



LABORATÓRIO NACIONAL
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Instituto de Pesquisas Tecnológicas
do Estado de São Paulo

Proc. 0607/17/15488

ECOMANAGE

Integrated Ecological Coastal Zone Management System

Contaminant transport modelling in the Alemoa area aquifer on Santos estuary basin

(Deliverable 2.7: Santos Estuary – Groundwater quality modelling)

Study developed for the European Commission DG
Research INCO-CT Programme under contract number
INCO-CT-2004-003715.

Study developed within the framework of LNEC Research
Plan for 2005-2008, referring to the study "Optimised
management of coastal aquifers and interaction
between groundwater and surface water"

Lisbon • March 2008

I&D HIDRÁULICA E AMBIENTE

RELATÓRIO 148/2008 – NAS

MINISTÉRIO DAS OBRAS PÚBLICAS, TRANSPORTES E COMUNICAÇÕES



Laboratório Nacional de Engenharia Civil, I.P.

Departamento de Hidráulica e Ambiente
Núcleo de Águas Subterrâneas

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IPT

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CONTAMINANT TRANSPORT MODELLING IN THE ALEMOA AREA AQUIFER ON SANTOS ESTUARY BASIN**(Deliverable 2.7 : Santos Estuary – Groundwater Quality Modelling)****ABSTRACT**

This report presents the conceptual model, the mathematical model and the computed results that allowed the quantification and mapping of the contaminant flow discharge of the illegal waste dumped in Alemoa area, at Santos Estuary, in Brazil. The physical data of the dumpsite was presented in terms of geology, hydrogeology, altimetry, evaporation and precipitation. From the results it can be concluded that groundwater and contaminant discharge of the Alemoa's wastes to Santos Estuary are mainly directed to the drains. Contaminant discharge of dumpsite to the Estuary was calculated in 1 750.49 mg/yr for benzene, 533.10 mg/yr for toluene, 8 247.04 mg/yr for lead and 646.03 mg/yr for cadmium.

MODELAÇÃO NUMÉRICA DE TRANSPORTE DE CONTAMINANTES NO AQUÍFERO NA ÁREA DO ALEMOA NO ESTUÁRIO DE SANTOS

(Deliverable 2.7: Estuário de Santos – Modelação da Qualidade das Águas Subterrâneas)

RESUMO

Este Relatório apresenta o modelo conceptual, o modelo matemático e os resultados obtidos que a quantificação da massa de contaminante transportada pelas águas subterrâneas, da área do Antigo Lixão de Alemoa para o estuário do Porto de Santos, no Brasil. Apresentam-se os dados de meio físico da área terrestre drenante para o estuário, em termos de geologia, hidrogeologia, altimetria, e precipitação. Dos resultados obtidos pode concluir-se que a descarga de águas subterrâneas e contaminantes para o estuário se faz principalmente para as valas construídas e para a rede de linhas de drenagem naturais. A descarga de contaminantes advindos da área do Antigo Lixão de Alemoa para o estuário foi calculada em 1 750,49 mg/ano para o benzeno, 533,10 mg/ano para o tolueno, 8 247,04 mg/ano para o chumbo e 646,03 mg/ano para o cádmio.

ACKNOWLEDGEMENTS

The authors do acknowledge the support of the 6th Framework Program of the European Commission for ECOMANAGE “Integrated Ecological Coastal Zone Management System” Project, INCO-CT-2004-003715, (cf. <http://www.dha.lnec.pt/nas/english/projects/ecomanage.htm>) as well as Laboratório Nacional de Engenharia Civil, I.P. Portugal, and, Instituto de Pesquisas Tecnológicas S.A.- IPT, for supporting this work in the framework of their protocol, led by Dr. JP Lobo-Ferreira in LNEC and Dr. Malva Mancuso in IPT.

Special thanks are also due to:

- Alexandra Sampaio (UNISANTA) for searching and getting the authorization to use the groundwater data needed on this work;
- Companhia Docas do Estado de São Paulo - CODESP for allowing using groundwater data of the sedimentary aquifer located in Alemoa, Santos.

TECHNICAL NOTES

The accomplishment of the present work counted on the contribution of some colleagues of LNEC and of IPT to whom the authors are thankful, in accordance with the note below:

- Dr. Teresa Leitão (LNEC, I.P.) for the discussions on groundwater quality subject.
- Dr. José Luiz Albuquerque Filho (IPT/CETAE/LABGEO) and MSc Sérgio Gouveia de Azevedo (IPT/CETAE/LABGEO) for the discussions on groundwater system subject.
- Dr. Malva Mancuso (IPT/CETAE/LABGEO) for the discussions on groundwater flux modelling subject.

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CONTAMINANT TRANSPORT MODELLING IN THE ALEMOA AREA AQUIFER ON SANTOS ESTUARY BASIN

(Deliverable 2.7 : Santos Estuary – Groundwater Quality Modelling)

1 Introduction

ECOMANAGE project aims to push the capacity of assisting managers to join horizontally knowledge from ecological and socio-economic disciplines. The three key aspects of ECOMANAGE are the consideration that: (1) a coastal zone depends on local pressures, but also on pressures originated in the drainage basin, transported mostly by rivers and by groundwater; (2) socio-economic activities are the driving forces of those pressures and that their impacts on the ecosystem have feedback on socio-economics; and, (3) the impacts depend on physical characteristics of the ecosystem that together with the loads determine its ecological state.

Three coastal zones showing conflicting interests between urban, industrial and agricultural pressures and environmental maintenance have been selected for developing the system. The selected areas are: Aisén Fjord in Chile, Bahía Blanca estuary in Argentina and Santos estuary in Brazil.

The purpose of this deliverable is to report on the groundwater flow and contaminant transport modelling of the sedimentary aquifer at Alemoa area system for Santos Estuary basin. That allowed the evaluation of the contribution of the contaminant loads from the aquifer system at Alemoa's dump to the Estuary, on steady state conditions.

There was not enough quantitative data about contamination at Santos Estuary Basin. The illegal waste dumped in Alemoa area was the first modelling approach chosen to represent quantification of diffuse pollution loads, discharging to the Santos Estuary.

The model was developed using the following software: Ground Water Modelling System – GMS, with the modules MAP, MODFLOW, PEST, MODPATH, and MT3D.

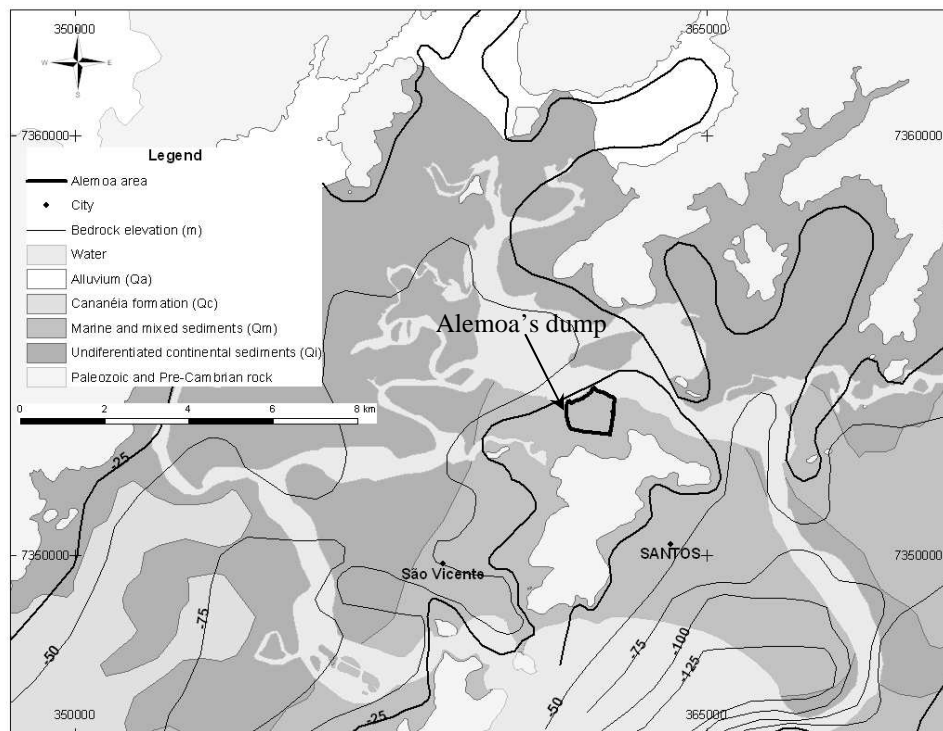
2 General Description

The dumpsite is placed at Alemoa quarter, one of the oldest of the city of Santos, in the coast of the State of São Paulo, Brazil. This area is inside of the limits of the Santos Port, where today is located an important industrial complex, with patios and deposits of containers used to transport loads to and from the Santos Port.

The area of this study is about 917 174.2 m², and in its neighbourhood predominates terminals of liquid granaries storage and small commerce. The Alemoa's dump is located inside the Estuary Basin area,

in the "Unidade de Gerenciamento de Recursos Hídricos" (Water Resources Management Unit) nr 7, called "Bacia Hidrográfica da Baixada Santista" ("Baixada Santista" Hydrographic Basin).

The dumpsite includes part of the land area that contributes with fresh water (flows at the surface or underground) to the Santos Estuary (Fig. 1).



Source: modified from Mancuso and Lobo Ferreira (2007)

Figure 1 – Map localization of the study area

The Alemoa's dump was used for more than 50 years as a disposal for solid waste related to the operation of Santos Port and domestic waste illegally dumped in the area. Beyond these activities, the area was used to store and move explosives on the access bridge made of armed concrete built in the extremity of the land, on the implantation of seedbed of workmanships for the magnifying of the wharf in the stretch Valongo-Paquetá and from the material dragged during the activities of implantation of Petrobras' terminal.

According to exposition scenes, the area was considered by ASTM 1739/95 as a type 1 scenario associated with immediate risks. This classification was determined once the area fits in the affirmation "A sensible habitat (e.g. mangrove, Atlantic Forest, etc.), environmental protected areas or sensible receivers (species economically important, species in danger or threatened species) are impacted or affected" (ESSENCIS, 2005).

3 Groundwater Conceptual Model

3.1 Introduction

A groundwater flow model was developed for the sedimentary aquifer. The conceptualization was based on the physical system, its geometry, geology and hydrogeology. The conceptual model also comprises groundwater recharge estimation and water budget understanding.

The area for modelling was defined in AutoCAD, using lithologic and hydrogeologic information of 35 boreholes. As a boundary condition for the sedimentary aquifer, it was considered the crystalline interface at -25 m deep. To delimitate this area a topographic map (AGEM, 1:1 000) was used. The data was used to produce a grid with 10 m x 10 m cells representing the elevation surface.

3.2 Geology and Hydrogeology

The geology of the area may be grouped into the basement formations (Palaeozoic and Pre-Cambrian) and Cenozoic cover (marine and mixed sediments).

The basement formations are the result of several tectonic phases, responsible for deformation, faulting, foliation, besides metamorphism and magmatic processes, combined with variations of climate and sea level. Inland, several faulting and epeirogenesis have produced the escarpment of the actual Serra do Mar. In the Cenozoic, the main events may be summarised in topography modelling, tropical humid climate, sea transgression and deposition of the sedimentary sequences (MANCUSO and LOBO-FERREIRA, 2007).

Data from hydraulic conductivity in the area was estimated as a function of the lithology (siltic clayey deposits): K_x , K_y , K_z = 0.1 to 0.5 m/d. Groundwater levels have been monitored for mapping of the piezometry (ESSENCIS, 2005). Groundwater levels are almost at surface and vary from 0 to 4 m elevation (Table 1).

3.3 Groundwater Recharge

Groundwater recharge, for modelling purpose ($R = 678$ mm/year), was estimated as 28.2% from precipitation (MANCUSO and LOBO-FERREIRA, 2007).

Table 1 – Monitored groundwater levels for the mapping of the piezometry

Well	X	Y	Topographic elevation (m)	Hydraulic Head (m)
S-11/PM	362 381.1790	7 353 714.1481	3.1785	1.5785
S-15/PM	362 205.2999	7 353 408.6719	1.5729	0.5
S-16/PM	362 194.5880	7 353 410.9418	1.5712	0.5
S-17/PM	362 361.8205	7 353 385.7727	1.7835	0.2835
S-18/PM	362 371.9807	7 353 383.6483	1.7689	0.3889
S-19/PM	362 659.9835	7 353 350.3634	1.6094	0.6794
S-20/PM	362 669.3322	7 353 349.2198	1.6821	0.7521
S-21/PM	361 612.8594	7 353 519.6963	1.5748	0.5
S-22/PM	361 627.2878	7 353 516.8373	1.5496	0.2596
S-24/PM	361 809.0861	7 353 549.9354	0.8947	0.5
S-25/PM	361 820.7692	7 353 549.0139	0.8391	0.5
S-26/PM	361 972.9756	7 353 410.2031	1.4878	0.7178
S-27/PM	361 982.6487	7 353 408.1024	1.4923	0.5
S-28/PM	362 530.4385	7 353 311.2870	0.9544	0.5
S-29/PM	362 540.3839	7 353 309.3671	0.9465	0.5
S-30/PM	362 219.2530	7 353 562.8653	3.2118	2.4118
S-31/PM	362 141.4904	7 353 499.4137	2.5203	1.1203
S-32/PM	362 046.3260	7 353 527.7851	1.8496	0.5296
S-33/PM	361 950.1086	7 353 602.3781	2.0011	0.8611
S-35/PM	362 236.5749	7 353 660.7956	3.0669	0.5
S-36/PM	362 098.3407	7 353 718.9518	1.3379	0.4979
S-37/PM	362 209.2419	7 353 753.7544	1.0398	0.4498
S-38/PM	362 288.1165	7 353 877.9594	1.3640	0.3640
S-39/PM	362 335.3982	7 353 940.6594	1.2161	0.4161
S-40/PM	362 259.0458	7 353 778.3469	1.2681	0.4681
S-41/PM	362 267.9424	7 353 776.0556	1.3550	0.6050
S-42/PM	362 334.3059	7 353 897.9153	1.2974	0.3774
S-43/PM	362 334.0463	7 353 906.4752	1.3275	0.4075
S-44/PM	362 327.6866	7 353 784.2366	1.0685	0.5
S-46/PM	362 313.4012	7 353 656.4726	3.6828	3.0228
S-47/PM	362 462.3715	7 353 663.6543	3.4739	2.6539
S-48/PM	362 286.7464	7 353 603.4566	4.6301	4.2301
S-49/PM	362 281.7879	7 353 538.4477	5.4615	1.4915
S-50/PM	362 290.7011	7 353 538.9316	6.0120	2.7820
S-55/PM	362 049.9415	7 353 647.6317	3.5050	1.4850

4 Groundwater Mathematical Model

4.1 Introduction

The total area modelled is 917 174.2 m² and comprises part of São Vicente island.

The mathematical groundwater flow model used in this study was MODFLOW. MODFLOW was first published by MCDONALD and HARBAUGH (1988). The flow model was developed considering flow as a

steady state, with lakes and the channel considered as constant head cells. Rivers were simulated as drains.

Considering the lithology, a two layers model was defined, with both layers on the porous aquifer. The bottom elevation of the first layer is -3.5 m, and the second is -25 m, so the first layer has a thickness of 4 m until 10 m.

4.2 Grid

The 3D model grid starts at the World Coordinates X = 361 606.269 m, Y = 7 352 826.235 m and Z = -25 m, ending at X = 362 878.551 m, Y = 7 354 058.188 m and Z = -25 m. The model has two layers subdivided into 123 rows by 127 columns. Each cell is 10 m by 10 m long in the xx and yy directions (Table 2). The thickness for layer 1 varies according to the topography.

Table 2 – Grid characteristics for Alemoa area groundwater model

Grid	Dimension		
	x	y	z
Origin	361 609.27 m	7 352 826.24 m	-25 m
Length	1 272.28 m	1 231.95 m	32 m
Number of Cells	127	123	2
Cell Size	10 m	10 m	

4.3 Layer Attributes

A layer was built to input recharge, hydraulic conductivity and a boundary in Modflow Model. The hydrogeological characterisation was accomplished using the geometry and hydraulic data from the geological formations.

4.4 Source/Sinks Attributes

Surface water from river, drains and Santos estuary was represented as drains, river and constant head on Modflow model. The drains were represented on the first layer as a partially penetrating water system. The river was represented as an interception system for groundwater flow, and the Santos estuary has been represented as a constant head and a fully interception system for groundwater flow. Considering the purpose of this work, the groundwater and sea water interaction was not simulated. The constant head boundary at 0 m allowed quantifying mean groundwater discharge from the sedimentary aquifer.

4.5 Groundwater Recharge

Calibration was obtained using recharge values of 678 mm/year.

4.6 Hydraulic Conductivity

Hydraulic Conductivity was obtained using an inverse model, named Modflow 2000 PES Process. This program adjusts a user-defined set of input parameters until the difference between the computed and observed values is minimized.

Figures 2 and 3 presents the parameters adopted by Modflow 2000 PES Process to obtain the hydraulic conductivity in Alemoa’s dump.

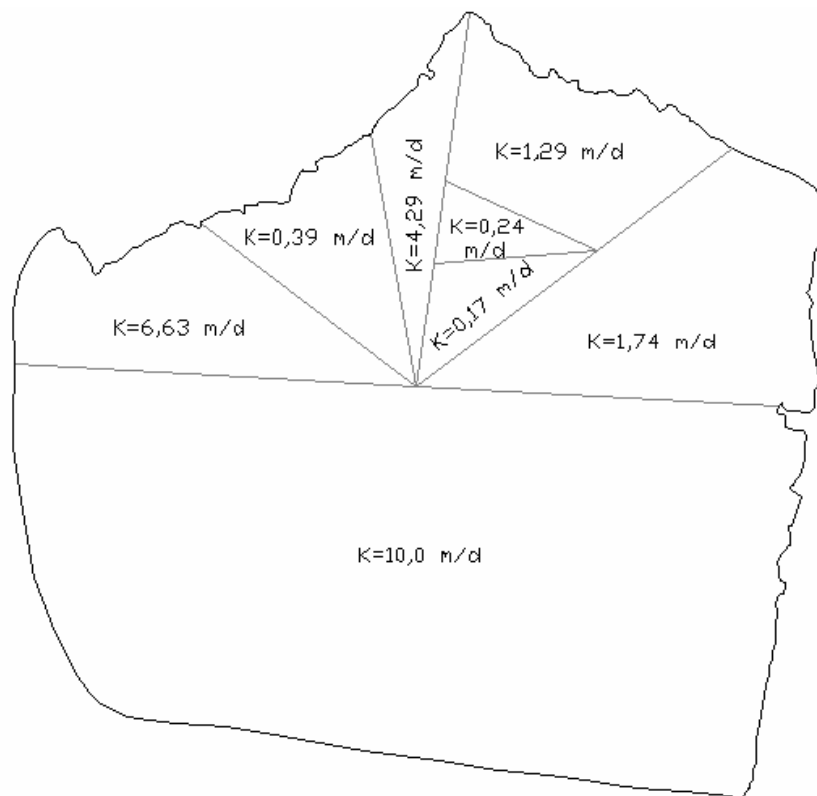


Figure 2 – Hydraulic conductivity (K) for layer 1 in Alemoa’s dump site

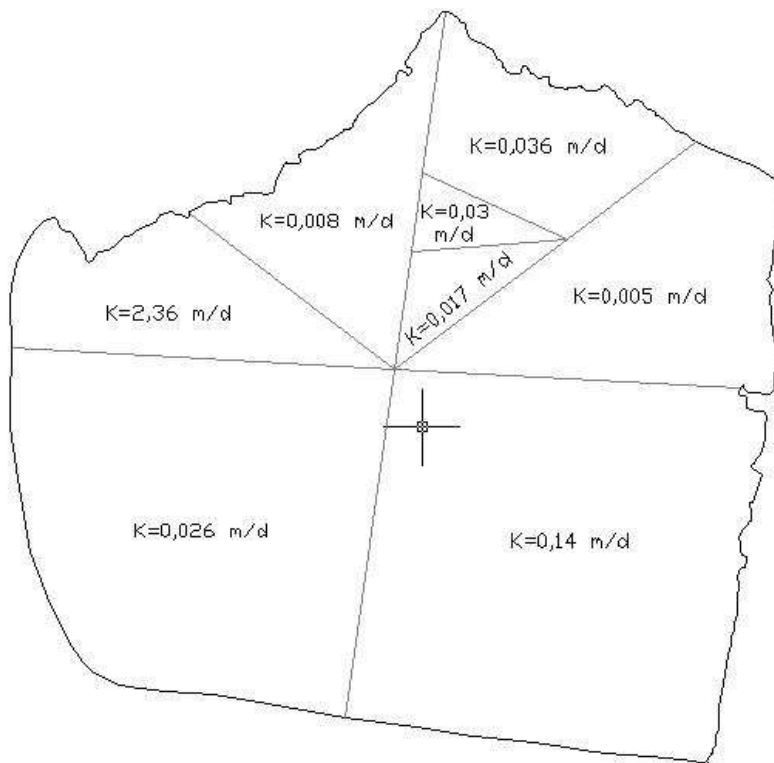


Figure 3 – Hydraulic conductivity (K) for layer 2 in Alemoa’s dump site

4.7 Results

The objective of the model calibration is to obtain a piezometric surface compatible with observed heads. In the Alemoa area, the groundwater flows towards the river and the drains opened according to the development needs from urban and Santos Estuary.

Water budget showed that flow in and out from the system are almost the same, with a discrepancy minor than 0.001%. According with the model results, total discharge from groundwater is 1 714 m³/d, 542 m³/d (24%) flows to the Estuary, 1 106 m³/d (56%) to the drains and 66 m³/d flows to the river (Table 3).

Table 3 – Water budget from Modflow model

CUMULATIVE VOLUMES (m ³)	
IN:	OUT:
STORAGE = 0.0000	STORAGE = 0.0000
CONSTANT HEAD = 3.3818	CONSTANT HEAD = 542.4811
DRAINS = 0.0000	DRAINS = 1 106.1559
RIVER LEAKAGE = 3.5751E-02	RIVER LEAKAGE = 66.1794
RECHARGE = 1 711.3975	RECHARGE = 0.0000
TOTAL IN = 1 714.8149	TOTAL OUT = 1 714.8163

IN - OUT = -1.3428E-03
 PERCENT DISCREPANCY = 0.00

5 Particle Trajectory

The particle trajectory was estimated using Modpath Processor. Modpath was originally created by David W. Pollack (1989) and uses the output files generated by Modflow model to calculate imaginary particle flow paths in the groundwater of the system.

Figure 4 presents the particle trajectories computed with Modpath Processor, representing the flow path using a dark blue arrow. The arrows in colour show the flow field obtained with Modflow model.

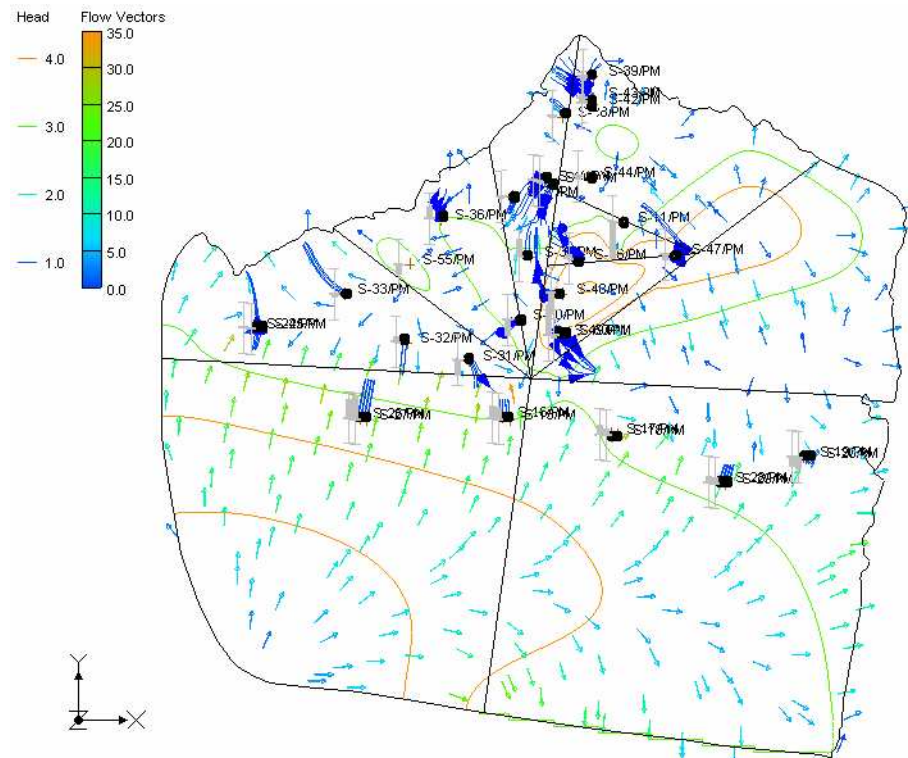


Figure 4 – Particle trajectory and flow vectors shaped using Modpath processor and Modflow

6 Results Computed with the MT3D Mathematical Model

The mathematical model used to represent the contamination plume was MT3D. The model was published by Zheng and Wang (1999) and it is used to calculate the transport of a contamination plume by solving the transport equations.

Four setups of the transport models were developed to assess the contamination plumes of benzene, cadmium, lead and toluene for a period of 100 years. The input data used by this model followed the same procedure used for Modflow model.

The concentration of contaminants obtained in each observation well has considered a constant load into the aquifer, which causes the contamination plume. Table 4 shows the concentration of contaminants used in each observation well for MT3D model development.

Table 4 – Contaminant concentration in observation well for MT3D model

	Cadmium (mg/l)	Lead (mg/l)	Benzene (mg/l)	Toluene (mg/l)
S11/PM	0.030	0.198	0.267	0.951
S15/PM	0.027	0.092	ND	ND
S16/PM	0.060	0.216	ND	ND
S17/PM	0.027	0.14	ND	0.0208
S18/PM	0.011	0.073	ND	0.0285
S19/PM	0.025	0.098	ND	0.0364
S20/PM	0.011	0.070	ND	0.013
S24/PM	0.02	0.097	ND	0.00939
S25/PM	0.012	0.127	ND	0.128
S26/PM	0.010	0.481	ND	ND
S27/PM	0.025	0.144	ND	ND
S28/PM	ND	0.062	ND	ND
S29/PM	0.022	0.101	ND	ND
S30/PM	ND	0.118	0.548	0.111
S31/PM	ND	0.298	0.213	0.0739
S32/PM	0.027	0.089	ND	ND
S33/PM	0.018	5.350	0.145	0.0188
S35/PM	ND	0.383	0.3	0.0486
S36/PM	ND	0.209	ND	ND
S37/PM	0.022	0.082	ND	ND
S38/PM	0.022	0.120	ND	ND
S39/PM	ND	0.084	ND	ND
S40/PM	0.030	0.096	ND	0.00304
S41/PM	ND	0.06	ND	0.00451
S42/PM	0.015	0.089	0.0781	0.00942
S43/PM	0.011	0.105	1.198	0.01
S44/PM	ND	0.437	0.0382	0.0234
S46/PM	0.011	0.181	0.597	0.0236
S47/PM	ND	0.104	0.0129	0.184
S48/PM	ND	0.155	0.0371	0.0149
S49/PM	0.025	0.096	0.0063	0.0104
S50/PM	ND	0.430	0.895	0.24
S55/PM	0.030	0.139	0.0881	ND
CETESB: Orienting Values	0.005	0.010	0.005	0.700

The development of the MT3D model allowed the assessment of groundwater contamination, and the computation of contamination loads flowing into rivers, drains and the Santos Estuary.

The contaminant balance showed that the contamination flow, in and out from the system, is almost the same, with a discrepancy smaller than 0.001%. Table 5 presents a synthesis of contaminant discharge to Santos Estuary, and Figures 5 to 8 and Tables 6 to 9 present the mass budget in 100 years for Benzene, Toluene, Cadmium and Lead.

Table 5 - Contaminant discharge to Santos Estuary

Compounds	Drains (mg)	Drains (mg/yr)	Santos Estuary (mg)	Santos Estuary (mg/yr)	Total Discharge (mg)	Total Discharge (mg/yr)
Benzene (C ₆ H ₆)	130 443.00	1 304.43	44 605.91	446.06	175 048.91	1 750.49
Cadmium (Cd)	59 247.54	592.48	5 355.097	53.55	64 602.637	646.03
Lead (Pb)	494 854.80	4 948.55	329 849.90	3 298.50	824 704.70	8 247.05
Toluene (C ₇ H ₈)	51 095.49	510.95	2 214.61	22.15	53 310.10	553.10

7 Conclusions

This Report presents a first approach for the evaluation of contaminant discharges from the illegal waste dumped in Alemoa area into Santos Estuary, in Brazil. It was based only on existing data. It is important to collect new data to improve this first modelling approach.

Considering the existing data, the contaminant transport model allowed the simulation of advection and dispersion into the aquifer system. The final aim was the quantification of diffuse pollution loads, discharging to the Santos Estuary.

From the results it can be concluded that the contaminant discharge of the Alemoa's dump to Santos Estuary are mainly directed to the drains, *i.e.* the values of directly flowing groundwater diffuse pollution into Santos Estuary are smaller than those values flowing to drains. Contaminant discharge of dumpsite to the Estuary was calculated as 1 750.49 mg/yr to benzene, 533.10 mg/yr to toluene, 8 247.04 mg/yr to lead and 646.03 mg/yr to cadmium.

The authors do suggest this research work to be further improved. This requires additional detailed field information, becoming available in terms of piezometry, inventory of wells, contaminant monitoring data, risk assessment, geophysical data, and hydraulic characterisation and remediation techniques alternatives studies.

Figure 5 – Contamination plume for Benzene

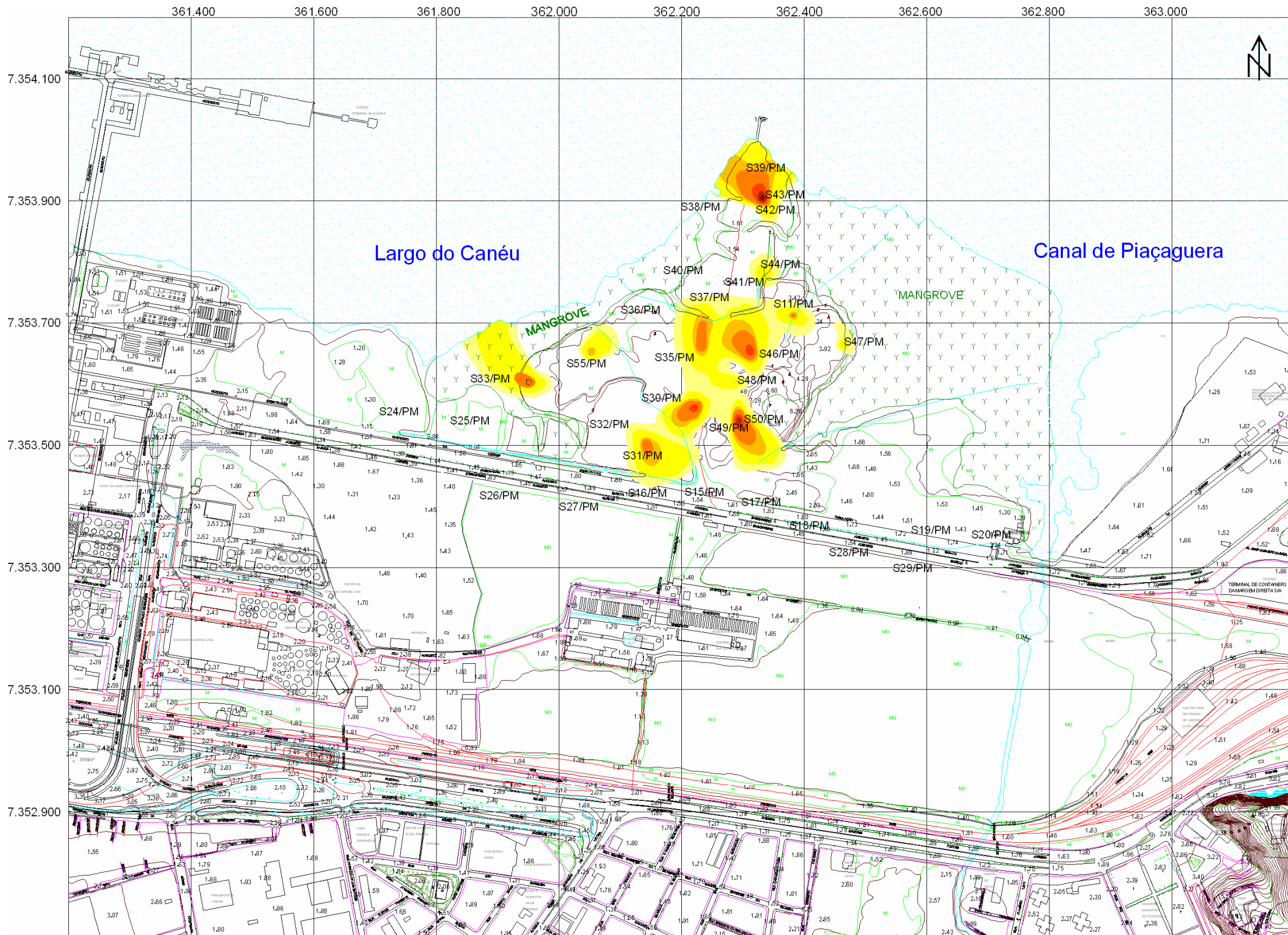


Table 6 – Mass budget for Benzene

	In (mg)	Out (mg)
CONSTANT CONCENTRATION	224 973.40	- 25 790.25
CONSTANT HEAD	0.000000	- 44 605.91
DRAINS	0.000000	- 130 443.00
RIVERS	0.000000	- 0.1913011 e-13
RECHARGE	0.000000	0.000000
MASS STORAGE (SOLUTE)	52.06100	-24 207.45
[TOTAL]	225 025.40	-225 046.60

NET (IN - OUT): -21.14062
 DISCREPANCY (PERCENT): -0.9394330E-02

Benzene concentration in groundwater (mg/L)

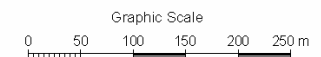
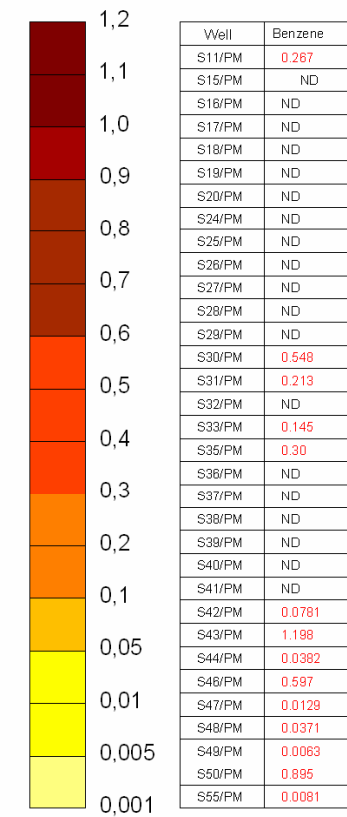


Figure 6 – Contamination plume for Toluene

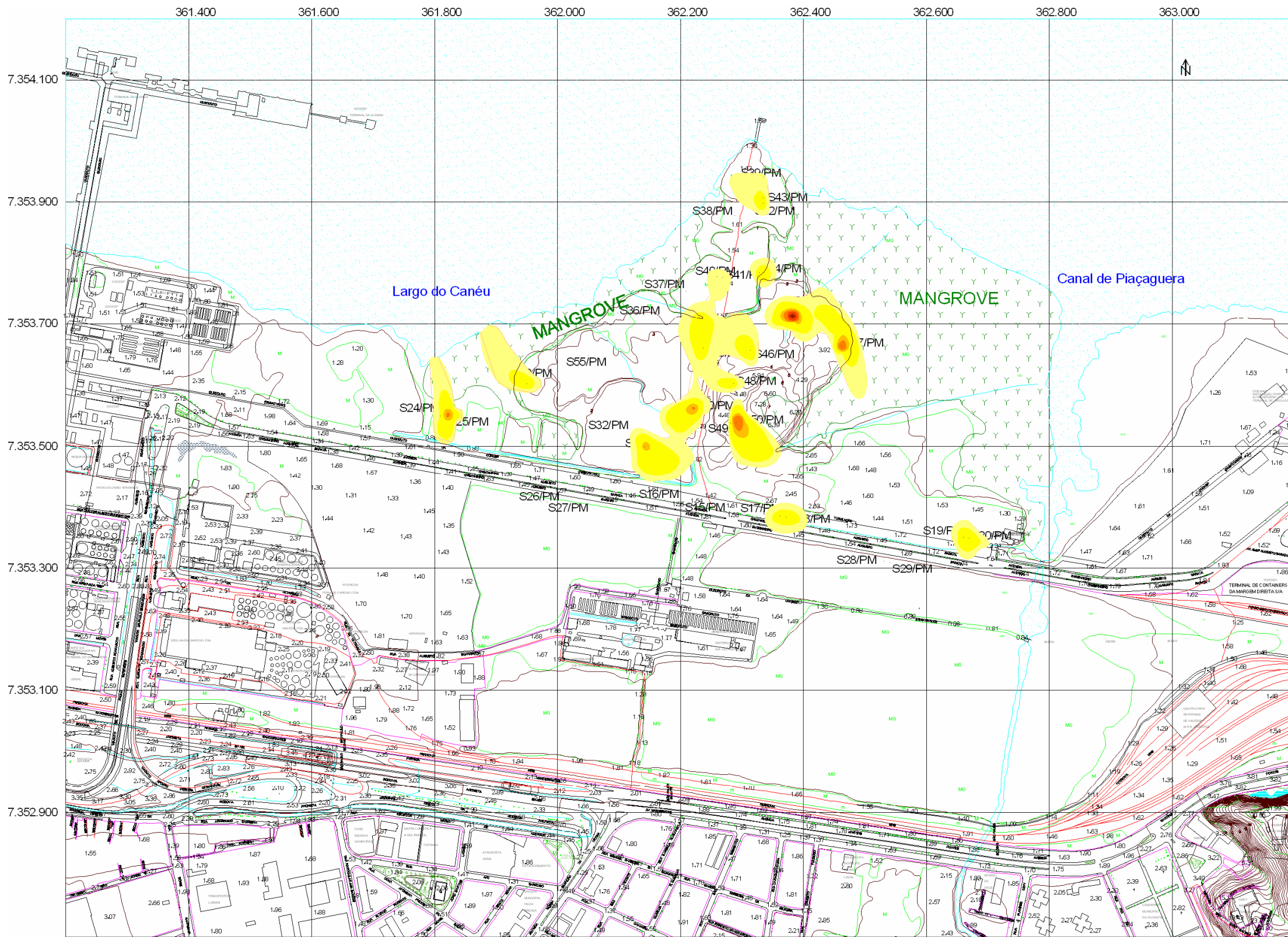
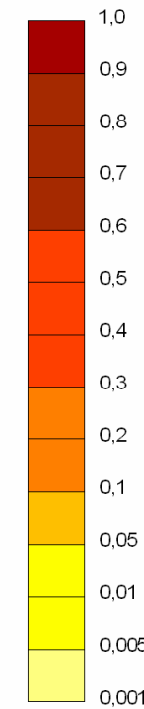


Table 7 – Mass budget for Toluene

	In (mg)	Out (mg)
CONSTANT CONCENTRATION	82 006.40	-22 891.92
CONSTANT HEAD	0.000000	- 2 214.610
DRAINS	0.000000	- 51 095.49
RIVERS	0.000000	- 0.6310048 e-6
RECHARGE	0.000000	0.000000
MASS STORAGE (SOLUTE)	13.82644	- 5 967.535
[TOTAL]	82 020.23	-82 169.55

NET (IN - OUT): -149.3203
DISCREPANCY (PERCENT): -0.1818874

Toluene concentration in groundwater (mg/L)



Well	Toluene
S11/PM	0.030
S15/PM	0.027
S16/PM	0.060
S17/PM	0.027
S18/PM	0.011
S19/PM	0.025
S20/PM	0.011
S24/PM	0.020
S25/PM	0.012
S26/PM	0.010
S27/PM	0.025
S28/PM	ND
S29/PM	0.022
S30/PM	ND
S31/PM	ND
S32/PM	0.027
S33/PM	0.018
S35/PM	ND
S36/PM	ND
S37/PM	0.022
S38/PM	0.022
S39/PM	ND
S40/PM	0.030
S41/PM	ND
S42/PM	0.015
S43/PM	0.011
S44/PM	ND
S46/PM	0.011
S47/PM	ND
S48/PM	ND
S49/PM	0.025
S50/PM	ND
S55/PM	0.030

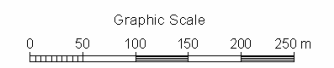


Figure 7 – Contamination plume for Cadmium

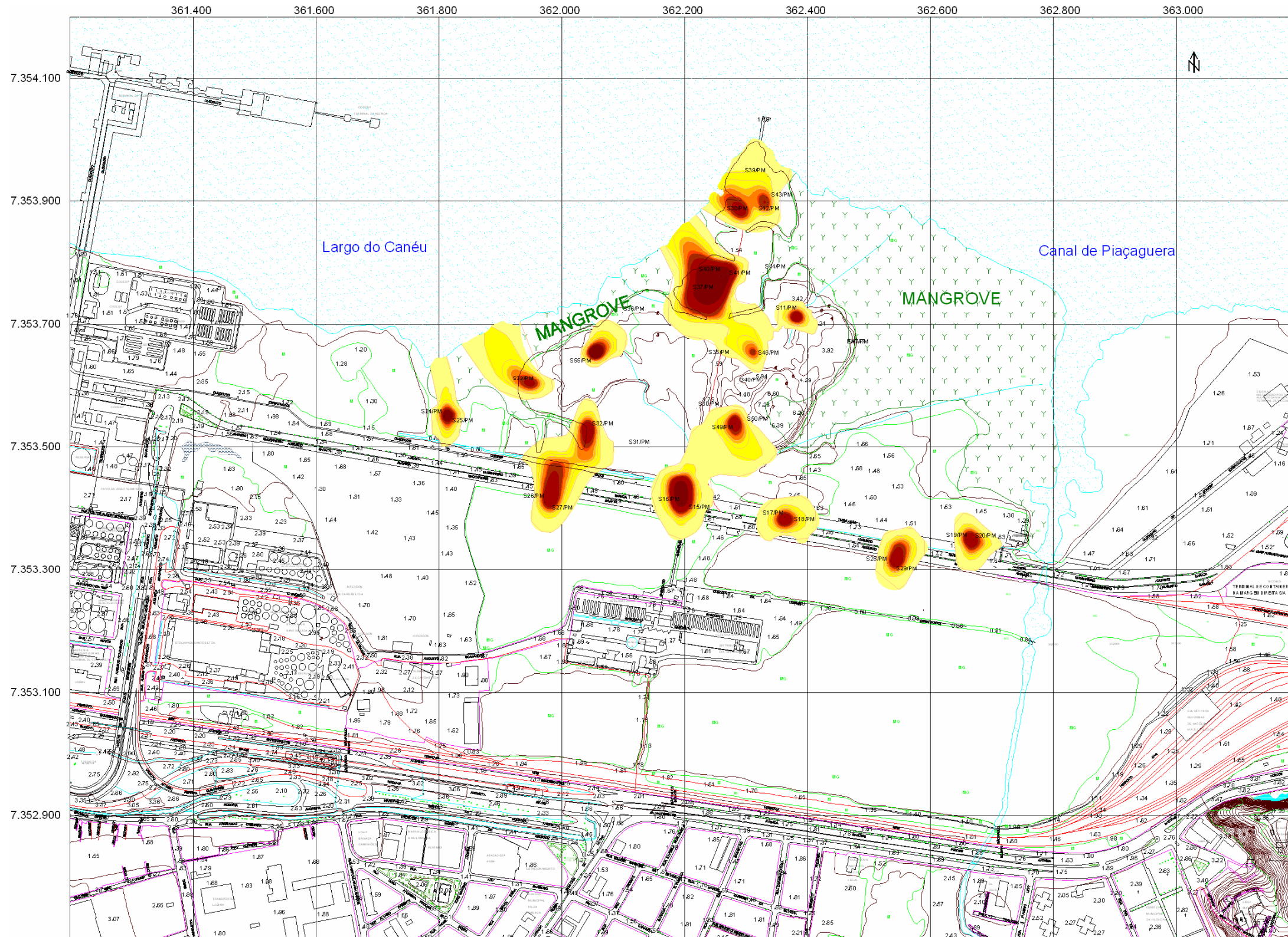


Table 8 – Mass budget for Cadmium

	In (mg)	Out (mg)
CONSTANT CONCENTRATION	76 920.11	- 8 057.009
CONSTANT HEAD	0.000000	- 5 355.097
DRAINS	0.000000	- 59 247.54
RIVERS	0.000000	- 0.5247957 e ⁻⁶
RECHARGE	0.000000	0.000000
MASS STORAGE (SOLUTE)	5.804924	- 4 282.970
[TOTAL]	76 925.91	- 76 942.62

NET (IN - OUT): -16.70312

DISCREPANCY (PERCENT): -0.2171090E-01

Cadmium concentration in groundwater (mg/L)

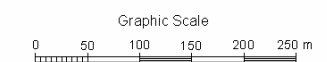
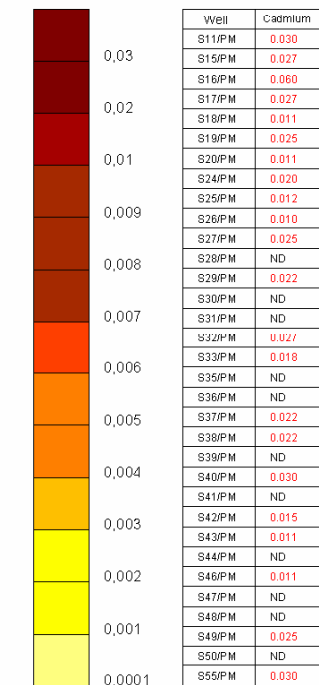


Figure 8 – Contamination plume for Lead

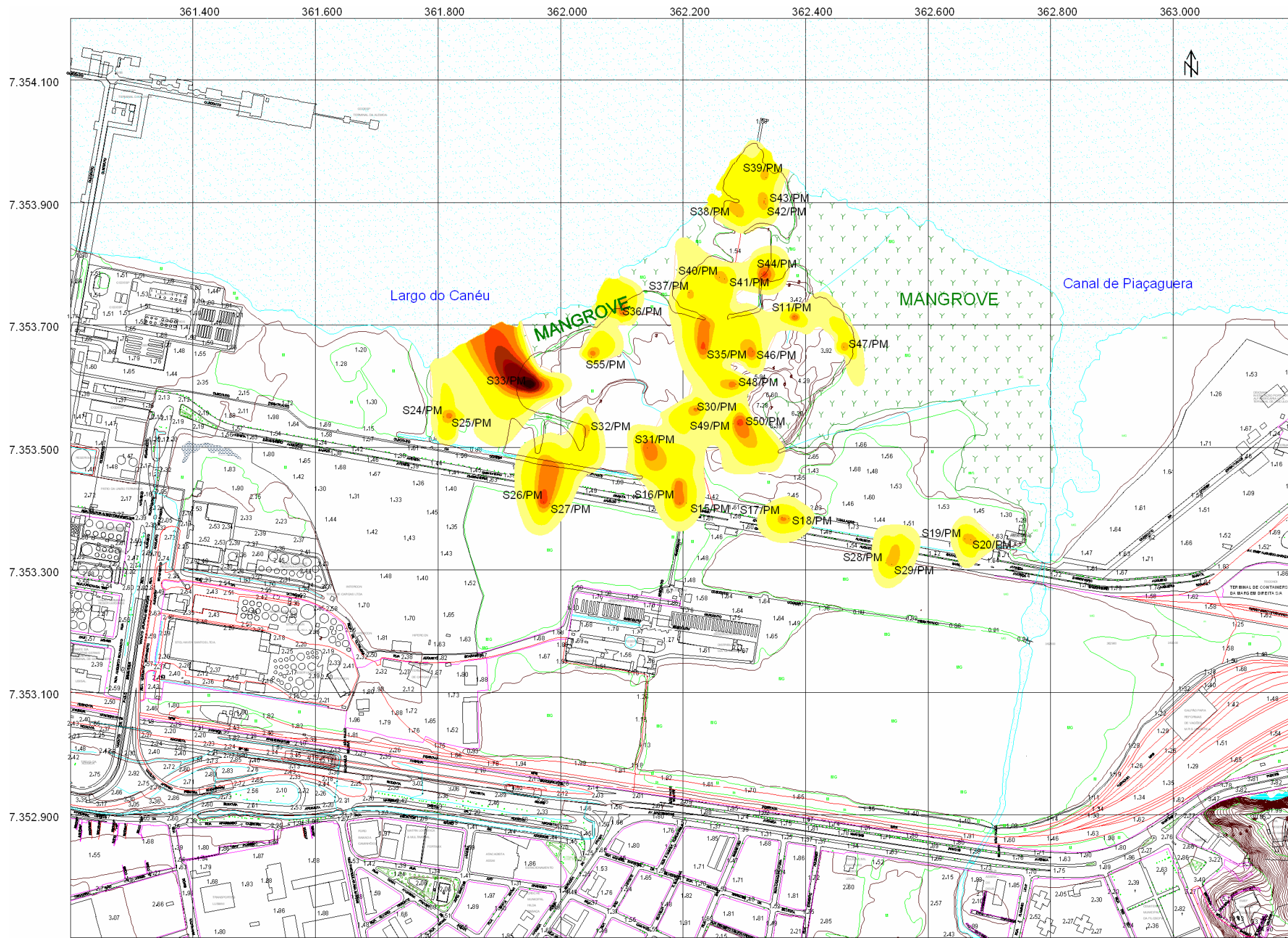
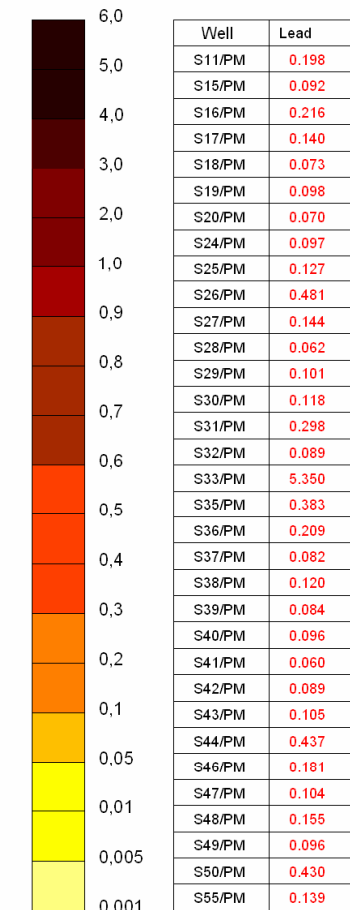


Table 9 – Mass budget for Lead

	In (mg)	Out (mg)
CONSTANT CONCENTRATION	963 184.6	- 57 823.38
CONSTANT HEAD	0.000000	- 329 849.9
DRAINS	0.000000	- 494 854.8
RIVERS	0.000000	- 0.2386230 e-5
RECHARGE	0.000000	0.000000
MASS STORAGE (SOLUTE)	120.4294	- 81 705.09
[TOTAL]	963 305.1	- 964 233.2

NET (IN - OUT): -928.1250
 DISCREPANCY (PERCENT): -0.9630159E-01

Lead concentration in groundwater (mg/L)



São Paulo, Instituto de Pesquisas Tecnológicas do Estado de São Paulo, Brazil
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