MODELLING OF TOXIC CONTAMINANTS IN THE NIAGARA RIVER PLUME IN LAKE ONTARIO

by
I. Stepien, D.C.L. Lam, C.R. Murthy,
M.E. Fox and J. Carey

National Water Research Institute Burlington, Ontario, Canada January 1986 NWRI Contribution #86-293

MANAGEMENT PERSPECTIVE

The work described in this report is predicated by the DOE concerns on the toxic contaminants in the Niagara River.

The distribution of organochlorine contaminants carried by the Niagara River into Lake Ontario has been simulated by a contaminant fate and transport model, as part of the NWRI Project on "Niagara River Toxics". The model was developed through interdisciplinary team work incorporating hydrodynamics of river-lake interactions and known chemical kinetics of the measured organochlorine contaminants. Extensive verification of the model with the observed field data has demonstrated its predictive capability which is one of the main goals of the DOE Toxics Management Program in general and Niagara River Toxics Project in particular. The model can be used to assess the concentration and exposure time of toxic chemicals for purposes of defining water quality standards.

PERSPECTIVE-GESTION

Les travaux décrits dans le présent rapport sont fondés sur les préoccupations du ministère de l'Environnement relatives à la présence de contaminants toxiques dans la rivière Niagara.

La distribution des contaminants organochlorés transportés par les eaux de la rivière Niagara dans celles du lac Ontario a été simulée au moyen d'un modèle sur le devenir et le transport des contaminants dans le cadre du projet de l'INRE (Institut national de recherche sur les eaux) portant sur les substances toxiques dans la rivière Niagara. Le modèle a été élaboré grâce à un travail d'équipe interdisciplinaire faisant appel à l'hydrodynamique des interactions entre les rivières et les lacs et à la cinétique chimique connue des contaminants organochlorés mesurés. Une vérification exhaustive du modèle avec les données obtenues sur le terrain a montré son pouvoir de prévision qui est l'un des principaux objectifs du Programme de gestion des produits chimiques toxiques du ministère de l'Environnement en général et plus particulièrement du projet d'étude sur les substances toxiques dans la rivière Niagara. Le modèle peut être utilisé pour évaluer la concentration des substances chimiques toxiques et le temps d'exposition en vue de formuler des normes sur la qualité de l'eau.

Le transport et la distribution locale des chloro-benzènes dans la zone de la barre du Niagara ont été simulés à l'aide d'un modèle bidimensionnel et les résultats ont été comparés aux données d'observation recueillies lors des expériences effectuées en 1982 et 1983. L'interaction entre les sédiments en suspension et les concentrations locales des polluants a été décrite au moyen d'un sous-modèle de fractionnement et les paramètres physiques du modèle (coefficient de fractionnement, vitesse de décantation) ont été étalonnés à l'aide de données obtenues sur le terrain. On a constaté que la dynamique du panache du Niagara dépend fortement du champ de courants poussés par le vent dans le lac Ontario. Le modèle peut être utilisé en vue de prévoir à court terme le devenir des susbstances toxiques à proximité de la côte et leur transport dans la zone côtière.

The transport and compartmental distribution of chlorinated benzenes in the Niagara Bar area were simulated using a two-dimensional model and the results were compared with observational data collected during 1982 and 1983 experiments. The interaction between suspended sediment and compartmental concentrations of pollutants has been described by a partitioning submodel and physical parameters of the model (partition coefficient, settling velocity) were calibrated with field data. It was found that the dynamics of the Niagara plume is strongly controlled by the wind driven field of currents in Lake Ontario. The model may be used for the purposes of nearshore and short-time prediction of fate and transport of toxic chemicals in the coastal zone.

INTRODUCTION

The coastal zone of Lake Ontario in the vicinity of the Niagara River is one of the International Joint Commission's high priority research areas. The main reason for this interest is the well-documented contamination of the Niagara River, mostly by chemical industry (Elder et al., 1981; Warry and Chan, 1981; Allan et al., 1983). The chemicals of industrial origin such as chlorobenzenes, chlorotoluenes, mirex, etc. enter the Niagara River by direct discharges (Oliver and Nicol, 1984) or by the leaching from chemical dump sites along the river (Elder et al., 1981). The Niagara River Toxics Committee Report (1984) catalogs at least 37 significant point sources of chemical contaminants recognized by Environment Protection Agency as priority pollutants.

Significant concentrations of chlorobenzenes, chlorotoluenes, PCB's and chlorostyrenes have been found in water and biota of the Niagara River (Kuntz and Warry, 1983; Oliver and Nicol, 1984; Fox and Carey, 1983). Sediments in Lake Ontario also contain elevated levels of these same compounds (Frank et al., 1979; Onuska et al., 1983; Kaminsky et al., 1983; Oliver and Nicol, 1984). However, little work has been done on tracing the pathway of contaminants from the river to the bottom sediment and also to the open waters of Lake Ontario. The contaminants enter the lake either dissolved or adsorbed on the suspended sediment. In the coastal zone, there will be a shift

towards a new equilibrium of the dissolved and adsorbed portions depending on the physio-chemical properties of the chemicals and on the open lake conditions. For example, if the sediment transport rate is slower than the settling rate, most of the contaminants will be transferred to the sediment in the adsorbed form. Otherwise, they will be transported to the open lake in both forms. Thus, the interactions of the sediment and water at the coastal zone strongly influence the pathway, composition and fate of the contaminants in the open lake.

The distribution of both dissolved and adsorbed forms of the contaminant at the mouth of the Niagara River is dominated by the strong river flow and the offshore lake currents. Sampling of both forms are not possible without the knowledge of the direction and shape of the river plume. An intensive experimental program has been carried out in 1982 and 1983 in which the collection of the chemistry data (Fox and Carey, 1985) was closely coordinated with physical measurements (Murthy et al., 1986). In particular, in 1983, the ship course pattern for sampling the toxic chemicals was determined by observing the real-time positions of the Lagrangian drifters released at the river mouth for the physical experiment. This maximizes the probability of sampling in the contaminant plume.

In this paper our hypothesis is that the distribution of the dissolved and adsorbed forms of the contaminants depends mainly on the interactions of water and suspended sediment including advection,

diffusion, net settling, adsorption and desorption. The relatively slower, long-term processes such as bioaccumulation and biodegradation (Halfon, 1984) are not important in the coastal zone. This hypothesis will be tested with the observed physical and chemical data collected from this intensive experimental program.

FIELD STUDY DATA BASE

The study area was covered by sampling stations arranged along several parallel transects forming a 40 km x 12 km parallelogram (Fig. 1), with the longer side along the south shore of Lake Ontario. The Niagara River mouth was located approximately at the centre of the south boundary. These boundaries were based on previous studies that had shown the Niagara River plume was most often developed in an easterly direction (Murthy, 1969).

In 1982, in a preliminary experiment, the network was sampled during seven intensive cruises between April 13 and November 12. On each cruise, sampling was begun on the westernmost transect and all the water samples were collected during one daytime period. At each site, 1-L water samples were taken at 1 m depth in precleaned glass bottles and 10 ml of hexane was added to initiate contaminants extraction. The bottles were sealed with teflon-lined screw caps and stored at 4°C in the dark until analysis. Concurrent temperature and light transparency profiles and measurements of surface conductivity were also obtained.

The analytical procedures for the water samples have been described in Fox and Carey, 1985. Briefly, the contaminants were extracted overnight by liquid-liquid extraction using hexane. The hexane extracts were dried by passing through anhydrous Na₂SO₄. After concentration by evaporation and cleanup on 40% H₂SO₄/silica gel column, the final 1 mL extracts were analyzed for the organochlorine contaminants by electron capture gas chromatography using capillary glass columns.

In order to study the transport of contaminants in the Niagara River Plume, it was necessary to identify compounds that could be used as tracers of Niagara River water. The most prominent chemicals observed by electron capture chromatography were: 1,2,4-trichlorobenzene, 1,2,3,5-tetrachlorobenzene, 1,2,4,5-tetrachlorobenzene, 1,2,3,4-tetrachlorobenzene, pentachlorobenzene, q-BHC, hexachlorobenzene, lindane (y-BHC). Of these compounds, the two BHC isomers were often present at uniform levels throughout the study area, and were not very useful as plume tracers. Of the remaining six chlorobenzenes 1,2,3,5-, 1,2,4,5-, penta- and hexa- isomers were eliminated since they were present usually at very low levels (for example, 90% of the hexachlorobenzene concentrations were below 1 On the other hand, the 1,2,3,4-tetrachlorobenzene (i.e 1,2,3,4-TeCB) and 1,2,4-trichlorobenzene (i.e. 1,2,4,-TCB) were present at significant levels in the plume and these two compounds were finally chosen as suitable plume tracers.

The 1983 field surveys were conducted during three cruises (May 11, August 10, October 4). The analytical procedure of water sampling was modified in order to determine more accurately the particulate and dissolved parts of total concentration. substantial improvement over the 1982 experiment occurs when, from a 10-L water sample collected at 1-m depth, a 4-L subsample was taken as whole water and a second 4-L subsample was filtered in the field through 1 µm glass fibre filter immediately after collection. initiate contaminant extraction and to preserve the sample from biological changes 200 mL of dichloromethane was added to each sample A further 1-L subsample was immediately filtered in the field. through a preweighed 1 um glass fibre filter in order to obtain weight of suspended solids. Extractions of the 4-L samples were completed in the laboratory with cleanup and analysis techniques similar to those The particulate contaminant concentrations were employed in 1982. computed by subtracting the 4-L filtered sample concentration from the The relative error of measured 4-L whole water concentration. concentrations was estimated to be 10% at the 95% confidence limit.

Occasionally, when the particulate contaminant concentration was less than the relative error of the measured total and dissolved concentration, this method resulted in a negative value of particulate concentration which was recorded as ND (no data, see Table I).

In order to determine the velocity field during each cruise up to 15 sail drogues were released near Niagara-on-the-Lake starting about 1-1/2 kilometers upstream of the river mouth. The trajectories

of drogues were established by fixes recorded on time-scales of the order of 1/2 hour increments. This was accomplished using a Mini-Ranger range-range system, four transponder stations and a small launch with a receiver aboard. The accuracy of this positioning system depends on the angles of intersection of signals radiating from the transponder station, but is in the order of ±10 meters as used in this study (Murthy et al., 1986). As a result the Lagrangian trajectories for each drogue and the corresponding horizontal velocity field in the area covered by the plume were computed. Details of the Lagrangian drogue technique are given in Simons et al. (1985), Murthy et al. (1986), and Murthy (1969)

MODEL FORMULATION

Because of the strong river flow and lake circulation, the chemicals associated with the Niagara River water remain in the Niagara River Bar area (see depth contours in Fig. 1) for only a few hours. Over such a short time frame, chemical processes such as biodegradation, bioaccumulation and volatization are relatively insignificant and can be neglected (Halfon, 1984). In the model formulation, it is more pertinent to consider the advection-diffusion, settling-resuspension and adsorption-desorption processes.

Central to the model formulation is the concept that the chemicals are present both in the aqueous phase (i.e. dissolved in the lake water), as well as in the solid phase (i.e. associated with the

suspended sediment particles). These interactions are depicted in Fig. 2 in which the suspended sediment contains the particular form of the chlorinated benzenes (solid phase) that can be absorbed from or desorbed into the dissolved form (aqueous phase). The hydrodynamical model will provide the computed currents for the advection of both the suspended sediments and the dissolved chemicals. We assume that the sediment—water system is at or near equilibrium. The exact proportion of dissolved to adsorbed form at equilibrium, is dependent on the properties of the individual chemicals and the characteristics of the suspended particles.

Thus,

$$c_{p} = \frac{\pi \cdot c_{ss}}{1 + \pi \cdot c_{ss}} c_{T}$$
 (1)

$$c_{d} = \frac{1}{1 + \pi \cdot c_{SS}} c_{T}$$
 (2)

where: C_m - total concentration (ng/L)

C - particulate concentration (ng/L)

C, - dissolved concentration (ng/L)

C_{SS} - suspended sediment concentration (mg/L)

Π - partition coefficient (L/mg)

Note that C_d refers to the dissolved form of the chemical in the lake water, C_p refers to the solid form of the chemical

adsorbed in the suspended sediment but calculated on the same per-unit-volume-of-water basis as C_d so that the total concentration is $C_T = C_d + C_p$. On the other hand, the partition coefficient π is defined in L/mg which is reciprocal to the unit of the concentration of the suspended sediment C_{SS} , so that their product, π^C_{SS} , is a dimensionless quantity in Eqs. (1) and (2). These definitions are necessary because the contaminant concentrations are many orders of magnitude less than the suspended sediment concentration.

In some cases, the suspended sediment concentration can be assumed as constant (e.g. Schnoor, 1982) and, if so, only one more equation is required, in addition to Eqs. (1) and (2), for the three unknowns C_d , C_p and C_T . However, in the case of the Niagara River area, C_{88} varies substantially from the river mouth to the offshore zone, with a decrease of over 60%, because the heavy load of suspended sediment contained in the river discharge settles rapidly by the time it reaches the offshore area. Thus, in our model, C_{SS} is allowed to vary in both space and time and constitutes one more unknown, making a total of four. As a result, two additional equations are required for describing the temporal and spatial changes of C_{SS} and C_T :

$$\frac{\partial hC_{SS}}{\partial t} + \nabla \cdot \dot{D}C_{SS} = K\nabla \cdot h \nabla C_{SS} - W \cdot C_{SS}$$
 (3)

$$\frac{\partial hC_{T}}{\partial t} + \nabla \cdot \vec{U}C_{T} = K\nabla \cdot h\nabla C_{T} - \frac{\Pi C_{SS}}{1 + \Pi C_{SS}}C_{T}$$
(4)

where \vec{U} is the two-dimensional, vertically integrated transport vector, h is the depth, ∇ is the two-dimensional spatial gradient operator, K is the turbulent eddy diffusivity and W is the net settling velocity.

The transport vector T is obtained from a hydrodynamical model (Simons and Lam, 1986) over the numerical grid shown in Fig. 1. Since Murthy et al. (1986) have shown that the physical regime in this region is virtually fully mixed at all times, the use of vertically integrated models is valid and can simplify the computation. that while net settling is applied to Css in Eq. (3), it is applied the particulate portion of CT in Eq. (4), i.e. Cp $\Pi C_{ss} \cdot C_T / (1 + \Pi C_{ss})$ To solve for the four unknowns CD, Cd, C_{ss} , C_{T} from the equations (1) - (4), C_{ss} can be conveniently obtained first from Eq. (3) by finite difference methods (e.g. Simons and Lam, 1986), as this equation is not dependent on the other Then, CT can be solved from Eq. (4), using the same numerical methods and the values of CSS just computed. Cp and Cd can be determined directly from Eq. (1) and respectively, using the computed values of CSS and CT. boundary conditions for Eqs. (3) and (4) are such that CSS and CT are specified at the inflow with no total flux at solid boundaries and no diffusive flux at open boundaries (Lam et al., 1984).

RESULTS AND DISCUSSION

The model has been applied to all three 1983 cruise periods because the 1982 data were no so adequate as discussed earlier. In one of the episodes (October 4, 1983), all four variables were measured and thus provided the necessary information for calibration of model parameters. The other two episodes were used for model confirmation purposes. Specifically, the physical parameters W and K were calibrated with the October 4 data. They were then held fixed in the confirmation runs. On the other hand, the chemical partition coefficient I was allowed to change according to the averaged value determined directly from the measured in situ concentration of the chemical concerned.

Model Calibration Results

As part of the model calibration, the measured values of dissolved and adsorbed 1,2,3,4-TeCB and 1,2,4-TCB for the October 4 episode are given in Table I. Averaged values of partition coefficient estimated from this set of data were 0.087 and 0.067 L/mg, respectively. These are higher (at least a factor of 10) than those predicted from Karickoff's empirical equations based on the chemicals water solubility and octanol-water partition coefficient (Karickoff, 1981). However, Karickoff's experiments were conducted on bottom sediments with "stabilized" organic carbon layer surrounding the

particles (Karickoff et al., 1979). Measurements on settling material in the Niagara Bar area (Oliver and Charlton, 1984; Charlton, 1983; Kuntz and Warry; 1983) indicated an organic carbon concentration 2-3 times bottom sediment TOC values and a significant part of the settling material was seston (algae, diatoms, etc.). It was shown in Fox and Carey (1983) that zooplankton and related biota are strong bioconcentrators of chlorobenzenes in the Niagara River.

The water samples of October 4 were collected during a six-hour time period from 14.50 GMT (station 612) until 21.00 GMT (station 276); a track plot of the survey vessel with exact timerecord is given in Fig. 3. In order to calibrate the settling velocity from such a quasi-synoptic set of data, an eight-hour simulation was performed and the "time series" of computed data corresponding to the observed "time series" was derived from 32 concentration maps (15 minute intervals). That is, only the computed values at the same location and time as the observed were selected, as shown in Fig. 4. The simulation was repeated for three values of settling velocity (W=1,2 and 3 m/day) and for each run standard error was determined. The minimum error (1.05 ng/L) was found for the case of W=2 m/day (Fig 4). The standard errors for the cases of W=1 m/day and 3 m/day were 1.07 and 1.12 ng/L, respectively (not shown). Thus, the model is relatively insensitive to the variations in the net settling velocity. The steady but large supply of the suspended sediment from the river and the strong current regime are two probable reasons for this insensitivity. The other physical parameter of the

model, eddy diffusivity ($K=0.1 \text{ m}^2/\text{s}$), was chosen for such an advection dominant case by a similar calibration procedure and on the basis of data available in the literature (Lam et al., 1984).

The contaminant-transport model (Eq. 1-4) was run for a 45-hour period from October 3, 2.00 GMT to October 4, 23.00 GMT. Time and space steps of computation were 100 seconds and 1000 m, respectively. Prior to this run, the hydrodynamic model (Simons and Lam, 1986) used the wind data from a meteorological buoy situated offshore from the river mouth (Fig. 1), and the computed currents were output in three-hourly intervals for use in the contaminant transport model. For example, figure 5 shows a map of such currents for October 4, 14.00 GMT; the field of horizontal velocity computed independently using drogue trajectories data is shown in the same figure for comparative purposes. The easterly orientation of the Niagara River plume is a consequence of the prevailing wind direction (generally westerly) and the semipermanent easterly flowing currents along the south shore of Lake Ontario (Simons et al., 1985; Murthy, 1969). This orientation produces the most coherent plumes.

Figure 6 shows the two-dimensional distributions of simulated 1,2,3,4-TeCB concentration (shown as contours) at 17.00 GMT, October 4, approximately corresponding to the midpoint of the period 14.50-2100 GMT for which the semi-synoptic observed values were sampled (shown in circles). Mean standard deviation between computed and observed data was 1.5, 0.7, 0.7 ng/L for total, dissolved and

particulate concentration, and 0.7 mg/L for suspended sediment concentration, respectively, well within the uncertainties of the observed data. Thus, the calibrated results were satisfactory.

Model Confirmation Results

As mentioned earlier, 1,2,3,4-TeCB and 1,2,4-TCB were found to be the best tracers of Niagara River water into the lake. However, interpretation of observed concentration patterns was made difficult by the fact that, for example, on five of seven 1982 episodes, the concentration of 1,2,3,4-TeCB at the location in the plume was approximately two times higher than those in the river. currently believed that these effects are due to the daily fluctuations in water diversions from the Upper Niagara River by U.S. and Canadian power authorities. As required by the Niagara River Treaty, the minimum flow over the Falls during the daylight hours is 2830 m³/s while the night-time minimum is 1410 m³/s. Thus, constant contaminant discharge between the diversion structure and hydroelectric plants would result in diurnal variations concentration in the river. Many of the point sources identified by the NRTC are located in this section of the river (NRTC, 1984). Unfortunately, hourly or even daily data of contaminant loading and are not available. The effects of these loading uncertainties can be tested in one of the model confrimation runs (e.g. the episode of May 10, 1983).

Indeed, one possible loading scenario is given by the following assumptions:

(A) The temporal values of flow Q_t and total 1,2,3,4-TeCB concentration C_t in the Niagara mouth fit the equation

$$Q_t \cdot C_t = Q_0 \cdot C_0 \tag{5}$$

where $C_0 = 10$ ng/L is the average concentration at the river mouth reported by Oliver and Nicol (1984) and $Q_0 = 6400$ m³/s is the average discharge.

(B) Flow conditions (discharge, depth of flow) on the lower Niagara River are assumed to be time-dependent and the contaminant concentration at the Niagara mouth is a result of the dilution effect as described by equation (5).

To test these hyptheses, data of discharge through Canadian and U.S. hydropower stations and Niagara River discharge at Ashland Avenue gauge were provided from Niagara River Power Diversion Authority (Falkenirk and Yee, personal communication, 1985). Figure 7 shows one-hourly data for period May 10-12, 1983, which demonstrated the diurnal cycles of the discharge resulting from the flow regulation of the water reservoirs at these stations approximately 10 km upstream. This influence was further confirmed by the computed results (Fig. 8) of a channel flow model (Stepien, 1984) for the discharge at the river mouth, using the upstream data (Fig. 7) as

inputs. Thus, if we assume that most of the contaminant sources (Allan et al., 1983) are upstream of the intake points of these reservoirs, then the dissolved contaminant concentration (Fig. 8) at the river mouth would indeed behave reciprocally to the flow as required by Eq. (5). Hence, the concentration time series presented in Fig. 8 was used as an input forcing function for simulating the concentration in the Niagara Bar area for period May 10-11, 1983, as part of the model confirmation test.

The quasi-synoptic and observed distributions (shown in circles) of total dissolved and adsorbed 1,2,3,4-TeCB (May 11, 14.00-21.00 GMT) are shown in Fig. 9. Again, the computed distributions (shown as contours) at 17.00 GMT, which is the midpoint of the observation period, are also shown. The isolated patch of higher concentration shown in the observed data was reconstructed by model and this pattern was repeated during the next cycle. The travelling time of the patch from the river mouth to the observed location in Fig. 9 corresponds approximately to the sampling time of May 11. Note that according to simulated scenario, maximum concentration at the river mouth should be detected during the morning hours, local time (Fig. 8) and the patch would move to the northwest part of the grid by afternoon (Fig. 9).

As a control test, we made a second run performed for the same episode with a constant value of concentration (8 ng/L) in the Niagara mouth for the entire 48 hours of computation. The results of this control test are shown in Fig. 10; the computed concentrations of

the dissolved 1,2,3,4-TeCB are approximately 30% lower than those computed for the first case and the offshore maximum is not present at all time.

Thus, our hypothesis that diurnal flow fluctuations could induce patches or maximas in the dissolved concentration field is apparently supported by the results of these two scenario runs. However, further confirmation of this hypothesis is needed when more accurate information about the loading is available.

In the August 10th episode, the direction and shape of the Figure 11 shows the plume were controlled by an easterly wind. distribution of the horizontal velocity field derived from drogue trajectories data and the current field produced by hydrodynamic model for August 10, 1983. As before, the quasi-synoptic observed values of another chlorinated benzene 1,2,4-TCB are shown in circles in Fig. 12 and the corresponding computed values as contour. We used the same model coefficients as those used for the case of October 4 (Fig. 6), except for the partition coefficient, in which case, a value of 0.067 L/mg determined from the October 4 data of 1,2,4-TCB is used The observed decreasing concentration gradient is (Table I). The simulation also shows an reflected in the computed values. eastward movement of the plume, but unfortunately this part of the study area was not sampled because the sample stations were chosen according to an anticipated plume direction determined during the experiment.

It is difficult to quantify rigorously the accuracy of the model results because of the limited number of observational points. For example, if we used the mean standard deviation between computed and observed total concentrations, then we found that the calibration results produced a value of 1.5 ng/L as discussed earlier (Fig. 6) and the confirmation results produced 1.1 ng/L, 1.2 ng/L and 2.3 ng/L for Figs. 9, 10 and 12, respectively. Thus, the confirmation runs seemed to produce results of comparable accuracy as those from the calibration run, showing that the physical parameters so calibrated were quite appropriate for the Niagara Bar area. However, with only seven observational points, for example, for the total concentration of 1,2,4-TCB in the case of Fig. 12, careful interpretation of these statistical measures are often warranted. Alternatively, we have lumped all computed and observed data (Figs. 6, 9, 10 and 12) and evaluated the combined data with the regression method (Thomann and The regression coefficients between the computed and Segna, 1980). observed results for the total and for the dissolved concentration in the combined data were found to be 0.75 and 0.71, respectively. These quite encouraging, in view of results were regression uncertainties in the boundary conditions and in the observed data.

CONCLUSIONS

Under assumed conditions of settling velocity, river flow and diurnal concentration fluctuations, the model adequately simulates

observed behaviour. Analysis of the observed data and results of simulations indicated that the key factors controlling the deposition and transport of the contaminants were partition coefficient and concentration of suspended solids. Under conditions of high suspended solids concentration, most of the adsorbed contaminants would be deposited in the Niagara Bar area. Otherwise, a significant proportion of the contaminants are carried in the dissolved form in the plume; the direction of this transport will be determined by the current and wind conditions.

The compartmental distribution and transport of toxic materials in the vicinity of the Niagara River plume may be simulated using the simple partitioning hypothesis. This approach is useful in the short term analysis of the pathway and transport of contaminants in the coastal zones. The model results also confirmed the use of a viable modelling framework to which more detailed processes or boundary conditions can be incorporated provided that adequate data are available.

ACKNOWLEDGEMENT

The authors have benefited by the constructive reviews provided by Drs. J.S. Bonner and B.M. Lesht. One of the authors (I.S.) was supported by a National Science and Engineering Research Council Postdoctoral Fellowship.

REFERENCES

- Allan, R.J., Murdoch, A. and Sudar, A. 1983. An introduction to the Niagara River/Lake Ontario pollution problem. J. Great Lakes, 9(2), 111-117.
- Charlton, M.N. 1983. Downflux of sediment, organic matter and phosphorus in the Niagara River of Lake Ontario. J. Great Lakes Research, 9(2), 201-211.
- Elder, V.A., Proctor, B.L. and Hites, R.A. 1981. Organic compounds near dump sites in Niagara Falls, New York. Environ. Sci. Technol., 15, 1237-1243.
- Fox, M.E. and Carey, J.H. 1983. Compartmental distribution of organochlorine contaminants in the Niagara River and the western basin of Lake Ontario. J. Great Lakes Res., 9(2), 287-294.
- Fox M.E. and Carey, J.H. 1985. Transport of selected organochlorine contaminants in the Niagara River plume. National Water Research Institute Report, Burlington, Ontario.
- Frank, R., R.L. Thomas, M. Holdrinet, A.L.W. Kemp and M.E. Braun.

 1979. Organochlorine insecticides and PCB's in surficial

 sediments (1968) and sediment cores (1976) from Lake Ontario.

 J. Great Lakes Res., 5, 18-27.
- Halfon, E. 1984. Predicting the environmental fate of toxic contaminants in large lakes: data requirements for mathematical models. In QSAR in Environmental Toxicology, Kaiser, K.L.E., (Ed.), D. Reidel Publishing Company, Dordrecht, Holland, 137-152.

- Kaminsky, R., Kaiser, K.L.E. and Hites, R.A. 1983. Fate of organic compounds from Niagara Falls dump sites in Lake Ontario. J. Great Lakes Res., 9(2), 183-189.
- Karickoff, S.W., Brown, D.S. and Scott, T.A. 1979. Sorption of hydrophobic pollutants on natural sediments. Water Res. 13: 241-248.
- Karickoff, S.W. 1981. Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. Chemosphere 10(8), 833-846.
- Kuntz, K.W. and Warry, N.D. 1983. Chlorinated organic contaminants in water and suspended sediments of the lower Niagara River. J. Great Lakes Res. 9(2), 241-248.
- Lam, D.C.L., Murthy, C.R. and Simpson, R.B. 1984. Effluent transport and diffusion models for the coastal zone. Lecture Notes on Coastal and Estuarine Studies, Series No. 5, Springer-Verlag, N.Y., 168 pp.
- Murthy, C.R., Lam, D.C.L. and Simons, T.J. 1986. Dynamics and transport modelling of the Niagara River plume in Lake Ontario.

 Rapp. P.-V. Reun. Cons. Int. Explr. Mer. (in press).
- Murthy, C.R. 1969. Large-scale diffusion studies in the Niagara

 River mouth, Lake Ontario. Proc. 12th Conf. Great Lakes

 Research, Int. Assoc. Great Lakes Res., pp 635-651.
- Niagara River Toxics Committee (NRTC), 1984. U.S.-Canada Niagara
 River Toxics Committee Report, Inland Waters Directorate, Ontario
 Region, Burlington, Ont.

- Oliver, B.G. and Charlton, M.N. 1984. Chlorinated organic contaminants on settling particulates in the Niagara River vicinity of Lake Ontario. Environ. Sci. Technol., 8: 903-908.
- Oliver, B.G. and Nicol, K.D. 1984. Chlorinated contaminants in the Niagara River, 1981 to 1983. Sci. Total Environ., 39: 57-70.
- Oliver, B.G. and Bothem, K.D. 1980. Determination of chlorobenzenes in water by capillary gas chromatography. Anal. Chem., 52, 2066-2069.
- Onuska, F.I., Mudroch, A. and Terry, K.A. 1983. Identification and determination of trace organic substances in sediment cores from the western basin of Lake Ontario. J. Great Lakes Res., 9(2), 169-182.
- Simons, T.J. and Lam, D.C.L. 1986. Documentation of two-dimensional x-y model package for computing lake circulations and pollutant transports. In W.G. Gray (Ed.), Physics-based modeling of lakes, reservoirs, and impoundment, ISBN 0-87262-531-1, A.S.C.E., N.Y., pp. 258-308.
- Simons, T.J., Murthy, C.R. and Campbell, J.E. 1985. Winter circulation in Lake Ontario. J. Great Lakes Res., 11(4), 423-433.
- Schnoor, J.L. 1982. Fate and transport modelling for toxic substances. In Modelling the Fate Chemicals in the Aquatic Environment. Ann Arbor Science, 145-163.
- Stepien, I. 1984. On the numerical solution of the Saint-Venant equations. J. of Hydrology, 67, 1-11.

- Thomann, R.V. and Segna, J.S. 1980. Dynamic phytoplantkon-phosphorus model of Lake Ontario: ten years verification and simulation.

 In Phosphorus Management Strategies for Lakes, Ann Arbor Science, 153-234.
- Warry, N.D. and Chan, C.H. 1981. Organic contaminants in suspended sediments of the Niagara River. J. Great Lakes Res., 7, 394-403.

Table I. Estimation of partition coefficient from October 4, 1983 field data. Total, compartmental and suspended sediment concentrations for 1,2,3,4-TeCB (I) and 1,2,4-TCB (II).

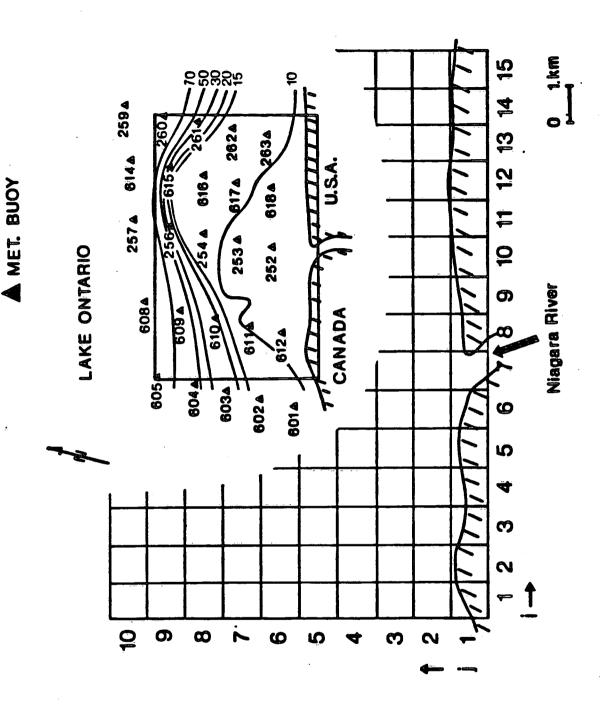
Station	Total [ng/L]		Dissolved [ng/L]		Adsorbed [ng/L]		Suspended Sediment [mg/L]	Partition Coefficient [L/mg]	
	I	II	I	II	ī	II		I	11
252	6.6	5.8	6.4	4.6	0.2	1.2	3.8	0.008	0.068
253	6.7	11.0	5.4	10.0	1.3	1.0	3.7	0.065	0.027
251	0.7	2.6	0.6	2.4	0.1	0.2	1.9	0.088	0.044
618	8.3	14.6	ND	ND	ND	ND	3.5	ND	ND
617	6.9	19.8	7.4	16.8	ND	3.0	3.9	ND	ND
616	2.7	7.0	5.5	13.4	ND	ND	2.7	ND	ND
263	7.6	18.7	5.3	12.6	2.3	6.1	3.7	0.117	0.130
262	5.2	4.6	4.7	10.1	0.5	ND	3.4	0.031	ND
261	2.9	7.0	3.0	8.1	ND	ND	3.5	ND	ND
260	0.7	2.4	0.6	2.9	0.1	ND	0.8	0.209	ND
612	ND	ND	4.2	11.0	ND	ND	2.8	ND	ND
276	6.3	12.8	6.9	16.0	ND	ND	4.8	ND	ND
	· · · · · · ·					Αν	erage	0.087	0.067

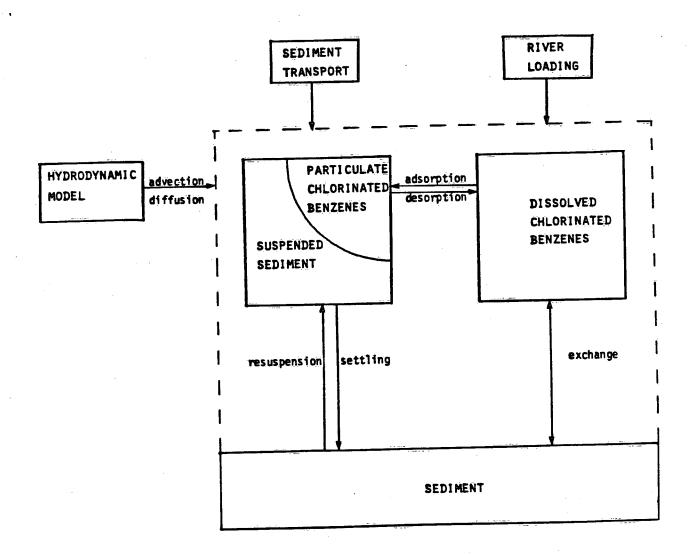
ND - No data

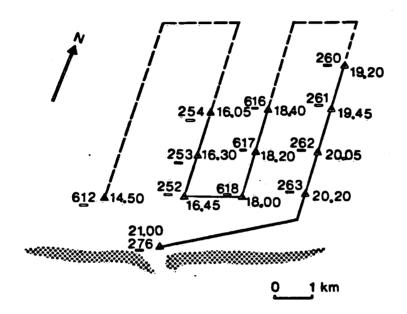
FIGURES

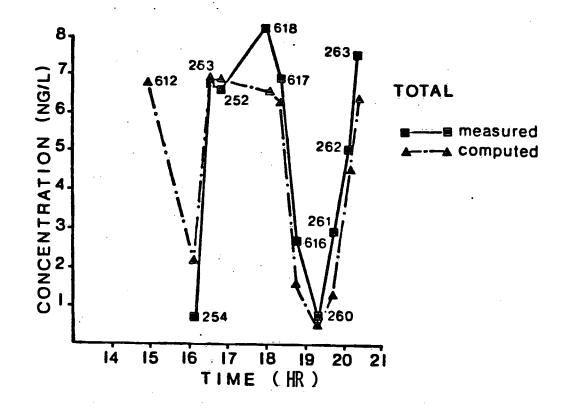
- Fig. 1 Computational mesh of the Niagara plume model. Inserted figure: depth contours (m) and samples sites (numbered triangles) arranged along parallel transects.
- Fig. 2 Schematic of the model framework.
- Fig. 3 Track plot of survey vessel and time record (starting at 14.50 GMT and ending at 21.00 GMT) of sampling sites (starting at station no. 612 and ending at 276) on October 4, 1983.
- Fig. 4 Observed and computed 1,2,3,4-TeCB (ng/L) concentrations for calibration run (October 4, 1983) for W = 200 m/day. Time shown is hr. GMT. (See Fig. 3 for positions of the numbered stations).
- Fig. 5 Vertically integrated field of current (hydrodynamical model, October 4, 14.00 GMT) and horizontal velocities computed from drogue trajectories.
- Fig. 6 Total and fractional 1,2,3,4-TeCB concentration (ng/L) and suspended sediment concentration (mg / L) . The observed values (circles) were sampled between 14.50 and 21.00 GMT; the computed values (contours) were for 17.00 GMT, October 4, 1983.

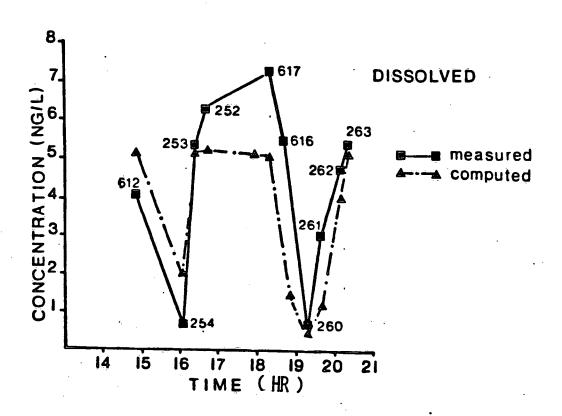
- Fig. 7 Discharge through hydropower stations: Canada (o), USA (Δ) and Niagara River discharge, Ashland Av. gauge (+). Upper diagram total discharge (cms) below the reservoirs, approximately 10 km upstream of the river mouth. Time shown is local EST, starting at 0 hr., May 10, 1983.
- Fig. 8 The computed discharge in the Niagara mouth and time scenario for the dissolved 1,2,3,4-TeCB concentration (May 10-11, 1983). Time shown is local EST, starting at 0 hr., May 10, 1983.
- Fig. 9 Time-dependent loading concentration scenario: total, dissolved and particulate 1,2,3,4-TeCB (ng/L) concentrations, May 11, 1983. The observed values (circles) were sampled from 14.00 to 21.00 GMT; the computed values (contours) were for 17.00 GMT.
- Fig. 10 Constant loading concentration scenario: total dissolved and particulate 1,2,3,4-TeCB concentration (ng/L), May 11, 1983 (cf. Fig. 9).
- Fig. 11 Vertically integrated field of current (hydrodynamic model,
 August 10, 14.00 GMT) and horizontal velocities computed
 from drogue trajectories.
- Fig. 12 Computed (contours) and observed (circles) of total, dissolved and particulate 1,2,4-TCB (ng/L) concentration, August 10, 1983.

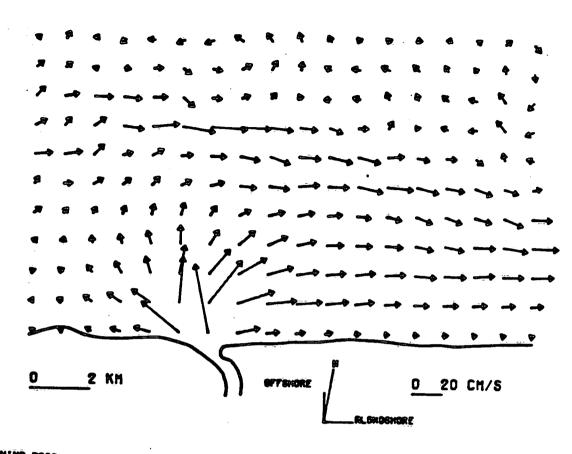


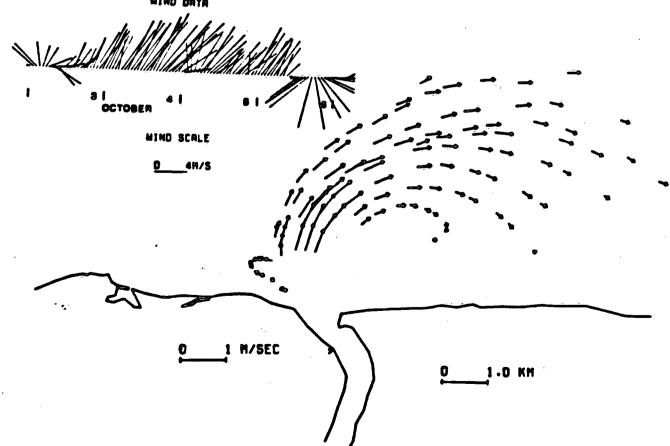


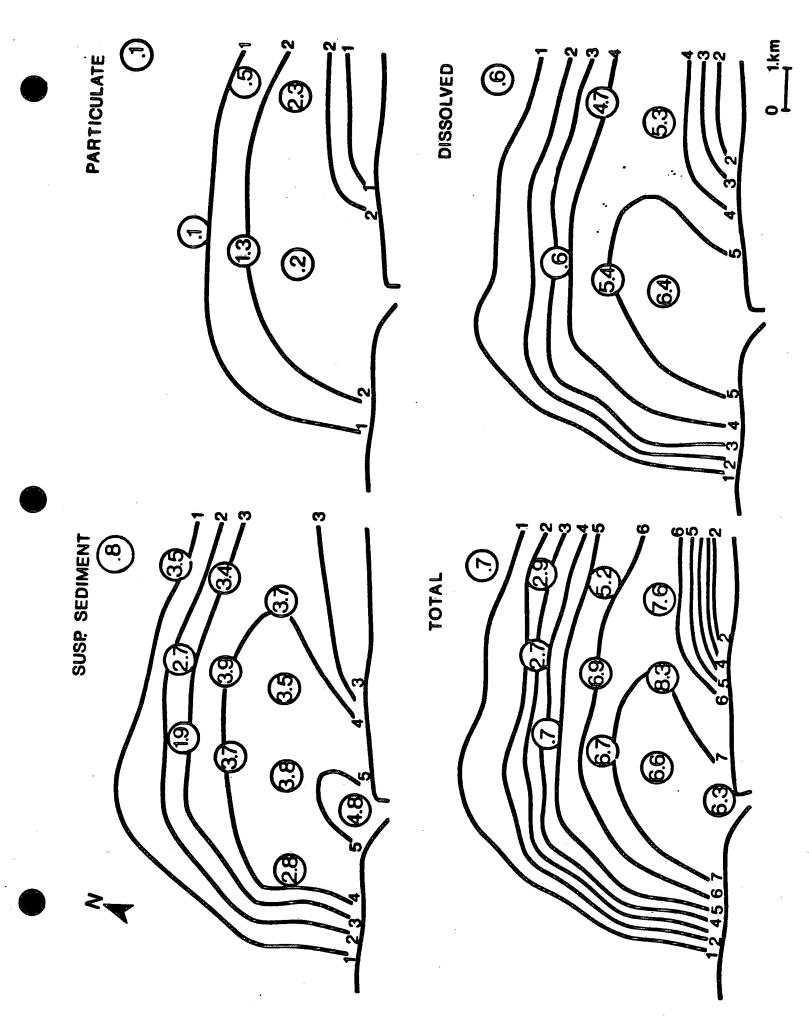


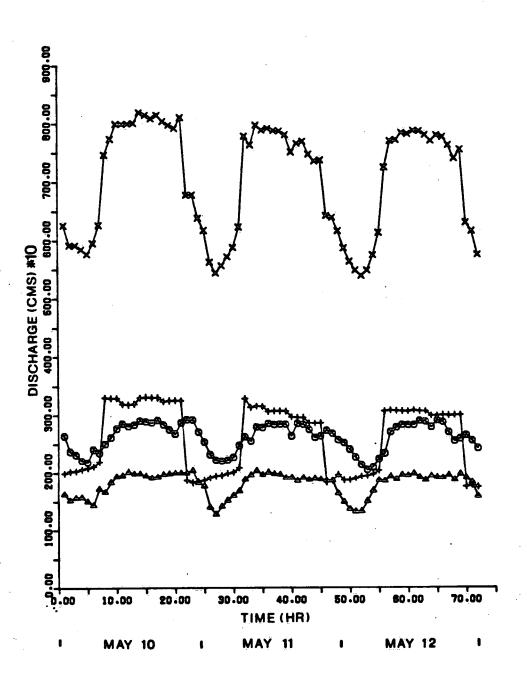


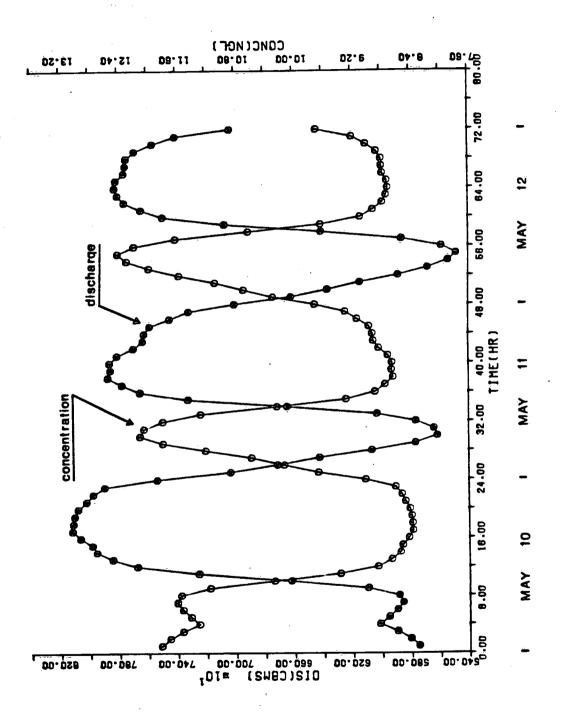


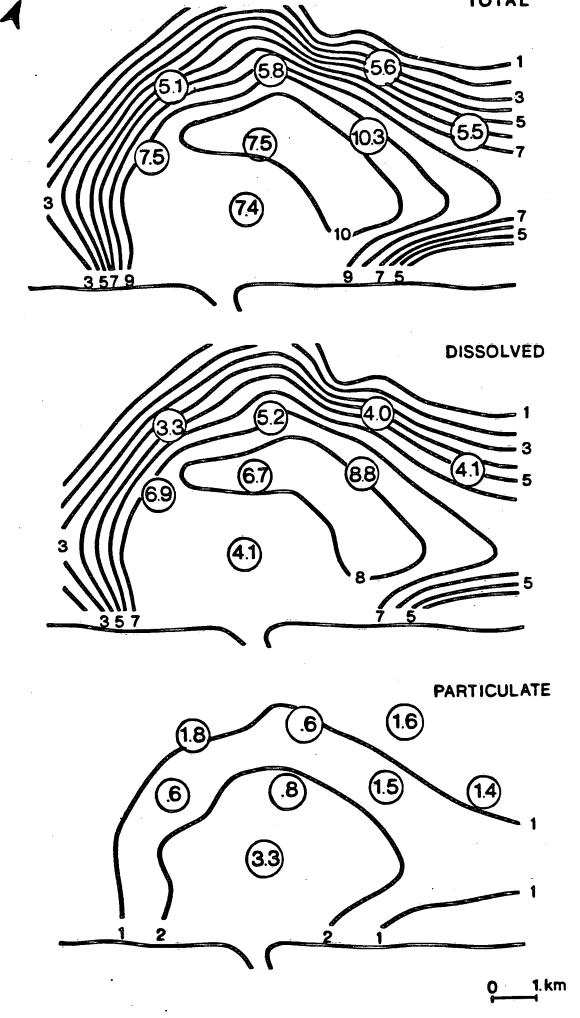


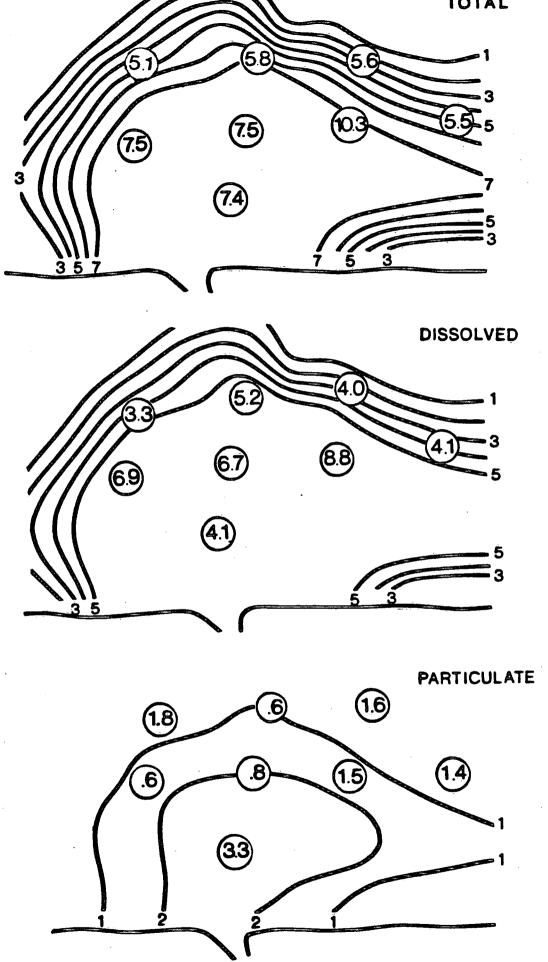


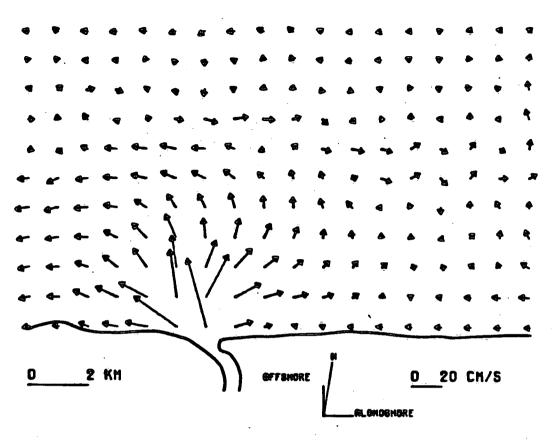












AUGUST 10.1983

