a preliminary effort of using the EXAMS framework (5) was partially successful (6). In its present configuration (4,7) which includes the water circulation of Lake Ontario, TOXFATE describes and predicts the fate of a toxic contaminant which enters Lake Ontario from the Niagara River; the river receives large discharges from industries and leachings from dumps located along its shores and has been a source of contaminants to the lake

since the beginning of the century (8). TOXFATE has been developed and verified (4) by simulating the fate of nine toxic contaminants, some of which have been detected in the lake, such as mirex, lindane and pentachlorophenol; at the time, however, validation was not possible because of the lack of long term loadings and concentration data. From the analysis of a radiodated sediment core from Lake Ontario (8) and measurements of contaminant loadings to lake Ontario from 1981 to 1983 (9) we have been able to estimate past loadings of several contaminants to Lake Ontario from the Niagara River. In this paper the predictive ability of the model is tested and compared to field data for four chlorobenzenes. The model includes degradation processes but biodegradation and photolysis terms were set to zero since these processes are negligible for the studied chlorobenzenes.

#### PAST LOADINGS ESTIMATES

The approximate loadings of chlorinated contaminants to Lake Ontario from the Niagara River for the period 1981 to 1983 can be estimated using the weekly sampling data of Oliver and Nicol (9). During the course of that study, a sediment core was also collected, analyzed and dated using radiochemical methods (8). The major chlorinated compounds found in both of these studies were chlorobenzenes, or CB's, so we chose the four chemicals, hexachlorobenzene (HCB), pentachlorobenzene (QCB), 1,2,3,4-tetrachlorobenzene (1,2,3,4-TeCB), and 1,2,4-trichlorobenzene (1,2,4-TCB) to test and validate the model. In addition to their presence in all samples, these compounds span a fairly wide range of physical chemical properties.

Present loadings (1981-1983) and historical loadings (1909-1981) were estimated from the sediment core analysis (8) using the assumption that a constant percentage of incoming contaminants were sequestered to settling particulates, which became bottom sediments. For example, the 1,2,4-TCB

concentration in the 7 to 8 cm interval of the sediment core (1966-67) was approximately 3 times higher than in the surficial sediment (0 to 1 cm). Thus, loadings for this compound in 1966/67 were estimated to be 7400 kg per year, three times the measured 1981 to 1983 loadings of approximately 2400 kg per year. These year to year loadings estimates were used in the modeling exercise (Table 1) and these data compare well with the overall loadings estimates made by Oliver (10) and reported in Table 2. The laboratory studies of Karickhoff (11) have shown that at low concentrations, such as those observed in the river (ng/L), the sorption of hydrophobic pollutants by sediments is linear, reversible and characterized by a partition coefficient. Therefore, our assumption should be correct, but, since no historical records or concentrations of these contaminants in the river exist, we can not test our hypothesis.

#### LAKE ONTARIO DATA

Table 2 shows the model's computed masses of CB's in the various lake compartments as well as the computed percentage losses of chemicals due to sedimentation, volatilization and transportation (St. Lawrence River). The measured CB masses in the lake compartments from the field data by Oliver (10) are also listed in Table 2. In that study, the masses of CB's lost via the St. Lawrence River were estimated by analyzing two large volume water samples near the outflow of the lake. The CB's in suspended sediments were estimated by analyzing centrifuged material from three stations at two depths on one occasion. The CB's in lake biota were taken from the literature (12,13). Bottom sediments were sampled more extensively - one core from each of the major sedimentation basins (Niagara, Mississauga, Rochester) was analyzed in detail together with 15 surficial sediment samples from each of these basins

as well as three samples from the Kingston Basin to obtain the CB masses in lake bottom sediments (10).

Also included in Table 2 are estimates of the CB's associated with downfluxing material. Oliver and Charlton (14) measured the proportion of Niagara River contaminant input that was sedimenting in Lake Ontario using sediment traps over a six month period in 1982. This short term study yielded somewhat lower amounts of CB's sedimenting than Oliver's other study (10). The average suspended sediment concentration in the Niagara River over the trap deployment period was 5 mg/L, somewhat lower than values reported in other studies - 8.4 mg/L (15) and 22 mg/L (16). Higher suspended sediment concentrations in the river would tend to increase the percentage of CB's sedimenting to the lake bottom. In any case, considering the limited number of measurements in both field studies, the agreement between them can be considered fairly good.

The estimation of volatilization losses from the field data can be obtained by difference in two ways. The sum of the short term (May to November, 1982) downfluxing material (14) plus the amount of material lost via the St. Lawrence River (10) can be subtracted from the total loading to give volatilization: 1,2,4-TCB (96%), 1,2,3,4-TeCB (96%), QCB (93%) and HCB (80%). Volatilization losses calculated from long term bottom sediment masses (10) and the same losses via the St. Lawrence River (10) are somewhat different: 1,2,4-TCB (93%), 1,2,3,4-TeCB (93%), QCB (79%) and HCB (38%).

#### MODEL SIMULATIONS

The four chemicals represent a class of volatile contaminants that may remain in the lake temporarily or possibly be persistent: their final sink may be the atmosphere rather than the bottom sediments or the lake waters. The prediction of their fate would therefore be helpful in determining permissible

loadings and to find the maximum chemical load permissible to Lake Ontario before exceeding the limits set by the International Joint Commission. TOXFATE was used to predict their fate and to compute the percentage of the loadings that would be lost to the atmosphere or remain in the lake; a good agreement between predicted and observed processes and between predicted and observed mass balances would be considered a validation of the model, given the fact that the model was only allowed to see the estimated inputs and was not further tampered with. Resuspension rates from the bottom sediments were set at  $5 \text{ g m}^{-2} \text{ day}^{-1}$  (17); the chemical properties used in the model for 1,2,4-TCB, 1,2,3,4-TeCB, QCB and HCB were: molecular weight [amu] 181.5, 215.9, 250.3, 284.9; octanol-water partition coefficient,  $\log K_{ow}$ , 4.0, 4.5, 4.9, 5.5; water solubility [mole/L]  $1.7 \times 10^{-4}$ ,  $2 \times 10^{-5}$ ,  $2.2 \times 10^{-6}$ ,  $3.5 \times 10^{-8}$ ; vapour pressure at 20 C [torr] 0.42, 0.01,  $1.7 \times 10^{-3}$ ,  $1.1 \times 10^{-5}$ , respectively. The simulations were run from the period of 1909 to 1983 and took seven hours each on a CDC Cyber 171 computer.

#### Masses of contaminants in Lake Ontario

Table 2 shows the masses of the four chlorobenzenes in four lake compartments, water, suspended sediments, biota and bottom sediments. The agreement between Oliver's estimates (10) and the model's are quite good; masses are within a factor of two for bottom sediments and water and within a factor of three for suspended sediments and biota. Given the very low percentage of loadings that remains in the lake - 0.28 % and 0.40 % in the water compartment for 1,2,4-TCB and for HCB, respectively, and in suspended sediments 0.003 % and 0.03 %, respectively - the agreement is quite good, indeed any agreement within one order of magnitude would have been considered excellent, since the model was run blindly beginning at 1909 to obtain 1983 data. Similar good comparisons were obtained for the other contaminants (Table 2). Notwithstanding the very large inputs to the lake (150000 to 310000

kg over the 74 year period for the examined compounds), the water fraction in 1983 contains only a minute proportion, 60 to 800 kg for each of the chemicals over the whole lake, resulting in very low water concentrations in the order of 0.1 ng/L or 0.1 ppt. The amount in fish is much lower, 0.1 to 6 kg in the whole lake for each contaminant, but concentrations are higher than in water because of the low fish biomass.

#### Concentrations of contaminants in Lake Ontario

A mass balance of contaminants in the lake is important to assess the fate of the chemicals once they enter the lake. From a practical or management point of view the prediction of concentrations, especially in water used as potable water supplies, in fish used for human consumption and in bottom sediments which can remain as a major source of internal loadings after external inputs are reduced, is of fundamental importance in a large lake that may respond very slowly (average water residence time is 7.8 years) to reduced contaminant loadings. The problem of predicting concentrations is very difficult because by definition a concentration is a ratio between the mass of a contaminant and the mass of the compartment of interest, for example, fish, benthos, suspended sediments etc. For some compartments this mass can be estimated fairly readily, even if within reasonable limits; for example, suspended sediments are on average 0.4 mg/L in Lake Ontario and this corresponds to 400,000 metric tons of suspended sediments in the whole lake assuming that the lake is homogeneous. Conversely, the estimation of biomass is very difficult and estimates can range within a factor of five; for example Oliver (10) estimates biota at  $10 \text{ g/m}^2$  in the whole lake or 190,000 metric tons dry weight, with an estimate as low as 85,000 metric tons or as high as 450,000 metric tons. When either number is used as an estimate of biomass, the predicted concentrations in fish can vary over the same range.

Therefore, if we were satisfied with the prediction of the mass of contaminants within a factor of two, we should be equally pleased if we can estimate concentrations in biota within one order of magnitude.

Given the previous assumptions and limitations, Table 3 shows predicted and literature value concentrations for several lake compartments. Water concentrations agree well with measured values since the water mass is well known and Table 2 showed that contaminant masses were in good agreement, even if only a very small percentage of the input of these volatile CB's remained in the lake. Suspended sediment concentrations vary widely in the lake with standard deviations almost as large as the mean value; in this respect the estimated concentrations are close to the mean lake values. Concentrations in bottom sediments are predicted within a factor of two, similar to the agreement for masses.

In a large lake the most difficult prediction to make is the bioconcentration in fish, benthos and plankton because of the above mentioned problem of not knowing the biomass. For some contaminants, such as QCB the agreement is within a factor of two and for the others the agreement is within a factor of three and certainly within an order of magnitude. The only discrepancy seems to be the low concentration predicted for HCB in fish. A similar discrepancy between environmental residue levels and concentrations calculated from bioconcentration factors has been reported for HCB (12). Some type of food chain transfer coefficient must be incorporated into the model for chemicals such as HCB which have a long half life in fish and, therefore, may never reach chemical equilibrium with the surrounding water. Improved estimates of biomass in the lake are also required before more precise concentrations can be predicted.

### Contaminants' fate and the lake's self-cleaning ability

The fact that only a low percentage of the four contaminants is found in the water confirms Oliver's (10) estimate that most of these contaminants leave the lake system by volatilization from the surface. Volatilization rates vary according to the chemical, more for 1,2,4-TCB and less for HCB. For example the average yearly loadings since 1977 have been about 120 kg for HCB and 2300 kg for 1,2,4-TCB (Table 1) but concentrations in the bottom sediments top layer are very similar for the two compounds, about 0.1 ug/g, indicating that 1,2,4-TCB is much less persistent than HCB. As for fluxes, TOXFATE predicts that during the period 1977 to 1983 about 67% of HCB loadings were lost from the lake by volatilization processes, while Oliver (10) estimated 80% during the period May-November 1982. Similarly for the other contaminants, the model produces lower volatilization estimates than Oliver's.

The model predicts that the half life of the volatilization process is only 0.3 years for 1,2,4-TCB and 1.5 years for HCB, while the half life of the physical transport out of the St. Lawrence river is 3 years for 1,2,4-TCB, i.e. similar to the lake water half life, and 12 years for HCB. Lake Ontario is a transition zone for the other volatile chemicals analyzed in this study but not for others, such as Mirex, which does not volatilize and is very persistent (1).

One last question that was investigated with the model was the time frame that it would take for some contaminants to be permanently buried in the bottom sediments if loadings were completely stopped. Two chemicals HCB and 1,2,4-TCB were chosen as representative of relatively persistent and more volatile compounds. As mentioned above, 1,2,4-TCB is very volatile and therefore only about 1 to 3% of the loadings are in the bottom sediments; if loadings were completely stopped it would take about 19 to 38 years for 1,2,4-TCB to be buried under 8 cm of clean sediments. This estimate is fairly

uncertain given the very small amounts which remain in the sediments. In comparison it will take about 150 years to completely eliminate from active circulation mirex (1), and about 26 years for HCB.

#### DISCUSSION

A simulation model, TOXFATE, has been employed to quantify the behaviour of four chlorobenzenes, 1,2,4-TCB, 1,2,3,4-TeCB, QCB and HCB, in Lake Ontario. The purpose of this study was to validate and to verify the prediction ability of the model using data, not used in model development. The predicted and observed data in the different components of the ecosystem agree within a factor of two; a very satisfactory conclusion considering the four orders of magnitude range between fish and bottom sediments, 2 to 3 kg of contaminants and 10,000 to 11,000 kg, respectively, the uncertainty of the data set and the uncertainty in some model parameters, e.g. resuspension. Computed sedimentation, volatilization and transport rates from the St. Lawrence River agree within a few percentage points with field estimates (Table 2). Given the good agreement with the data, TOXFATE, originally developed and verified for nine other contaminants, can be considered validated and a useful tool to predict the fate of persistent and/or volatile compounds in large lake systems where physical effects, such as wind driven water circulation, play an important role. From a management perspective, TOXFATE could now be used to predict the fate of other contaminants entering lake Ontario from the Niagara River and to assess the environmental effects of different loadings reduction alternatives.

## CONCLUSIONS

As pointed out by Halfon (1) large lake toxic contaminant models are sensitive to one parameter, mainly the resuspension rate from the sediments; fiddling or calibrating the model with that parameter allows an almost perfect fit to the data, within a few percentages for the mass of the four contaminants. Therefore, the question is whether the model should be calibrated using the resuspension parameter or whether we should only use measured parameters, such as those available from Charlton (17). In this exercise the measured value was used even if a calibrated model would have given a better fit. Comparison with other contaminant data in the future will permit the resolution of this problem. The inescapable conclusion, however, is that resuspension rates should be measured accurately wherever possible since they have fundamental role in controlling contaminants fate in Lake Ontario (see also Halfon (6)).

The main problem of the prediction of toxic contaminants fate, once a model has been satisfactorily validated for a few compounds, is the lack of loading data; this problem is particularly evident in a large lake system. Presently, the Niagara River is regularly monitored for compounds in the water and in suspended sediments (15), however, such monitoring has taken place only since the late 1970's and earlier loadings data can only be inferred from bottom sediments data. For new or recently released compounds, or for compounds not yet identified in the lake, these data are not available and may not be available for a foreseeable future; for contaminants which are already entering the lake, the bottom sediments are a good source of past loadings data provided that a comprehensive data base with concentrations and dating is available, as shown by Oliver (10).

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Table 1: Estimated loadings (kg/year) to Lake Ontario from the Niagara River 1909-1983.

Year/Compound	1,2,4-TCB	1,2,3,4-TeCB	OCB	HCB
1909-1920	1500	150	60	46
1921-1931	2400	290	140	230
1932-1939	3300	490	160	150
1940-1946	2800	500	410	180
1947-1949	4400	880	450	180
1950-1953	3900	670	280	110
1954-1956	3900	1000	440	190
1957-1959	6100	1200	560	260
1960-1962	8900	2100	770	920
1963-1965	9000	3800	870	710
1966-1967	7400	3200	710	390
1968-1969	5700	1400	420	350
1970-1972	3900	1300	300	200
1973-1974	3700	940	200	160
1975-1976	3700	880	200	100
1977-1978	2400	610	150	100
1979	2200	760	240	140
1980	2400	760	240	140
1981	2400	760	240	160
1982-1983	2400	760	240	120

Table 2: Comparison of simulations and field estimates for the year 1983.

Contaminant	Method	Input	Water	Suspended	Biota	Bottom	Sedimentation	Volatilization	Transport
		(kg)	(kg)	Sediments (kg)	Sediments	Sediments			
1,2,4-TCB	Model	273,000**	770	7	3	9,100	3	89	8
	Ref. 10	310,000	700	10	2	11,000	4 (1)*	93	3
1,2,3,4-TeCB	Model	63,000**	260	8	4	6,000	13	79	8
	Ref. 10	66,000	210	4	2	3,300	5 (2)*	93	2
OCB	Model	22,200**	86	4	2	6,900	21	72	7
	Ref. 10	23,000	90	4	2	4,100	18 (4)*	79	3
HCB	Model	16,300**	61	4	3	4,300	29	67	4
	Ref. 10	15,000	90	9	8	8,500	57 (15)*	38	5

\* From Reference 14.

\*\* From core data (8) using one centimetre slices and used as inputs to the model. Model inputs are different from Oliver's (10) estimates since they are based on yearly estimates rather than on a global 74 year estimate.

Table 3: Measured and estimated (in parenthesis) concentrations of chlorobenzenes in Lake Ontario water, sediments and biota. Units are in ng/g dry weight but for water [ng/L]. Where applicable, ranges of values are indicated where biomass estimates in Lake Ontario are uncertain.

Compartment/Contaminant	1,2,4-TCB	1,2,3,4-TeCB	QCB	HCB
Water	.44 (.49)	.13 (.17)	.057 (.055)	.057 (.039)
Suspended Sediments	15 (11)	5.3 (13)	5.3 (6)	14 (6)
Bottom Sediments	97 (56-44)	36 (102-116)	36 (54-63)	100 (53-57)
Macroinvertebrates	80 (24-120)	50 (6-32)	40 (24-120)	170 (22-110)
Plankton	6 (5-22)	6 (4-17)	9 (5-24)	10 (3-15)
Fish	3 (5-23)	4 (9-42)	14 (5-24)	130 (4-22)