Tracer dispersion study: Diffusion coefficient and modeling results

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Abstract
This work compared the outcome of tracer dispersion experiments with the results of a far field numerical modeling. The studies were carried out on two different locations from Rio de Janeiro coast: the first near the city of Maricá, approximately 30 km east from the Guanabara Bay, and the second inside the bay, at São Gonçalo. For the tracer experiment, it was used a *Rhodamine, Amidorhodamine G*®. The experiment released approximately 50 liters of the compound into the water. The release was made by an instantaneous injection into the system. Three ships were used during the operation to release the compound, to monitor the movement and the dilution of the *Rhodamine* on the water and to collect environmental data. To measures the concentration of the tracer on the field, the boats has done line measures along the movement axis of the plume. The results from the tracer experiment were used to estimate the vertical and horizontal diffusion coefficient. These coefficients were used in the far field model and the results of the modeling were compared with what was measured. The far-field model used was CHEMMAP, a model that can simulate the dispersion and distribution of chemical products on the surface and water column. It was considered the same meteorological and oceanographic conditions found by the field team. The results were similar, with little difference on the dispersion cloud. In the experiment inside Guanabara Bay, the linear correlation coefficient was 0.84 while in Maricá region it was 0.73.

Keywords
Tracer experiment; tracer dilution; diffusion coefficient, far-field model; far-field transport

INTRODUCTION

This paper will compare the outcome of dispersion studies of a fluorescent tracer (Rhodamine) with the results of a far field numerical modeling. The studies were carried out in two different locations along Rio de Janeiro coast: at São Gonçalo, inside the Guanabara Bay, and the second at ocean coast, approximately 30 km east from the Bay, at Maricá.

Study Area

Winds. Predominant winds over Rio de Janeiro coast are from NE, with moderate intensity, typically from South Atlantic Subtropical High (SASH). Periodically this condition is disturbed by frontal systems follow in a SW-NE (Kousky, 1979, apud Castro Filho & Miranda, 1998). Pinho (2003) also describes prevailing winds from NE and strong gusts from SW, associated with frontal systems. Inside the Guanabara Bay a pre-frontal condition is predicted by winds from N and NE, the low pressure system changes wind direction at counterclockwise to SW (Kjerfve et al., 1997).

Currents: The pattern inside the bay is highly dominated by the tides, with a preferential N-S circulation (Guimarães et al, 2007). Regarding the area outside the bay, the predominating currents are to SW in the surface and NE in the bottom during the summer and to NE in the whole water column during the winter (Mano, 2007).

Temperature and Salinity. Bérgamo (2006) analyzed data inside Guanabara Bay for different seasons and present temperature values between 20 and 29ºC. Araujo et al (2004) present salinity of São Gonçalo beaches raging between 20 and 24.3, with mean value of 22.83. At Maricá, according NODC database, the water temperature at summer is 23.8 ºC with salinity of 35.5. During the winter the water temperature is 21.3 ºC and salinity 35.8.

MATERIAL AND METHODS

Tracer Experiment

Three boats were used to conduct the experiment: one to inject the tracer on the water and collect the ADCP data, one to dynamic monitor the movement of the tracer cloud in the ocean and the last one to collect water samples to measure the concentration of the tracer on the water and collect the CTD data. The measures were done along the movement axis of the plume to better capture the dispersion of the tracer.

One kilogram of Rhodamine, *Amidorhodamine G*® was diluted into 3 liters of alcohol and 47 liters of water, until a homogeneous solution with concentration of approximately 2%. The release of tracer was made by an instantaneous injection into the system, table 1 shows the location and information of injections carried at São Gonçalo and Maricá.

The set of concentration values was considered to calibrate the computer model. Were compared the concentration values measured at each point and at each moment to the values calculated by the model for these same points and instants.

Models

Delft3D, developed by *Delft Hydraulics*, was the model used to create the hydrodynamic base. To calculate the dispersion and distribution of the tracer on the water, was used CHEMMAP model, developed by *ASA*. Both models were forced with the same meteorological and oceanographic conditions found by the field team during the tracer experiment.

RESULTS AND DISCUSSION

Environmental Data

Inside Guanabara Bay, São Gonçalo region, the ADCP data indicate moderate currents during the experiment, averaging around 11 cm/s and ranging from 6 to 29 cm/s. The CTD data indicate two layers in water column, the first up to 6 m with temperature ranging from 26 to 23 ºC, density values between 1,011.00 kg/m^3 e 1,022.00 kg/m^3 and salinity from 20 to 32. In the deeper layer, more homogeneous, the temperature values ranged from23 to 21 ºC, the density remained constant at around 1,022.00 kg/m^3 and salinity been constant around 33.

During the Maricá experiment the magnitude of currents increased from 20 cm/s to 30 cm/s. The mean direction measured with ADCP is East-West. The data show a current variation between the bottom and surface during the experiment period. The CTD data indicate a layer up to 20 m with temperature values ranging from 25.3 to 22 ºC, density varied smoothly from 1,022.00 to 1,024.00 kg/m^3 and salinity between 33 and 35. In the deeper layer, between 20 and 28 m, the temperature values varied rapidly from 22 to 15 ºC, the density remained constant at around 1,025.00 kg/m^3 and salinity around 35.

Tracer Behavior and Dilution

At São Gonçalo the concentration measurements indicated that the tracer injected on sea surface mixed vertically up 2 m. Near the injection locate the highest concentration measured was about 30 mg/m^3 and at the distant points the highest concentration was about 6 mg/m^3. The tracer flows to 220º (relative true north). The analyses results in two clouds of dispersion inside de Guanabara Bay, the first one indicate a displacement of 1,700 m in the East-West axis (away from São Gonçalo) and 4,700 m in the North-South axis (toward the Bay mouth). For the second cloud the displacement was about 400 m in E-W and 1,000 m in N-S.

At Maricá the transport and dispersion tracer was strongly influenced by meteorological and oceanographic conditions and the swell. Initially the cloud presents an elongated format dispersing with the local currents. About 45 minutes after injection, with the south-southeast winds and the waves, the cloud stretched toward the beach with a length around 100 to 200 m and width of a few tens of meters. With the reduction of wind speed (1 hour after injection) the cloud tracer concentrated in circular shape and continued moving to west. With the increase of wind speed the cloud again showed an elongated format transverse the coast, the observed length was around 30 to 50 m. The measurement indicated a tracer flow to 60º (relative true north), equivalent to 7,300 m in East-West axis (parallel to coast line) and 2,500 m in North-South (approaching the coast). The highest concentration measured was 63 mg/m^3.

Far-field Model

The simulated scenarios intended to reproduce the meteorological and oceanographic conditions of the experiment period. Initially was developed the hydrodynamic model for the same date of experiment, using Delft3D model. These results were used at far-field model (CHEMMAP). Then were estimated the coefficients of horizontal dispersion to both studied areas to compare the concentration curves of environmental data and model results.

Estimation of horizontal diffusion coefficient. To calculate the diffusion coefficients were used three different methods: one based on the variance of the measured concentration; the second based on the temporal variation of the area; and the last, calculate the diffusion coefficient by the angular coefficient between the area values and time dispersion.

The first method presented was developed by Roberts & Webster (2002) where diffusion coefficient is based on variance.

Considering the equation: $E_L = \frac{1}{2}\frac{d\sigma_L^2}{dt}$, where σ^2_L is the space variance of the concentration distribution and it is also a measure of instantaneous scattering of the tracer and E_L is the diffusion coefficient.

This definition is based on the solution of the fundamental equation of the advection-dispersion (Okubo, 1966 and Okubo, 1971) and for its application are necessary information for field experience with tracers. Thus for obtaining the E_L from the field data, it is necessary to know the spatial distribution (longitudinal and transverse) of the concentration.

The procedure adopted for calculating the diffusion coefficient use the estimated spatial variance of concentration distribution. This calculation is presented below for the third navigation line of collected data at Maricá, selected as example.

Figure 1 shows the concentration values as a function of the distance, on this line. The distance is measured from the starting point of transect. For this spatial distribution of concentration the 50% percentile corresponds to 96.8 m and the 68% percentile correspond to 139.6 m (and 139.6 - 96.8 = 42.8 m), the Standart Deviation for this case is 42.8 m. The calculated variance is 1,829.0 m^2. This procedure was applied to all navigation lines. The values of variance along the lines are presented in Figure 2.

The second step was calculate the average times of each navigation line. With the time values and variance were calculated diffusion coefficient (Figure 3). The average dispersion coefficient for the period and scale of sampling was 0.88 m^2/s.

These indicate that as the tracer cloud increases as time goes, it feels the turbulent movements of increasing range and consequently the diffusivity increase too. This was observed by Okubo (1971), the author describes an apparent increase of horizontal turbulent diffusivity with increasing range of movement.

Another methodology used to calculate the diffusion coefficient consists on estimate the temporal variation of tracer cloud area. Considering the equation $A_k = \frac{Vol_k}{H} = \frac{m}{C_k \times H}$ Where, C_k is the average concentration on navigation line *k*, *H* is the thickness of plume and *m* is the tracer mass.

For each thickness the diffusivity was calculated with the variation of the area along the lines and the variation of average time. The diffusion coefficient varies between 0.01 m^2/s and 7.4 m^2/s. The average coefficient is 0.65 m^2/s, considering plumes thickness ranging from 0.1 to 6.0 m and along the lines (Figure 4).

Finally, the other way to calculate the diffusion coefficient is by calculating the angular coefficient from linear regression between the values of area and time. Figure 5 shows the range of areas along lines and for different thickness, against the average instants of sampled lines. The average angular coefficient was 0.76 m^2/s.

These same methods were applied to data sampled at São Gonçalo. For the coefficient calculated by the variance, the average value obtained was 1.56 m^2/s; for the coefficient calculated by temporal variation of area, the average value was 0.82 m^2/s and; for that obtained by the angular coefficient the value was 0.46 m^2/s.

Based on these studies and considering the results of dispersion, it was concluded that the best results were obtained using the diffusion coefficient equal to 1.0 m^2/s.

Simulation results and comparisons with environmental collected data. To illustrate the comparison between the results of far-field modeling and the collected data were selected one navigation line for each studied area.

To São Gonçalo scenario the tracer concentration were compared with the sampled concentration on the first navigation line (Figure 6). The modeling results show concentration values similar to the collected data, but displaced about 150 m. Noting that this line is distant 2.5 km of ejection point, an 150 m displacement can be neglected when analyzing the model behavior. The calculation of linear correlation coefficient does not considered these displacement, the calculation were carried independently of the line position. The correlation coefficient on São Gonçalo scenario was 0.84.

To Maricá scenario the tracer dispersion were illustrated with the sampled concentration on the fifth navigation line (Figure 7). The linear correlation coefficient (independent of line position) was 0.73.

CONCLUSIONS

The comparison between the far-field model results and sampled concentration data indicates that the model can reproduce the tracer behaviour and dilution on water satisfactorily. The linear correlation coefficient between results and collected data was 0.84 for São Gonçalo simulation and 0.73 for Maricá simulation.

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Table 1 - Information about the experiment.

Location	Date	Time (h) (UTC)	Mass (kg)	Volume (L)	Coordinates (WGS-84)	
					º West	º South
São Gonçalo	07/12/09	10:10	1	50	43,133	22,803
Maricá	09/12/09	13:30	1	50	42,944	22,999

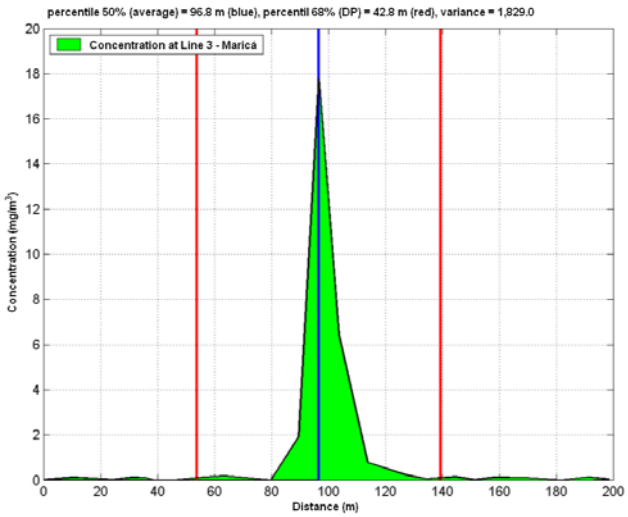

Figure 1 Navigation line nº 3 at Maricá, concentration and distance. The blue line shows the 50% percentile and red lines the 68% percentile.

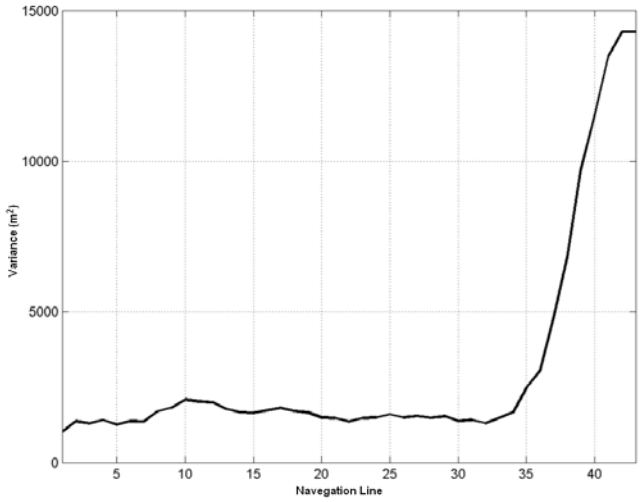

Figure 2 Variance along lines navigation.

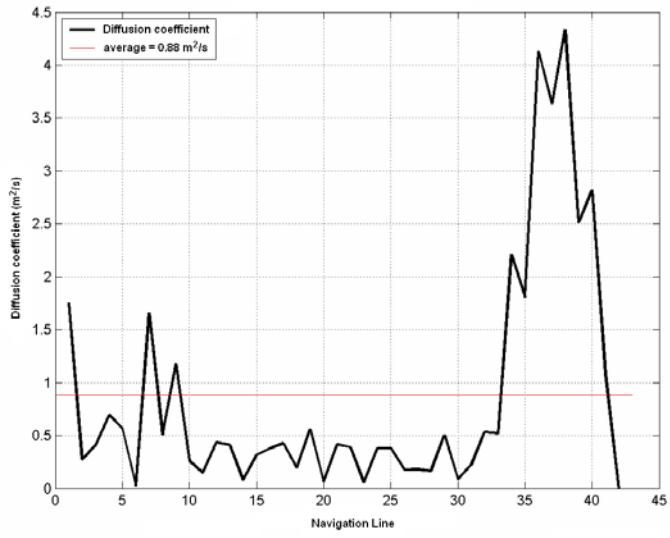

Figure 3 Estimative of diffusion coefficient.

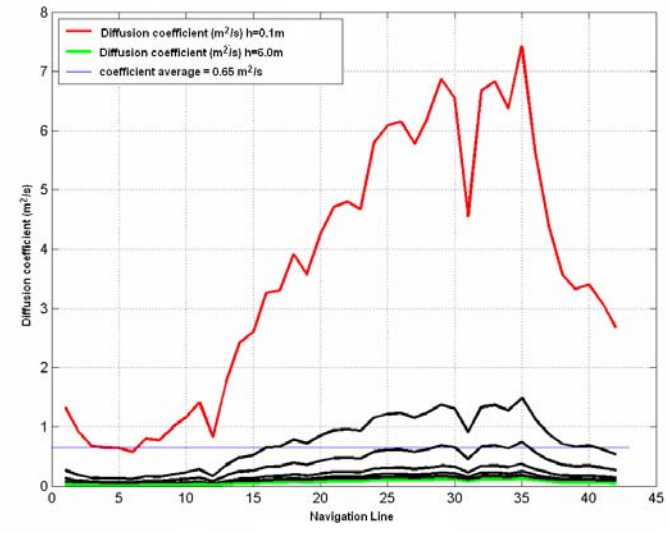

Figure 4 Estimative of horizontal diffusion coefficient.

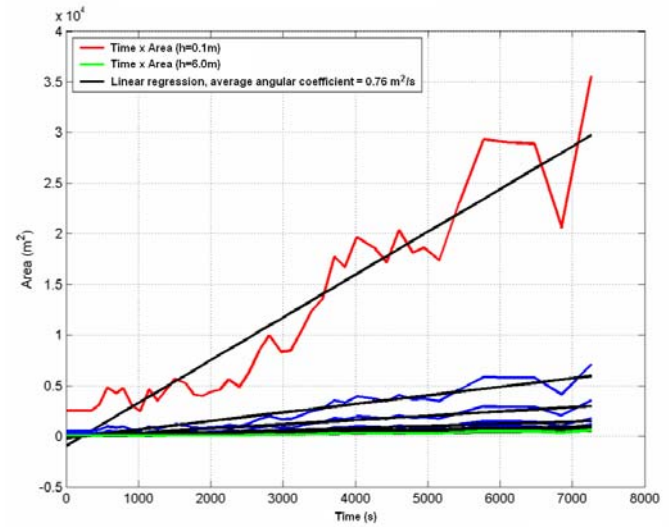

Figure 5 Estimative of horizontal diffusion coefficient by linear regression.

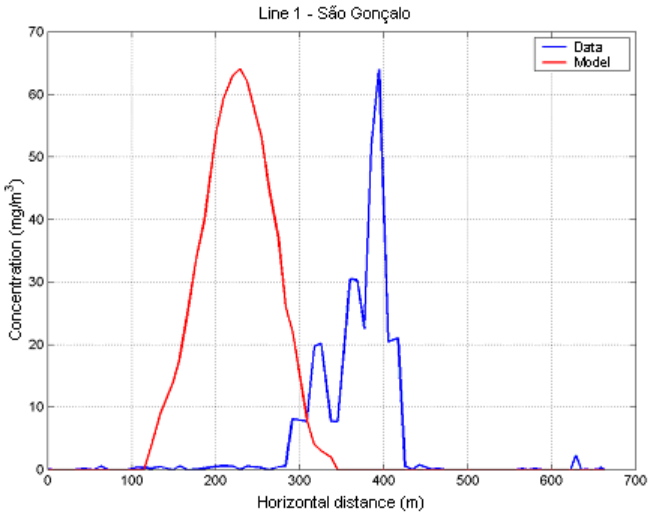

Figure 6 Compare of collected concentration and model results along the line 01, at São Gonçalo.

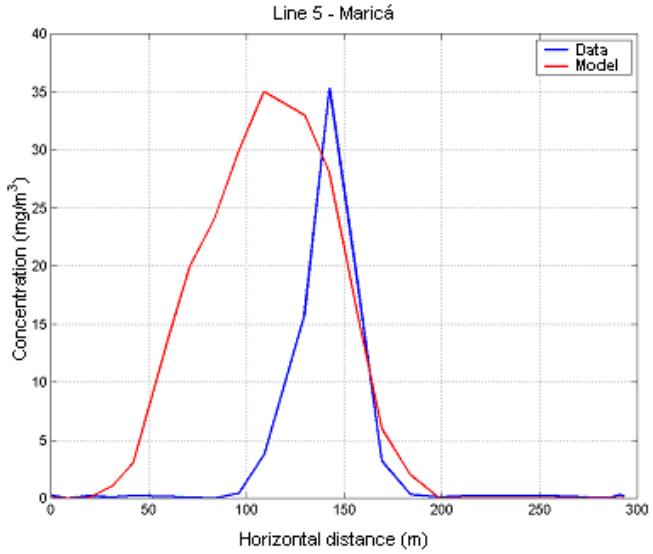

Figure 7 Compare of collected concentration and model results along the line 05, at Maricá.