

**SOFTWARE FOR THE ASSESSMENT OF MASS BALANCE AND
BIODEGRADATION IN AQUIFERS
USER'S GUIDE – VERSION 1.0**

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FRENCH SUMMARY

Le logiciel SAMBBA (Software for the Assessment of Mass Balance and Biodegradation in Aquifers) a été créé pour faciliter la mise en œuvre de la méthodologie MACAOH relative à l'étude de la faisabilité de l'Atténuation Naturelle comme mesure de gestion d'un site pollué (Côme et al, 2006a). Outre une base de données, il est composé de deux modules correspondant chacun à une étape de la méthodologie :

- Le module « qualitative assessment » permet d'évaluer qualitativement si le mécanisme de biodégradation est actif sur le site d'étude et, s'il l'est, sous quelles conditions (aérobie, anaérobie en zone méthanogène, sulfato- ou ferri-réductrices...) (étape 2 de la méthodologie) ;
- Le module « quantitative assessment » est dédié au calcul de la proportion de chaque mécanisme participant à l'atténuation naturelle d'un panache de polluant (convection, dispersion, dilution, volatilisation et lessivage...). Il est basé sur le principe de bilan des flux et permet de calculer des taux de biodégradation (étape 3 de la méthodologie).

Le présent ouvrage est le guide de l'utilisateur pour ce logiciel (SAMBBA, version 1.0). Il est composé d'instructions pour lancer l'application, d'une description des différentes fenêtres de l'interface et d'un tutorial pour chacun des modules.

Ce logiciel a été développé par BURGEAP avec l'aide de l'Institut de Mécanique des Fluides de Toulouse (IMFT) dans le cadre d'un projet de Recherche & Développement cofinancé par l'ADEME. BURGEAP est propriétaire des sources de ce logiciel. Le logiciel SAMBBA est distribué gratuitement.

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1. Getting Started with SAMBBA

The only system requirement for SAMBBA to run on your computer is the .NET framework which commonly comes with Windows. The supported systems are Windows XP and further. Space requirement (for SAMBBA to be installed) is **85.4MB**. There is no set up procedure to install the application.

The first time you use SAMBBA, follow the steps below:

- Copy the SAMBBA folder called *SAMBBAApp_v1.0* on your computer;
- Check that the whole folder is present. It should include four folders: *Icons*, *Release*, *Template and Tutorial* for a total size of **85.4MB**;
- Run *SAMBBA.exe* located in the *Release* folder.

2. What does SAMBBA do?

SAMBBA is an application to help users to proceed through the MACAOH methodology when assessing the feasibility of the monitored natural attenuation (MNA). This methodology is fully described in the technical guide "MACAOH - Atténuation naturelle" for French readers (Côme et al, 2006a)¹. An extended abstract of this guide is also available in English². The methodology includes four successive steps (Figure 1):

- **step 1:** preliminary data analysis to specify the spatial structure and temporal evolution of the pollution at the identified receptors;
- **step 2:** qualitative evaluation of the biodegradation mechanisms of dissolved and gaseous compounds in the plumes;
- **step 3:** quantitative evaluation, based on mass balances, of natural attenuation processes in the source zone and the plumes (vapour and dissolved in groundwater);
- **step 4:** prediction of the temporal evolution of NAPL saturations (source zone) and of concentrations in the groundwater and vadose plumes. The MACAOH "Modeling" guide (Côme et al, 2006b) proposes various recommendations concerning the choice of computational tools, the data required, the implementation of numerical codes, and the information that should be included in the study report.

After completing these steps, responsible parties (the consulting company, the industry and the public administration) must decide whether MNA is accepted as a remediation strategy, either implemented as a stand-alone technique or in combination with an "active" technique.

SAMBBA addresses steps 2 and 3 of the MACAOH methodology.

¹[http://www.ademe.fr/lien_internet_vers_guide_MACAOH / atténuation naturelle ?](http://www.ademe.fr/lien_internet_vers_guide_MACAOH_att%C3%A9nuation_naturelle%20?)

²http://www.ademe.fr/sites/default/files/assets/documents/%255B69418%255D%25206833_MACAOH_Natural%2520attenuation_Summary.pdf

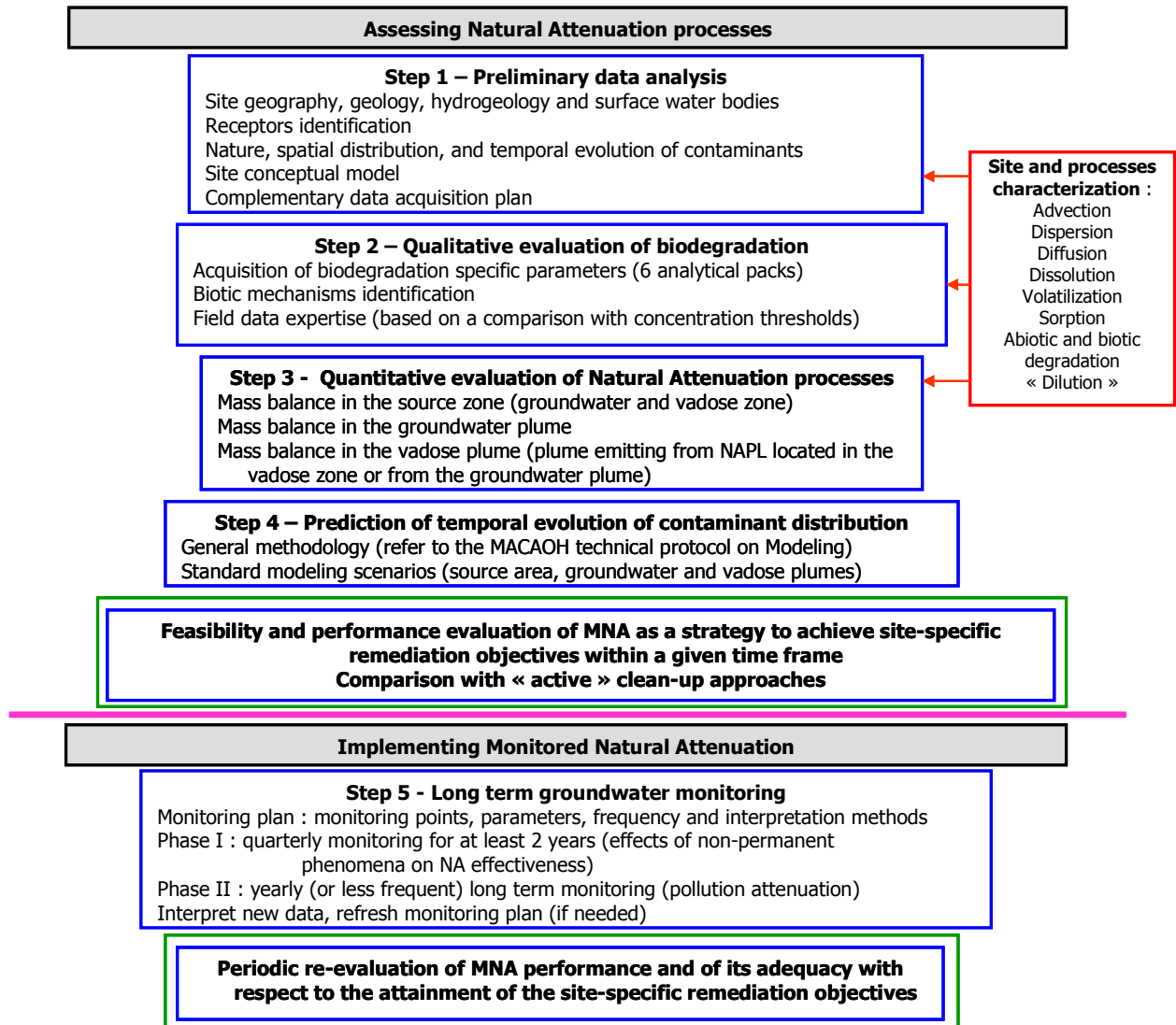


FIGURE 1 – METHODOLOGICAL FLOWCHART FOR ASSESSING NATURAL ATTENUATION (NA) AND IMPLEMENTING MONITORED NATURAL ATTENUATION (MNA). THE BLUE BOXES SHOW THE STEPS CARRIED OUT BY THE CONTRACTOR (E.G., CONSULTANTS), AND THE GREEN BOXES SHOW THE STEPS PERFORMED BY THE CLIENT AND THE PUBLIC ADMINISTRATION

The qualitative evaluation (**step 2**) aims at assessing whether or not the biodegradation of the chlorinated solvents is active, and if so, to specify under which redox conditions biodegradation occurs. The method consists in analysing a list of parameters organized as analytical packages (Table 1) and to be measured in at least 7 monitoring wells (1 up-gradient from the source zone, 2 in the source zone, and 4 down-gradient wells located at increasing distance from the source). The measurements characterize the chlorinated solvents and their degradation products, the dominant redox conditions in groundwater, the carbon sources, and the geochemical conditions of the aquifer.

The evaluation focuses on the reductive dechlorination of chloroethenes, chloroethanes and chloromethanes (Figure 2). It is conducted as a thorough data analysis that relies on the computation of a "dechlorination rate" and a comparison between the measured concentration and a proposed threshold value for each parameter (Table 3).

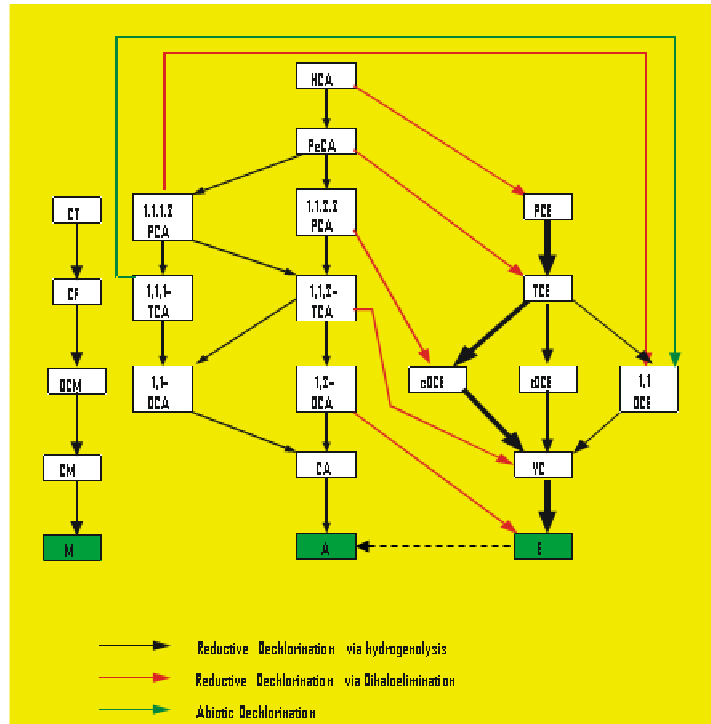


FIGURE 2 – DEGRADATION OF CHLORINATED ALIPHATIC HYDROCARBON VIA BIOTIC AND ABIOTIC PATHWAYS (CT TETRACHLOROMETHANE, CF TRICHLOROMETHANE, DCM DICHLOROMETHANE, CM CHLOROMETHANE, M METHANE, HCA HEXACHLOROETHANE, PeCA PENTACHLOROETHANE, 1112-PCA 1,1,1,2-TETRACHLOROETHANE, 1122-PCA 1,1,2,2-TETRACHLOROETHANE, 111-TCA 1,1,1-TRICHLOROETHANE, 112-TCA 1,1,2-TRICHLOROETHANE, 11-DCA 1,1-DICHLOROETHANE, 12-DCA 1,2-DICHLOROETHANE, CA CHLOROETHANE, A ETHANE, PCE TETRACHLOROETHENE, TCE TRICHLOROETHENE, 11-DCE 1,1-DICHLOROETHENE, C-DCE CIS-1,2-DICHLOROETHENE, T-DCE TRANS-1,2-DICHLOROETHENE, VC VINYL CHLORIDE, E ETHENE

Analytical packages	Parameters measured
"VOCs" Package: chlorinated and petroleum hydrocarbons	Chloroethenes, chloroethanes, chloromethanes, BTEX and petroleum derivatives
"Anions" Package	Chlorides
	Nitrates
	Sulfates
"M-E-E" Package	Methane, ethene et ethane
"DOC-NPOC" Package	Dissolved Organic Carbon (Non Purgeable Organic Carbon: VOCs excluded, already measured in the VOCs Package)
"Electrochemical" Package (on-site measure)	Dissolved Oxygen (mg/L)
	pH
	Redox Potential (mV)
	Temperature (°C)
	Conductivity (µS/cm)
"Colorimetric" Package (on-site measure)	Alkalinity (mg/L of CaCO3)
	Ferrous Iron (mg/L)

TABLE 1 - DESCRIPTION OF THE "ANALYTICAL PACKAGES" REQUIRED FOR THE QUALITATIVE EVALUATION OF THE BIODEGRADATION OF CHLORINATED HYDROCARBONS IN GROUNDWATER.

The quantitative evaluation (**step 3**) is based on a mass flux balance computation of each process involved in Natural Attenuation (NA) and allows for the calculation of the biodegradation rates. In the present version (v1.0), the evaluation can be conducted in the groundwater plume only and for the Chloroethenes family only. Note that the method of assessment in the source zone and / or for others hydrocarbons families is quite similar and might be supported in future versions of the application.

In the plume of dissolved contaminants (groundwater), the mass flux balance is computed between two aquifer transects delineated by groundwater elevation contours and characterized by a set of monitoring wells located on a plane perpendicular to the flow direction (Figure 3). This approach consists in an analytical

evaluation of the relative contributions from advection, volatilization, and vapour washout between two plume transects. The contributions of hydrodynamic dispersion and "dilution," on one hand, and biodegradation processes on the other hand are then computed by difference. This method also allows for the calculation of biodegradation rates based on the site-specific data.

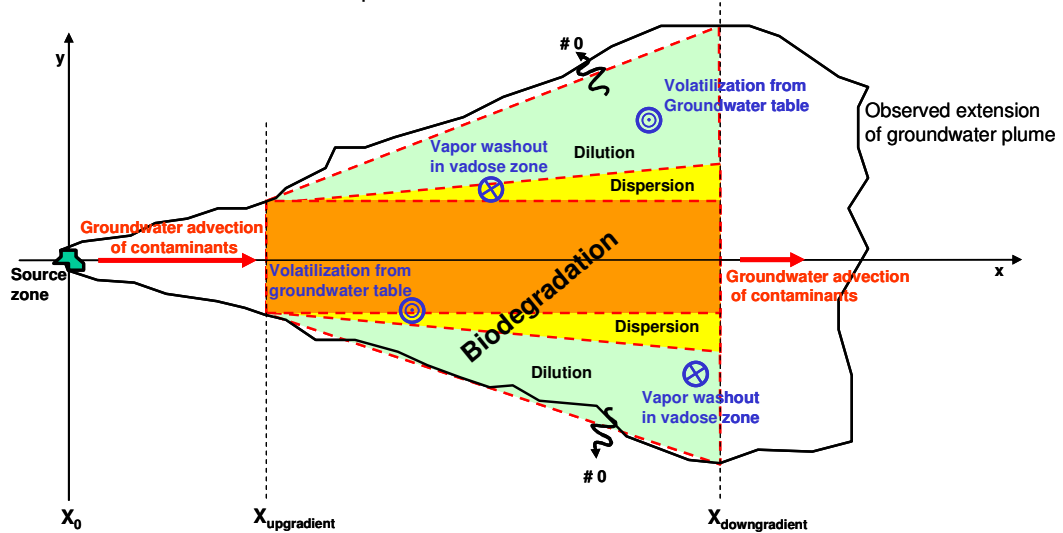


FIGURE 3 – A SCHEMATIC OF THE MASS BALANCE COMPUTATION FOR THE QUANTITATIVE EVALUATION OF NA PROCESSES IN THE PLUME OF DISSOLVED CONTAMINANTS

The application of the method is demonstrated in the tutorial section (Section 4). The reader might also refer to the technical guide for more details (Côme et al, 2006a).

3. Dealing with the SAMBBA interface

The application is composed of three modules: *Database*, *Qualitative Assessment* and *Quantitative Assessment*. These modules are described below. In the main window, clicking on one of the module box allows to open it. Once one module is opened, navigation between modules is possible by clicking on another module box (the former module stays open) in the main menu. Only one form for each module can be opened at the same time. If the user wants to start a new study, he/she will have to close the previous one first. SAMBBA informs the user about it when opening a new study.

In both *Qualitative Assessment* and *Quantitative Assessment* modules, SAMBBA requires GIS³ files (shape format) as input. The user must prepare these files in (any) GIS tool first. Note that a *shape* file always goes with a *dbf* file that includes the attribute table and a *shx* file for geometric features. SAMBBA requires these 2 files with each *shp* input file.

3.1. GIS input files

Four different shape files are needed as input (see Figure 4 for an example):

- The *plume centerline* file (polyline shape file);
- The *monitoring wells* file (point shape file);
- The *sections* file (polylines shape file);
- The *control volume* file (polygon shape file).

The first two are required for both the qualitative and the quantitative assessment modules and the last two only for the quantitative assessment. **The coordinate reference system (CRS) of these shape files must be a unique metric system (same CRS for all the files).**

³ Graphical Information System

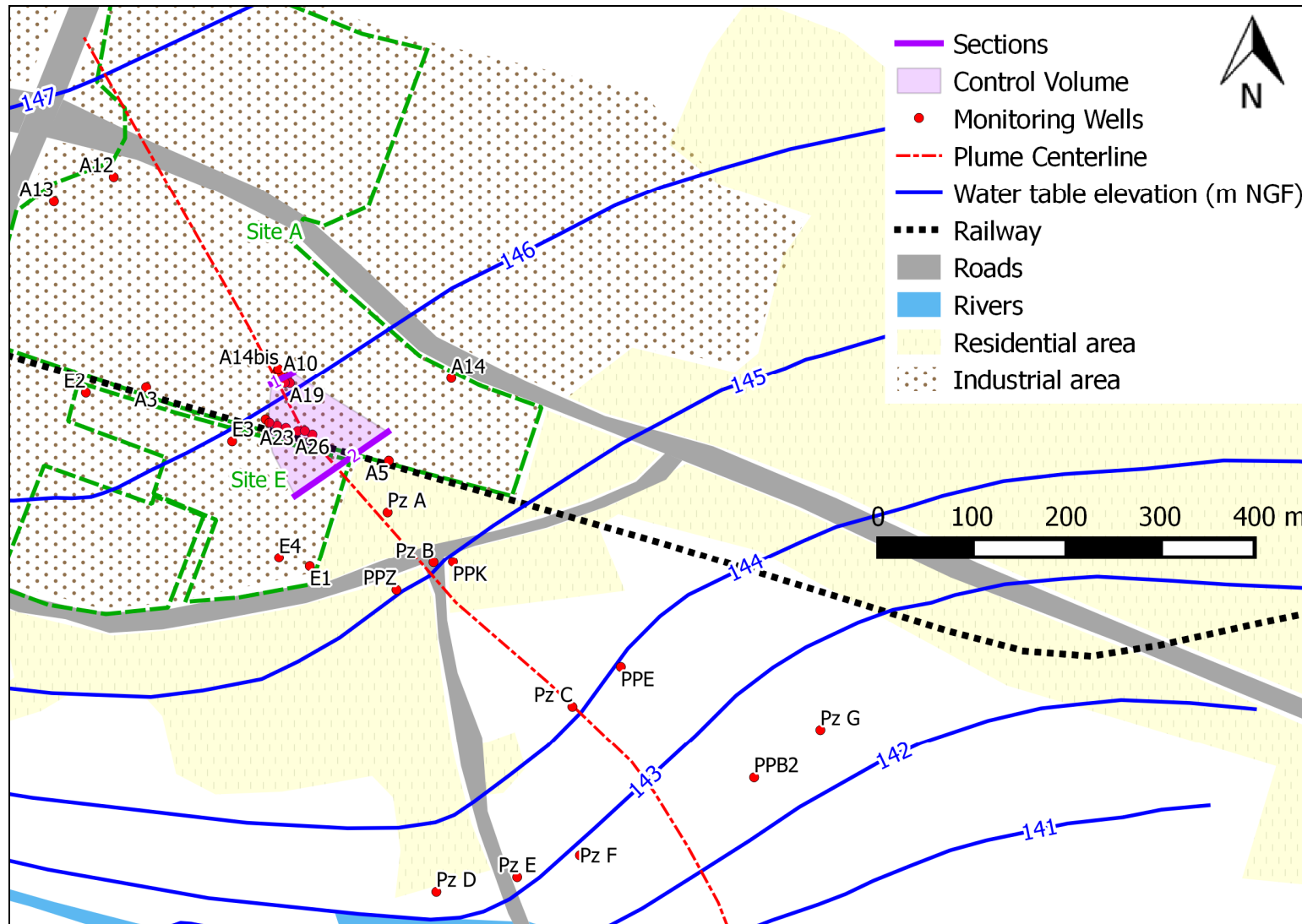


FIGURE 4 – EXAMPLE OF THE FOUR SHAPE FILES REQUIRED BY THE APPLICATION

3.1.1. The plume centerline file

The *plume centerline* file must include only one polyline object that represents the plume centerline. It passes through the source zone of pollution (located around the monitoring wells A10 and A14bis in Figure 4) and extends upstream and downstream to cover the investigated area (where the monitoring wells are located). This file is used by SAMBBA for its geometric features; there are no special requirements for its attribute table.

3.1.2. The monitoring wells file

The *monitoring wells* file is a point shape file. It must include the monitoring wells and many associated parameters that must be set in a special order in the attribute table. The file *TABLE_WellsData.csv* included in the SAMBBA material (in the *Template* folder) presents the data that are required in the attribute table. The order, the titles and the number of fields must be as in this file. It is strongly recommended to prepare the shape file from this csv file. The required fields and their units are described in Table 2. Note that some fields are optional or contain output data; nonetheless the columns of these fields must appear in the input file and might stay empty. Note that some data are optional because the application does not need them to compute and to display results. However some of these data are important for the user to analyse the results in the qualitative assessment module.

The user might refer to the technical guide (Côme et al, 2006a) for details on the calculation of output data.

3.1.1. The sections file

The *sections* file must include two polylines. These two polylines represent transects that delineate the portion of plume on which the mass balance is computed. They follow groundwater elevation contours and are chosen so that they can be represented by a set of nearby monitoring wells. There is no special requirement for its attribute table. This file is used to compute the advection mass flux flowing through each transect, SAMBBA computes the length of each section for that purpose.

3.1.2. The control volume file

The *control volume* file must include a polygon. Note that if the file contains many polygons, SAMBBA will consider only one polygon (the last one in the attribute table). This polygon represents the horizontal extension of the plume between the two transect. The surface of this polygon is used by SAMBBA to compute the volatilization and the vapour washout flux (or rain recharge flux). There is no special requirement for its attribute table.

Field Name	Description	Units	Input / Output	Optional?*
WELL_NAME	Well name	-	Input in shape file	QAL / QAT
X_GEOREF	X coordinate	m	Input in shape file	QAL / QAT
Y_GEOREF	Y coordinate	m	Input in shape file	QAL / QAT
PCE	Concentration of Tetrachloroethylene (PCE)	µg/l	Input in shape file	QAL / QAT
TCE	Concentration of Trichloroethylene (TCE)	µg/l	Input in shape file	QAL / QAT
CIS_DCE	Concentration of Cis-1,2-dichloroethene (c 1,2-DCE)	µg/l	Input in shape file	QAL / QAT
TRANS_DCE	Concentration of Trans-1,2-dichloroethene (t 1,2-DCE)	µg/l	Input in shape file	QAL / QAT
11_DCE	Concentration of 1,1-Dichloroethene (1,1-DCE)	µg/l	Input in shape file	QAL / QAT
VC	Concentration of Vinyl Chloride (VC)	µg/l	Input in shape file	QAL / QAT
ETHENE	Concentration of Ethene	µg/l	Input in shape file	QAL / QAT
HCA	Concentration of Hexachloroethane (HCA)	µg/l	Input in shape file	0
PECA	Concentration of Pentachloroethane (PeCA)	µg/l	Input in shape file	0
1122_PCA	Concentration of 1,1,2,2-Tetrachloroethane (1,1,2,2-PCA)	µg/l	Input in shape file	0
1112_PCA	Concentration of 1,1,1,2-Tetrachloroethane (1,1,1,2-PCA)	µg/l	Input in shape file	0
112_TCA	Concentration of 1,1,2-Trichloroethane (1,1,2-TCA)	µg/l	Input in shape file	0
111_TCA	Concentration of 1,1,1-Trichloroethane (1,1,1-TCA)	µg/l	Input in shape file	0
12_DCA	Concentration of 1,2-Dichloroethane (1,2-DCA)	µg/l	Input in shape file	0
11_DCA	Concentration of 1,1-Dichloroethane (1,1-DCA)	µg/l	Input in shape file	0
CA	Concentration of Ethyl Chloride (CA)	µg/l	Input in shape file	0
ETHANE	Concentration of Ethane	µg/l	Input in shape file	0
CT	Concentration of Carbon Tetrachloride (CT)	µg/l	Input in shape file	0
CF	Concentration of Trichloromethane (Chloroform) (CF)	µg/l	Input in shape file	0
DCM	Concentration of Dichloromethane (Methylene Chloride) (DCM)	µg/l	Input in shape file	0
CM	Concentration of Chloromethane (Methyl chloride) (CM)	µg/l	Input in shape file	0
A_ACID	Concentration of Acetic Acid	µg/l	Input in shape file	0
CHLORIDE	Concentration of Free Chloride	mg/l	Input in shape file	0
METHANE	Concentration of Methane	mg/l	Input in shape file	0
SULFATES	Concentration of Sulfates	mg/l	Input in shape file	0
SULFIDE	Concentration of Sulfide	mg/l	Input in shape file	0
FE_TOTAL	Concentration of Total Iron	mg/l	Input in shape file	0
FE_ION	Concentration of Ferrous Iron	mg/l	Input in shape file	0
MANGANESE	Concentration of Manganese	mg/l	Input in shape file	0
NITRATES	Concentration of Nitrates	mg/l	Input in shape file	0
AMMONIUM	Concentration of Ammonium	mg/l	Input in shape file	0
OXYGEN	Concentration of Dissolved Oxygen	mg/l	Input in shape file	0
EH	Eh - corrected value***	mV	Input in shape file	0
TEMP	Temperature	°C	Input in shape file	0
ORP	ORP - read value***	mV	Input in shape file	0
ALCALINITY	Alcalinity	mg/l	Input in shape file	0
PH	pH	-	Input in shape file	0
COND	Electrical conductivity	µS/cm	Input in shape file	0
DOC	Dissolved Organic Carbon (Non Purgeable organic Carbon: VOCs excluded) (DOC- NPOC)	mg/l	Input in shape file	0
CHEMOXD	Chemical oxygen demand	mg/l	Input in shape file	0
ALCOHOLS	Concentration of Alcohols	mg/l	Input in shape file	0
VOC	Concentration of Non halogenated Volatile Organic Compounds (VOC) (BTEX**** + Alkyl-benzenes + Naphtalene)	mg/l	Input in shape file	0
HC_C5_C10	Concentration of Hydrocarbons C5-C10	mg/l	Input in shape file	0
HC_C10_C40	Concentration of Total Hydrocarbons C10-C40	mg/l	Input in shape file	0
H_C10_C16	Concentration of Hydrocarbons C10-C16	mg/l	Input in shape file	0
H_C16_C22	Concentration of Hydrocarbons C16-C22	mg/l	Input in shape file	0
H_C22_C30	Concentration of Hydrocarbons C22-C30	mg/l	Input in shape file	0
H_HEAVY	Concentration of Hydrocarbons >C30	mg/l	Input in shape file	0
COMPOUND1	to be specified		Input in shape file	0
COMPOUND2	to be specified		Input in shape file	0
COMPOUND3	to be specified		Input in shape file	0
COMPOUND4	to be specified		Input in shape file	0
COMPOUND5	to be specified		Input in shape file	0
COMPOUND6	to be specified		Input in shape file	0
COMPOUND7	to be specified		Input in shape file	0
COMPOUND8	to be specified		Input in shape file	0
COMPOUND9	to be specified		Input in shape file	0
COMPOUND10	to be specified		Input in shape file	0
NOTE	to be specified	-	Input in shape file	0

Field Name	Description	Units	Input / Output	Optional?*
LOCATION	Location of the well compared to the contamination source zone		Input in the QUALI interface**	QAL
DSOURCE	Distance of the well from the source	m	Output	
BIOZONE	Type of biodegradation zone	-	Input in the QUALI interface**	O
TX_CEMAX	Maximum dechloration rate of Chloroethenes	%	Output	
TX_CEMIN	Minimum dechloration rate of Chloroethenes	%	Output	
CS_PCE	Ratio Concentration / Solubility of PCE	%	Output	
CS_TCE	Ratio Concentration / Solubility of TCE	%	Output	
R_DCE_A	Rate of DCE as a product of TCA	%	Output	
R_CV_A	Rate of VC as a product of TCA	%	Output	
R_E_A	Rate of Ethene as a product of TCA	%	Output	
R_A_A	Rate of Ethane as a product of TCA	%	Output	
CM_CE	Total molar concentration of Chloroethenes	μmol/l	Output	
CMS_PCE	Total chloroethenes molar concentration / PCE Solubility	%	Output	
CMS_TCE	Total chloroethenes molar concentration / TCE Solubility	%	Output	
TX_CA	Dechloration rate of Chloroethanes	%	Output	
CS_HCA	Ratio Concentration / Solubility of HCA	%	Output	
CS_PECA	Ratio Concentration / Solubility of PeCA	%	Output	
CS_22PCA	Ratio Concentration / Solubility of 1,1,2,2 PCA	%	Output	
CS_12PCA	Ratio Concentration / Solubility of 1,1,1,2 PCA	%	Output	
CS_12TCA	Ratio Concentration / Solubility of 1,1,2-TCA	%	Output	
CS_11TCA	Ratio Concentration / Solubility of 1,1,2-TCA	%	Output	
CM_CAT	Total molar concentration of Chloroethanes	μmol/l	Output	
R_PAR_CA2	Ratio (HCA+PeCA+PCA) molar concentration / Total molar concentration of chloroethanes	%	Output	
CMS_HCA	Total chloroethanes molar concentration / HCA Solubility	%	Output	
CMS_PECA	Total chloroethanes molar concentration / PeCA Solubility	%	Output	
CMS_22PCA	Total chloroethanes molar concentration / 1,1,2,2 PCA Solubility	%	Output	
CMS_12PCA	Total chloroethanes molar concentration / 1,1,1,2 PCA Solubility	%	Output	
CMS_12TCA	Total chloroethanes molar concentration / 1,1,2 TCA Solubility	%	Output	
CMS_11TCA	Total chloroethanes molar concentration / 1,1,1 TCA Solubility	%	Output	
TX_CMMAX	Maximum dechloration rate of Chloromethanes	%	Output	
TX_CMMIN	Minimum dechloration rate of Chloromethanes	%	Output	
CS_CT	Ratio Concentration / Solubility of CT	%	Output	
CS_CF	Ratio Concentration / Solubility of CF	%	Output	
CM_CMTOT	Total molar concentration of Chloromethanes(w/o Methane)	%	Output	
CMS_CT	Total chloromethanes molar concentration / CT Solubility	%	Output	
CMS_CF	Total chloromethanes molar concentration / CF Solubility	%	Output	
C_EA	Concentration of Ethene + Ethane	μg/l	Output	

* QAL : Required for the Qualitative Assessment Module, QAT : Required for the Quantitative Assessment Module, O : Optional

** The parameter can be set in the input data tab of the Qualitative Assessment Interface

*** see specifications given by the probe manufacturer

**** Benzène, Toluène, Ethylbenzène, Xylènes

TABLE 2 – REQUIRED FIELDS IN THE MONITORING WELLS FILE

3.2. The Database module

The database includes the physical parameters (molecular weight and water solubility) of chloroethenes, chloroethanes and chloromethanes (22 compounds included). These parameters are needed for the calculation of the other modules. The *database* module was created for visualization purpose only. The user can visualize (click *open*) and print it (click *print* or *print preview* to prepare the print).

3.3. The Qualitative Assessment module

The *Qualitative Assessment* window consists in 5 tabs. The first one is dedicated to the input data and the next four to the visualization of results through graphics. The latter are activated once the input data have been filled in. In the *Qualitative Assessment* menu, standard actions are available: *New*, *Open*, *Save*, *Save as*, *Print Data Results* and *Save Graphics*. Note that the format for saving a qualitative assessment study is *xml*. The last action (*Save Graphics*) is available once the input data have been filled in and graphs tab activated. *Print Data Result* consists in printing the main table of the *Input Data* tab. *Save Graphics* allows to save every graphics of the four last tabs in JPEG format.

3.3.1. The Input Data tab

The Input Data tab window is divided in 4 areas (Figure 5).

DataBase Qualitative Assessment Quantitative Assessment ?

Input Data Chloroethenes Graphs Chloromethanes Graphs Chloromethanes Graphs Other Graphs

Select plume centerline file : TUTOCenterline.shp

Select monitoring wells file : TUTOWellsData.shp

Inform the number of wells : 7

MONITORING WELLS	A12	A9	A11	A25	Pz A	Pz C	PPB2
Location	Upstream (ref)	Source	Downstream	Downstream	Downstream	Downstream	Downstream
Distance from the source	-384	0	7	62	188	474	658
EA / ED Zone		Iron-reductio...	Methanogen...	Methanogen...	Iron-reductio...	N/O inteme...	Min/N litem...

BIODEGRADATION OF CHLORINATED ALIPHATIC HYDROCARBONS

>> CHLOROETHENES, ETHENE & ETHANE

PCE (µg/L)	0.00	129.00	537.00	26.00	18.00	114.00	17.00
TCE (µg/L)	0.00	22153.00	147.00	71.00	55.00	313.00	99.00
cis-DCE (µg/L)	0.00	8734.00	21665.00	265.00	281.00	990.00	112.00
trans-DCE (µg/L)	0.00	51.00	49.00	0.00	15.00	0.00	0.00
1,1-DCE (µg/L)	0.00	18.00	0.00	0.00	0.00	0.00	0.00
VC (µg/L)	0.00	172.00	3207.00	96.00	202.00	3.00	12.00
Ethene (µg/L)	0.00	58.00	1026.00	18.00	24.00	0.00	0.40
Ethane (µg/L)	0.00	3.00	84.00	135.00	4.00	27.00	0.90
Max dechloration rate (%)	NC	34.62	59.59	76.88	64.64	46.57	42.44
Min dechloration rate (%)	NC	12.96	46.93	70.81	54.08	31.92	25.96

>> More details

>> CHLOROETHANES & ETHANE

>> CHLOROMETHANES & METHANE

>> FINAL PRODUCTS

Ethene + Ethane (µg/L)	0.00	61.00	1110.00	153.00	28.00	27.00	1.30
Acetic Acid (µg/L)	-	-	-	-	-	-	-
Free chloride (mg/L)	469.00	323.00	237.00	162.00	279.00	174.00	78.70

OXYDATION-REDUCTION CONDITIONS

Methane (mg/L)	0.01	0.85	17.00	21.06	0.66	1.01	0.02
Sulfates (mg/L)	102.00	96.60	73.20	22.70	128.00	36.00	62.30
Sulfide (mg/L)	0.03	0.26	0.06	0.02	ND	0.00	ND
Total iron (mg/L)	-	-	-	-	-	-	-
Ferrous iron (mg/L)	1.20	6.30	10.20	18.10	2.08	0.14	0.02
Manganese (mg/l)	-	-	-	-	-	-	-
Nitrates (mg/L)	0.00	2.75	0.00	0.00	0.00	9.30	0.00
Ammonium (mg/L)	0.00	1.84	5.41	518.00	0.00	0.00	0.00
Dissolved oxygen (mg/L)	0.16	0.07	0.00	0.11	0.00	1.29	3.22

>> Redox potential

Eh (mV) - corrected value	225.68	1.52	-54.01	25.14	274.04	298.24	414.17
Temperature (°C)	12.50	15.40	18.80	18.60	14.70	10.40	7.80
ORP (mV) - read value	10.00	-212.00	-265.00	-186.00	60.00	81.00	195.00
Alcalinity (mg/L)	160.00	200.00	260.00	1260.00	280.00	260.00	160.00

Workflow for the qualitative assessment of natural attenuation

- Before starting, make sure that the input data files are prepared. Two files are required :
 - a shape file defining the main plume centerline (one polyline file only)
 - a shape file defining monitoring wells and their associated data (point file) - these number and type of data are listed in TABLE_POLLUANTS.xlsx (template folder)
- Import the plume centerline shape file and the monitoring well shape file
- Enter the number of wells to consider in the qualitative assessment
- In the table, select the wells to consider (Name' combobox) along the centerline (wells should be ranked from upstream to downstream) and select their location from the source (Location' combobox)
- Analyse the results displayed on the table and check out the graphics tab for their visualization
- Choose the electron acceptor / donor zone according to the analysis of results (EA / ED zone' combobox)
- Don't forget to save the ongoing work!

Legend

Dechloration rate (%): < 5 | 5 - 20 | 20 - 40 | 40 - 60 | > 60

Ethene + Ethane (µg/l): < 20 | 20 - 200 | > 200

Free chloride (mg/l): < 2 x C_{upstream} | > 2 x C_{upstream}

Methane (mg/l): < 1 | > 1

Sulfates (mg/l): > 2 x C_{upstream} refer to UG* | < 20

Ferrous iron (mg/l): < 2 | > 2

Nitrates (mg/l): > 1 | < 1

Dissolved oxygen (mg/l): > 0.5 | < 0.5

Eh (mV): > +100 | < +100

ORP (mV): > -100 | < -100

Alcalinity (mg/l): < 2 x C_{upstream} | > 2 x C_{upstream}

DOC-NPOC (mg/l): < 10 | > 10

Non halogenated VOC (mg/l): < 2 | > 2

* the color classes for sulfate concentrations depend on the values of other parameters, please refer to the User's Guide for details

FIGURE 5 – INPUT WINDOW OF THE QUALITATIVE ASSESSMENT MODULE

On the right part of the window, two areas are dedicated to:

- instructions to use the sheet ("Workflow" area);
- a colour coded legend to help in the assessment of the main data table (see details in Table 3).

In the top left area, the user is invited to choose the two shape files needed for the evaluation: a *plume centerline* file and a *monitoring wells* file. The format and information that must contain these files are described in Section 3.1. Besides, the user must set the number of monitoring wells to consider in the study (this number will only be used in the *Qualitative Assessment* study). The application requires at least one monitoring well although it is recommended to work with 7 wells or more in the MACAOH methodology. Clicking *ok* allows sizing the main data table below with one column for each monitoring well.

The main table (located in the bottom left area of the input window) includes all the required information to conduct the qualitative evaluation of biodegradation. Some data are extracted from the input files and others are computed by the application. First the user must select monitoring wells among those of the *monitoring wells* shape file using the combo-boxes in the first line of the table. The method consists in selecting, from left to right, the monitoring wells from upstream to downstream along the plume centerline (cf. Côme et al, 2006a). The user must then choose the location of each monitoring well (combo-boxes in the second line) among *upstream (ref)*, *upstream*, *source*, *downstream*. At least one *upstream (ref)* well is needed for the table to colour properly (cf Table 3 for more details) and one *source* well is required to compute the *distance from the source* field (third line of the table). Once the first two lines are set, the input data are automatically updated, the output data are computed and the graphics tab are activated.

The *Distance from the source* field represents the distance between a monitoring well and the monitoring well selected as the "source" along the plume centerline. The application use the *plume centerline* shape file and the *monitoring wells* shape file to calculate this distance.

The *EA / ED zone* field is set by the user once he/she has analysed the results using the colour coded lines (see Table 3).

The next lines of the table consist of many parameters that are both input data (contained in the *monitoring wells* file) and computed data. Note that the last fields are free for the user to define; the title of these fields can be modified.

The user can refer to the tutorial for an example on how the data are analysed. Note that a double click on the ">>" allows to hide some group of lines in the table. No cells can be modified in the table except the title of the lines below "OTHERS COMPOUNDS". These lines are free to fill in by the user.

Information	Parameter	Color legend	condition for dechlorination	Interpretation
Reductive dechlorination performance	Dechlorination rates	>60%	very high	allow to quantify the degradation extent of chlorinated solvents. For Chloroethenes, the max. rate and min. rates are calculated from PCE and TCE as unique parent product respectively. For chloroethane, the parent product is the TCA (sum of the 2 isomers). For chloromethane, the max. and min rates are from CT and CF respectively.
		40 to 60%	high	
		20 to 40%	medium	
		5 to 20%	low	
Final product	Ethene + Ethane	> 200 µg/l	high	account for final product that are harmless for the environment. It highlights a the completion of the dechlorination for chloroethenes & chloroethanes
		20 to 200 µg/l	medium	
		<20 µg/l	low	
	Free chloride	> 2*C _{upstream} *	high	can lead to a chlore balance calculation if it is a conservative tracer
< 2*C _{upstream} *	low			
Methanogenesis	Methane	>1 mg/l	high	Highlight strong reductive conditions
		<1 mg/l	low	
Sulfate reduction	Sulfates	<20 mg/l	high	highlight sulfate reduction condition only if sulfate concentrations significantly decrease along the plume centerline
		< 2*C _{upstream} AND Ferrous iron > 2mg/l and POR < -100 mV	medium	
		>2*C _{upstream} *	low	
Iron (III) reduction	Ferrous iron	>2 mg/l	high	
		<2 mg/l	low	
Nitrates reduction	Nitrates	<1mg/l	high	
		>1mg/l	low	
anaerobic / aerobic	Dissolved oxygen	< 0.5 mg/l	high	if O2 > 0.5 mg/l and FeII <2 mg/l then the degradation is strictly in aerobic condition
		>0.5 mg/l	low	
	Eh	<+100 mV	high	confirm the electronic pressure in the medium
		>+100 mV	low	
	ORP	<-100 mV	high	
		>-100 mV	low	
Alcalinity	> 2*C _{upstream} *	high	informs on the production of CO2	
	< 2*C _{upstream} *	low		
Non purgeable (dissolved) organic	DOC-NPOC	> 10 mg/l	high	informs on the available non purgeable carbons (does not inform on the longevity of the DOC source)
		< 10 mg/l	low	
Purgeable organic carbons	Non halogenated VOC	> 2 mg/l	high	should be measured when there is a contamination by monoaromatic hydrocarbons (BTEX,...). These compounds are purgeable and are not included in the DOC-NPOC group. If present, they are a carbon source for degradation in the presence of dissolved oxygen
		< 2 mg/l	low	

* C_{upstream} is the parameter concentration (or value) at the monitoring wells identified by the user as *upstream (ref)* (in *location* field)

TABLE 3 – INTERPRETATION OF PARAMETERS FOR THE QUALITATIVE EVALUATION OF BIODEGRADATION (PLEASE REFER TO TABLE 2 FOR ABBREVIATIONS)

3.3.2. The Graphs tabs

These tabs are activated once the Input data tab is complete. All graphs represent some parameters of the main table (vertical axis) versus the distance from the source (horizontal axis).

The first three graphs tabs are dedicated to the three families of aliphatic chlorinated solvents (see Figure 6 for the chloroethenes family). They include:

- the mass concentrations of the family compounds including the final product of biodegradation (ethene, ethane or methane depending on the family);
- the molar concentration of the family compounds;
- the molar proportion of three groups of chlorinated compounds: the parent species, the metabolic intermediates and the final products. Table 4 presents the groups of compounds for each family;
- the dechlorination rates.

The last tab presents parameters for the visualisation of oxidation / reduction and inorganic electrons acceptor/donor along the centreline (Figure 7).

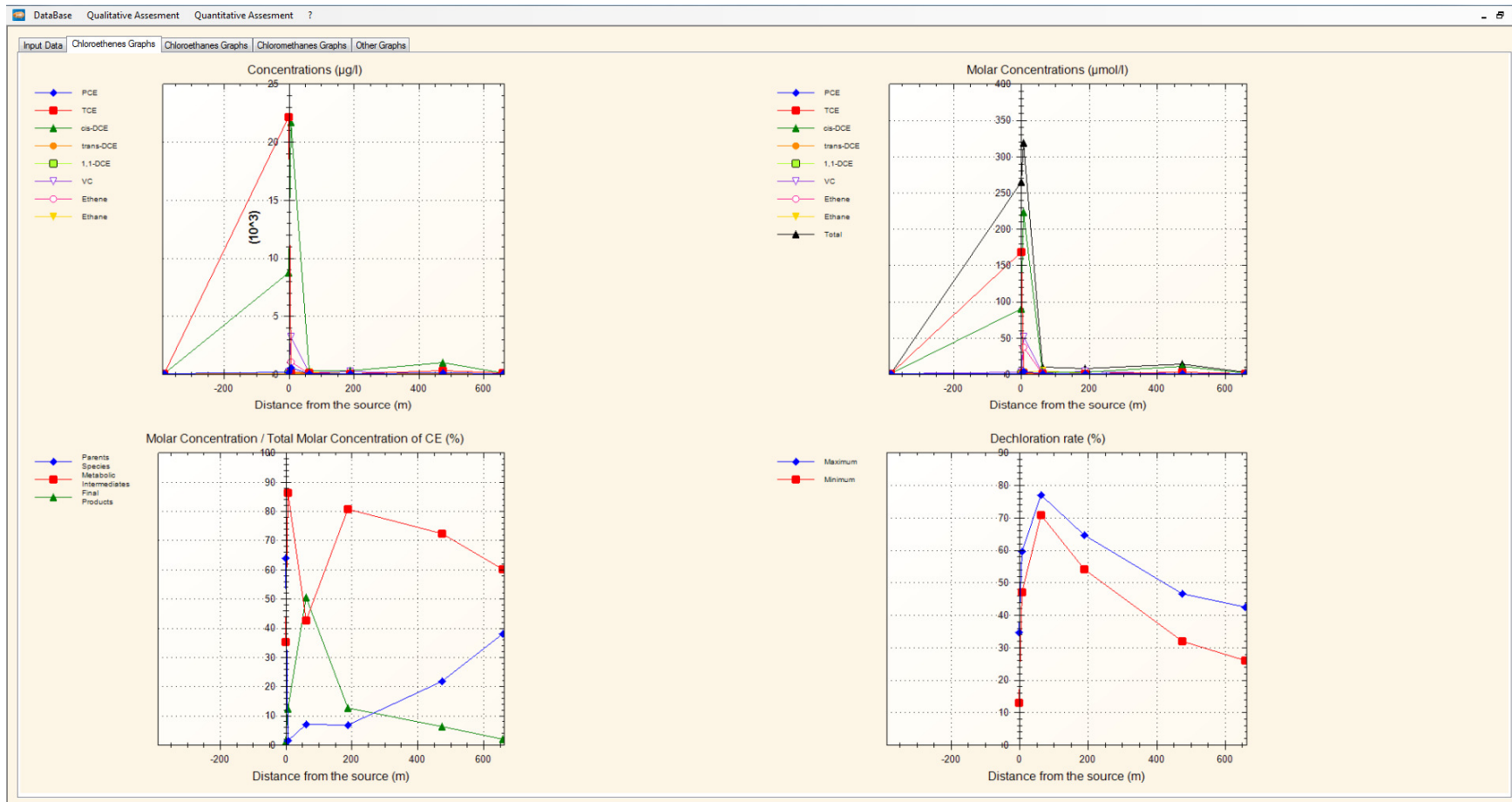


FIGURE 6 – CHLOROETHENES GRAPHS TAB OF THE QUALITATIVE ASSESSMENT MODULE

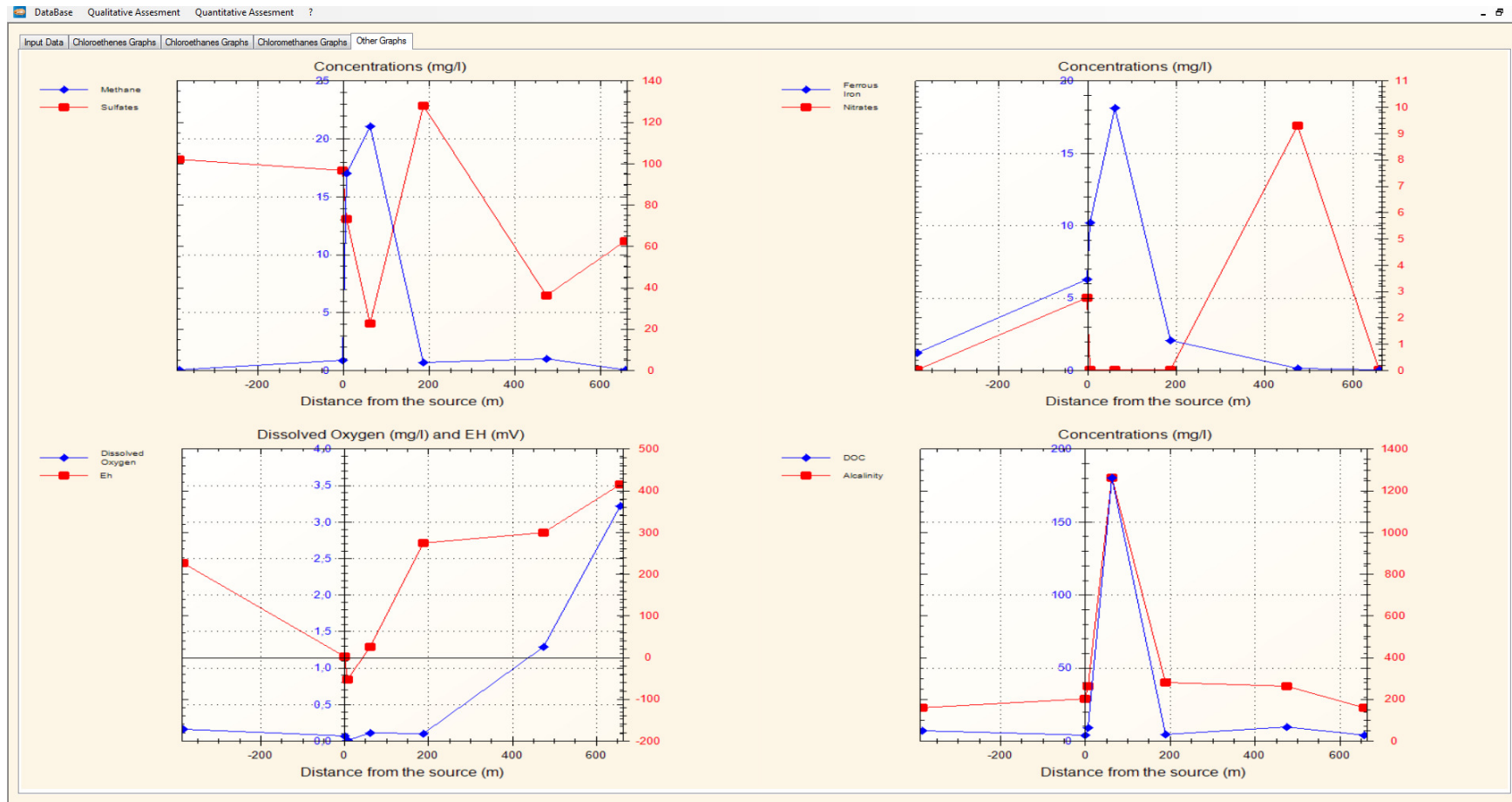


FIGURE 7 – OTHER GRAPHS TAB OF THE OF THE QUALITATIVE ASSESSMENT MODULE

	Chloroethenes	Chloroethanes	Chloromethanes
Parents species	PCE, TCE	HCA, PeCA, 1,1,2,2-PCA, 1,1,1,2-PCA, 1,1,2-TCA, 1,1,1,-TCA	CT, CF
Metabolic Intermediates	c 1,2-DCE, t 1,2-DCE, 1,1-DCE, VC	1,1-DCA, 1,2,-DCA, 1,1,-DCE (product of TCA), VC (product of TCA), CA	DCM, CM
Final products	Ethene, Ethane	Ethene (product of TCA), Ethane	Methane

TABLE 4 – GROUP OF CHLORINATED COMPOUNDS FOR EACH FAMILY

3.4. The Quantitative assessment Module

The *Quantitative Assessment* window consists in 2 tabs, one for inputs and the other for outputs called *Results in the plume*. In the *Quantitative Assessment* menu, standard actions are available: *New*, *Open*, *Save*, *Save as*. Note that the format for saving a quantitative assessment study is *xml*.

3.4.1. The Input tab

This tab is divided into 3 parts (Figure 8).

The first part is dedicated to general options:

- the *plume centerline* shape file and the *Sections* shape file must be prepared in a GIS tool beforehand (see section 3.1);
- the *Contaminants data file* is a shape file. It has the same format that the monitoring wells shape file (see Section 3.1.2). Note that the *monitoring wells* file used for the qualitative assessment can be used in the quantitative assessment module as well;
- *Biodegradation options*: the user can choose to work with *no biodegradation*, *aerobic biodegradation* or *anaerobic biodegradation*. According to the chosen option the mass balance will be computed in a different manner (see the technical guide for more details on the calculation, Côme et al (2006a));
- *Effective porosity*: this field must be set by the user between zero and 1 in accordance with its physical definition;
- *Distance between sections*: this field is automatically computed from the *sections* file and the *plume centerline* file. It represents the distance between the two transects included in the sections file along the plume centerline. The user cannot modify this value, it is only displayed for information (and used for computations of travel time);
- *Contaminant family*: the user might choose the contaminant family to work with (among aliphatic chlorinated solvents). In the current version of SAMBBA (v1.0), this option is not activated; the study can be conducted with chloroethenes only;
- *Location of the region*: the user might choose whether to work in the contamination source or in the plume. The mass balance is slightly different in the two zones (Côme et al, 2006a). The study can be conducted in the plume zone only in the current version of SAMBBA (v1.0), this field is then locked on the *plume* option;
- *Number of control volume*: the user might choose the number of control volume (1, 2 or 3). This field determines whether the mass balance is computed by considering convection, dispersion and dilution as three separated mechanisms (3 control volumes), by grouping together dispersion and dilution (2 control volumes) or by adding the three mechanisms (1 control volume). In the current version of SAMBBA (v1.0), the study can be conducted on two control volumes only; the field is then locked on 2.

The right top area of the window entitled *Source balance options* is dedicated to specific parameters required when conducting studies on the contamination source. As this option is not available on the current version of SAMBBA, this input area has been deactivated.

DataBase Qualitative Assessment Quantitative Assessment ?

Input Results in the Plume

Plume centerline shape file: TUTOCenterline.shp

Sections shape file: TUTOSections.shp

Contaminants data file: TUTOWellsData.shp

Biodegradation options: Anaerobic biodegradation

Effective porosity: 0.06

Distance between sections: 110.52

Contaminant family: Chloroethenes

Location of the region: Plume

of control volumes: 2

Source balance options:

Initial mass (kg):

Convection

Upstream section

Section name: 1

Section length (m): 24.83

Aquifer depth (m): 4

of subsections: 4

y1 (m)	y2 (m)	Well name	Darcy velocity (m/d)
0	10	A18	0.06
10	14	A16	0.06
14	18	A11	0.06
18	24.83	A20	0.06

Downstream section

Section name: 2

Central subsection

Section length (m): 24.83

Aquifer depth (m): 4

of subsections: 3

y1 (m)	y2 (m)	Well name	Darcy velocity (m/d)
0	10	A26	0.06
10	15	A4	0.06
15	24.83	A25	0.06

Total subsection

Section length (m): 119.50

Aquifer depth (m): 4

of subsections: 5

y1 (m)	y2 (m)	Well name	Darcy velocity (m/d)
0	75	Pz A	0.06
75	85	A26	0.06
85	90	A4	0.06
90	100	A25	0.06
100	119.50	Pz A	0.06

Intermediate subsection

Section length (m):

Aquifer depth (m):

of subsections: 1

Volatilisation and Rain Recharge

Total control volume shape file: TUTOControlVolume.shp

Surface of total area (m²): 8912.47

Surface of central area (m²): 2744.20

Recharge flux (m/s): 9.5e-10

Contaminant	Volatilized flux (µg/m ² /d)	Concentration of recharge (µg/l)
PCE	0.3	0.009
TCE	23.3	0.173
DCE	149	24
VC	12.4	0.0736
Ethene	26.1	0.009
Ethane	54.8	0.009

FIGURE 8 – INPUT WINDOW OF THE QUANTITATIVE ASSESSMENT MODULE

The second part is dedicated to the input data that are required to compute the convection mass fluxes. The data are similar on the upstream and the downstream sections:

- *Section Name*: the user can choose one of the two sections included in the *Sections* shape file that are loaded in the combo box;
- *Section length*: this field is computed by the application according to the geometrical property of the section selected above. As each section should encompass the entire width of the plume, the computed value actually refers to the width of the plume at the location of each section;
- *Aquifer depth (m)*: this field must be filled by the user;
- *Number of subsections*: each section can be divided in many subsections. As this number is set, the small table below is resized accordingly (one line for each subsection).
- In the table of subsections, one line corresponds to one subsection and requires the following information:
 - the length of the subsection along the main section (from y_1 to y_2). The value refers to the width to which each subsection parameter (groundwater velocity and contaminants concentrations) is applied;
 - the well associated with each subsection. The user must select the well among the list of monitoring wells included in the *Contaminants data* file. Note that concentrations of contaminants (C_i for compound i) included in this file are used for the computation (Eq. (1)) ;
 - the Darcy velocity on the subsection (vD).

The convection flux through the main section is then computed with the following equation:

$$Q_i = \sum_{\alpha} C_{i,\alpha} * vD_{\alpha} * (y2_{\alpha} - y1_{\alpha}) * e \quad (1)$$

α subsection index in the main section

e aquifer depth (m) for the main section

Note that in the downstream section, two subsections are defined:

- the central subsection corresponds to the central part of the downstream section which length equals the length of the upstream section. It is the width of the central tube of the plume;
- the total subsection corresponds exactly to the downstream section (total width of the plume due to dilution and dispersion processes).

The convection fluxes through these two subsections are required for the mass balance to compute. The convection input parameters for these two subsections can be set as described above (i.e. each subsection can be divided into many smaller subsections). Note that when working with three control volumes (option non available in the current version of the software), the downstream section contains an intermediate subsection that must be set as well. The parameter setting area for this last subsection is not activated in the current version (located on the right hand side of the convection area).

The last part of the window is dedicated to the input data required to compute the fluxes for the volatilisation and rain recharge mechanisms:

- *Total control volume shape file*: the *control volume* file must be prepared in a GIS tool beforehand (see section 3.1). It usually encompasses the surface area located between the two sections included in the *Sections* shape file. If this area intersects with a vapour impermeable layer (geological layer in the vadoze zone or a concrete slab for example) the user might need to delineate a surface area accordingly;
- *Surface of total area (m²)*: this field is computed by the application according to the geometrical property of the *control volume* file;
- *Surface of central area (m²)*: this field is computed according to the geometrical properties of the *plume centerline* file and the *sections* file. It represents the surface area of the central tube along the centerline which width equals the length of the upstream section;
- Recharge flux (m/s): this field must be set by the user. It usually equals the effective rain recharge;
- The table includes the volatilized flux and the concentration of recharge for the compounds of the chloroethenes family and its biodegradation by-products. These fields must be set by the user. The volatilized and rain recharge (or vapour washout) fluxes are computed according to the following equations:

$$Q_{i, volatilisation} = F_i * A \quad (2)$$

$$Q_{i, rain recharge} = C_i * A * r$$

F_i Volatilized flux of compound i

A Surface of total area through which the volatilized flux and the rain recharge is computed

C_i Concentration of compound i in vapour washout (dissolved phase)

r Rain recharge

At last, clicking on the *Compute* button at the bottom right of the window makes the application compute the mass balance and fills in or updates the *Results in the plume* tab.

3.4.2. The Results in plume tab

The *result in plume* tab presents the results (Figure 9). For each assumption (see Côme et al, 2006a, for the definition of these assumptions), the computed mass balance is presented in a table of results and a column chart. All the output parameters are described in the technical guide (Côme et al, 2006a) with two additional parameters:

- The residual total balance is the difference between influxes and outfluxes of the “input” mechanisms (convection, recharge and volatilization). This residual is assumed to be the remaining flux in the mass balance that is attributed to the dilution and biodegradation. If the residual is negative, it can mean that there might be an error in the input settings of the “influxes” mechanisms or that biodegradation results in production of the related compounds (which is a possible situation during dechlorination for metabolic intermediates and final products only) ;
- The dilution line of the tables actually equals the sum of the dilution and dispersion fluxes (the two processes are gathered when working with only 2 control volumes which is the only option supported in the current version of SAMBBA, cf. Section 3.4.1).

The convention in the flux table is that influxes are positive and outfluxes are negative.

The column charts present the results of the mass balance. Right clicking on this figure allows to access to standard options for the figures (copy, save, print, zoom...).

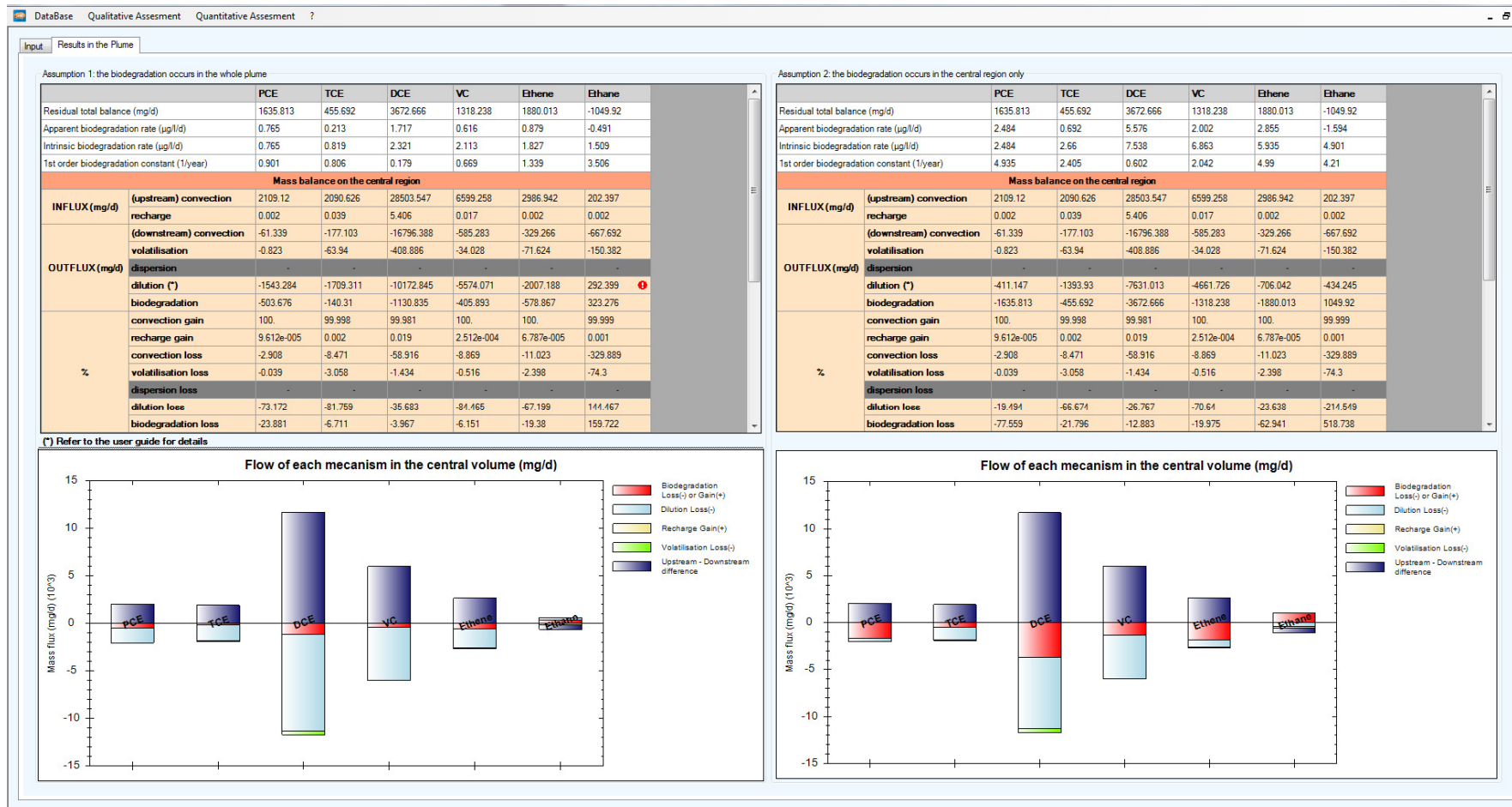


FIGURE 9 – OUTPUT WINDOW OF THE QUANTITATIVE ASSESSMENT MODULE

4. Tutorial

Make sure to copy the SAMBBA material on your computer first. Two tutorials are presented here, one for each main module.

4.1. Tutorial 1 - Qualitative evaluation

The industrial site presented in this tutorial is located on top of a sandy alluvial aquifer, which has an average thickness of 5 m to 7 m, lying on top of a clay-loam substratum. The groundwater table is at a depth of about 2 m. The average hydraulic conductivity of the aquifer is $3 \cdot 10^{-4}$ m/s and the average pore velocity of the groundwater is about 1 m/d. Private individuals located down-gradient from the site use groundwater for gardens and cattle (the closest wells are 300 m down-gradient from the source zone). The site situation is presented on Figure 4.

Pollution from chlorinated solvents has been present for about 30 years and is due to multiple overflows of a storage tank. The lateral extension of the main source zone is about 25 m² (located in a rectangular area including the monitoring wells A14bis, A9 and A16, Figure 4). The NAPL, consisting of a PCE/TCE mixture (about 60/40 molar fraction), was identified at the alluvial aquifer / substratum interface (with a maximum total concentration of about 60 g/kg dry weight). The plume of dissolved chlorinated compounds emitting from the main source extends over 650 m down-gradient with an end-point discharge in a river; the plume is also extremely wide, with a width of about 300 m near the river.

Before starting the user must always prepare the GIS input files (cf. Section 3.1). The data acquired for the qualitative evaluation of the biodegradation on this site were prepared in the required csv format (see *Tutorial\TABLE_TUTOWellsData.csv*). The required shape files were also prepared (in the **\Tutorial\GISfiles* folder: *TUTOCenterline.shp* and *TUTOWellsData.shp*). These shape files come with a Quantum-GIS project (0-TUTOmainGIS.qgs) so that you can visualize them⁴.

Click on *Qualitative Assessment* to start the tutorial. First you have to load the two required shape files. In the *Select plume centerline file* line, click on *browse* and load *TUTOCenterline.shp*. In the *Select monitoring wells file* line, click on *browse* and load *TUTOWellsData.shp*. We will conduct the study on 7 monitoring wells as recommended in the technical guide (Côme et al, 2006a); fill in the *number of wells* field accordingly and click *OK*. 7 columns are then created in the main table below and the monitoring wells of the shape file are loaded in the combo boxes of the first table line. On this line, select the monitoring well to work with from upstream to downstream (left to right) along the plume centerline: A12, A9, A11, A25, PzA, PzC and PPB2. When selecting a well, the associated data (contaminants concentrations, redox parameters, etc...) will automatically load in the column. On the second line, choose the location of each well compared to the source. There should be at least one well upstream (the first one is the upstream reference, or "upstream (ref)") and only one well in the source. Select A12 as the upstream reference well, A9 in the source and all the others as downstream. This will make the application to compute the distance of each well from the source well (in the third line). Now all the data are loaded and you are ready to analyse the displayed data in the table and on the graphs of the other tabs. Your screen should look like the one on Figure 5 (and the *Chloroethenes graphs* tab and the *Other graphs* tab are identical to Figure 6 and Figure 7, respectively). Note that the results of this tutorial are saved under *TUTOquali.xml* and distributed with the application (*Tutorial* folder).

Some cells are coloured to help you identify if the situation is suitable for biodegradation by reductive dechlorination (see the legend besides the table and some details in Table 3).

The analysis of the resulting table leads to the following comments:

- Regarding the chloroethenes data, the reductive dechlorination quickly leads to the production of large amounts of all metabolic intermediates, especially cis-DCE (in A11). Apparently, cis-DCE does not form a bottleneck in the source zone, since VC and ethene are also produced in large quantities.

⁴ Requires Q-GIS to be installed on your computer (<http://www.qgis.org>)

The calculated dechlorination rates are, therefore, quite high: maximum of 34 and 59% for A9 and A11, respectively. It is important to note the high quantities of ethene and ethane produced (1100 µg/L of ethane in A11), which indicate efficient and complete reductive dechlorination;

- Regarding the redox conditions:
 - Biological reductive dechlorination is efficient because the redox conditions are methanogenic at the presumed location of the source zone (A9). In this monitoring well, the methane concentration is slightly below the threshold value⁵, but the monitoring wells located down-gradient and near A9 (A11 and A25) indicate considerable production of methane (17 to 21 mg/L), which is confirmed by strongly negative redox potentials (Eh from -54 to +2 mV) that is associated to favourable conditions for reductive dechlorination;
 - The sulfate reduction is not as efficient; there are high sulfate concentrations in the most contaminated zone. It is possible that the very high sulfate concentrations prevent even more complete dechlorination due to competition between sulfate-reducers and halo respirators for electrons.
 - Measurements of ferrous iron (6 mg/L to 18 mg/L in A9, A11 and A25) confirm reductive conditions with, in addition, the absence or near-absence of nitrates and dissolved oxygen at locations up-gradient from the source zone. Lastly, alkalinity concentrations confirm high CO₂ production at A25 (the starting point of the plume);

Therefore, at this site, and at the most contaminated zones in particular (from A9 to A25), there is evidence of active biological degradation.

- The pollution caused by chlorinated solvents comes together with other carbon contamination, as shown by the high content of dissolved organic carbon that "fuels" the biological reactions. Methanogenesis will continue as long as carbon is available. The high production of ethene and ethane indicates that efficient dehalorespirators (in particular, *Dehalococcoides ethenogenes*) are present and benefit from suitable physic-chemical conditions.
- Regarding the variations of contaminant along the plume centerline, the contaminant concentrations are still high at the receptor locations (e.g. in the private well PPB2). Indeed, the spatial dimensions of the zone that shows strongly reductive conditions are too small to allow for a long enough residence time for complete reductive dechlorination of the chlorinated contaminants into the harmless end-products, i.e. ethene and ethane. In addition, cis-DCE and especially VC reach the identified receptors. Moreover, biological degradation of TCE, cis-DCE, and VC in the "remote" plume (more than 660 m away from the source zone) proves to be inefficient in aerobic conditions. The increase in TCE concentration at well PzC is due to the presence of a TCE plume from a nearby site (site E, Figure 4) mixing together with the main plume from site A.

4.2. Tutorial 2 - Quantitative evaluation

The following example is conducted on the same industrial site than the previous tutorial (see the site description in the first paragraph of Section 4.1). In the methodology, it is advised to compute the mass balance of the quantitative evaluation in each homogeneous redox condition zone independently. Therefore, the evaluation will be conducted in the area identified as a suitable zone for methanogen biodegradation in the qualitative evaluation (see the conclusion of tutorial 1). The area is located downstream but close to the source zone, it is delineated by (see figures below): a section passing through well A11 with a length fitting the source zone extension (~25m) and a section located between wells A25 and PzA (where the width of the plume is ~120m, see Figure 4).

Before starting the user must always prepare the GIS input files. The four required files are ready to use for this tutorial (*TUTOCenterline.shp*, *TUTOWellsData.shp*, *TUTOSections.shp*, and *TUTOControlVolume.shp*). Please refer to Section 3.1 for details on how to prepare these files. The site situation and the shape files can be visualize by opening the *0-TUTOmainGIS.qgs* Q-GIS project⁶ and on Figure 4.

⁵ Actually in this well, high ferrous iron production indicates at least iron reducing conditions and near full methanogen conditions

⁶ Requires Q-GIS to be installed on your computer (www.qgis.org/)

Click on *Quantitative Assessment* to start the tutorial. First you have to load the first three required shape files in the first three lines of the Input tab window. Note that the file *TUTOWellsData.shp* must be loaded on the *Contaminant data* line. Next, choose the biodegradation type you want to compute the mass balance with: select *Anaerobic Biodegradation*. Indeed, as the qualitative evaluation (tutorial 1) has showed previously, anaerobic biodegradation is active in the zone delineated by the sections. Fill in *0.06* for effective porosity ((measured by field pumping and tracer tests).

By following the above settings, the top area of the input window should look like the one below.

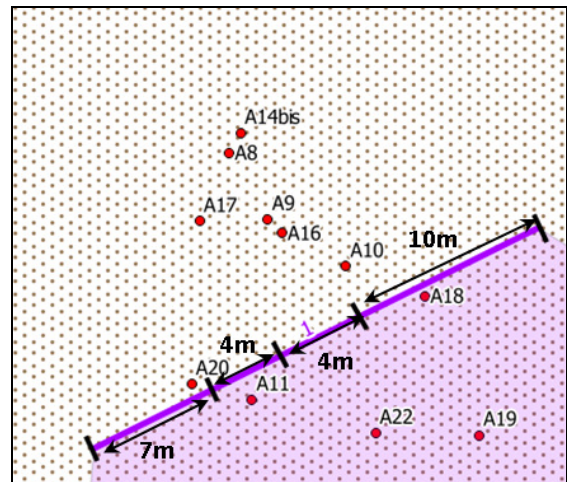
Plume centerline shape file	TUTOCenterline.shp	Browse		
Sections shape file	TUTOSections.shp	Browse	Distance between sections	110.52
Contaminants data file	TUTOWellsData.shp	Browse	Contaminant family	Chloroethenes
Biodegradation options	Anaerobic biodegradation		Location of the region	Plume
Effective porosity	0.06		# of control volumes	2

Let's move to the convection section.

The sections included in the *TUTOSection.shp* file has been loaded; assign the section name as 1 for upstream and 2 for downstream (1 and 2 are the ID of the polylines included in *TUTOSection.shp*). The downstream section must be wider than the upstream section. If not, SAMBBA will inform the user about it (an error icon will show up besides the downstream section length). The sections lengths are automatically computed by the application and are displayed for information. Next, set the aquifer depth to 4m on the three section / subsection areas: the aquifer depth is somewhat homogeneous on the studied plume portion of the industrial site (between the sections). Note that some sites can show variable aquifer depth, for instance because of substratum interface rise or decline. In such cases, specify different aquifer depths at the two sections. Next, the section can be divided into subsections; the convection flux through each section will be the sum of the convection flux through these subsections.

At the upstream section (section n°1), 4 subsections are set (note that the length entered in the input window is cumulative. For each new subsection only enter the y_2 value):

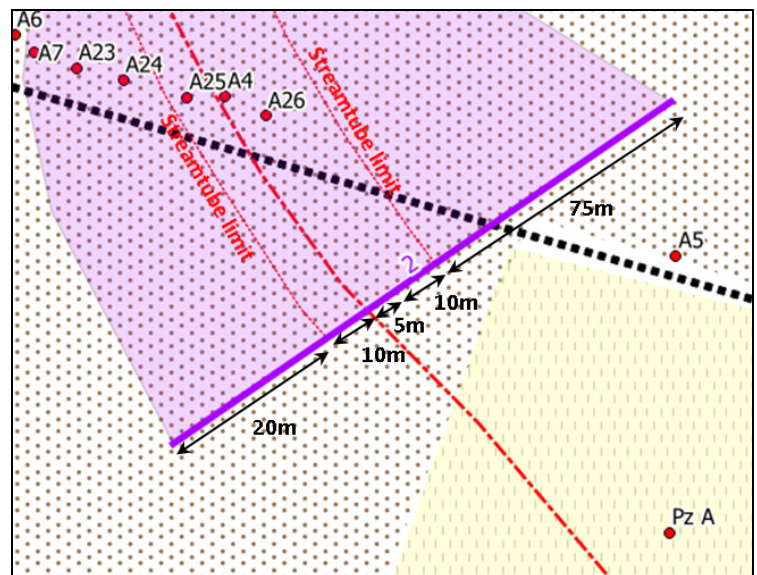
- The first one is 10 meters long ($y_2=10$) and the measurements at the nearby monitoring well A18 is used for the calculation of the influx convective flux on this subsection;
- The second one is 4 meters long ($y_2=14$); it is about the centre of the section and probably the place where the convection influx is the most important. There is no monitoring well close to it but well A16 seems relevant as it is representative of the observed concentration in the source zone;
- The next subsection is 4 meters long ($y_2=18$) and associated to the nearby monitoring well A11;
- The last one is 7 meters long and associated with the nearby monitoring well A20.



The downstream section (section n°2) is divided into 5 sections:

- In the *Central subsection* table (central stream tube), three subsections are considered with lengths of 10m, 5m and 10m ($y_2 = 10$ and 15). As there is no monitoring well near those subsections, we assume that there is small variations of concentrations along the stream tube (convection is dominant compared to the other mechanisms) and the upstream monitoring wells can be used. A26, A4 and A25 are then associated to the subsections;
- In the *Total subsection* table, the same central subsections are filled and 2 additional subsections are considered: one on the eastern side (75m length) and one on the western side (20m length). Since there is no monitoring well on either lateral subsections the same downstream monitoring well is chosen for both: well PzA (note that well A5 could be used too). In the *Total*

subsection table, the y_2 values for the 5 subsections (from east to west along the section) are: 75, 85, 90, 100, 119.50 (by default the total length of the section)



Finally, the Darcy velocity of groundwater is homogeneous and about 0.06 m/d.

By following the above settings, the *Convection* area of the input window should look like the one below.

Convection

Upstream section

Section name: 1

Section length (m): 24.83

Aquifer depth (m): 4

of subsections: 4

y1 (m)	y2 (m)	Well name	Darcy velocity (m/d)
0	10	A18	0.06
10	14	A16	0.06
14	18	A11	0.06
18	24.83	A20	0.06

Downstream section

Section name: 2

Section length (m): 24.83

Aquifer depth (m): 4

of subsections: 3

y1 (m)	y2 (m)	Well name	Darcy velocity (m/d)
0	10	A26	0.06
10	15	A4	0.06
15	24.83	A25	0.06

Total subsection

Section length (m): 119.50

Aquifer depth (m): 4

of subsections: 5

y1 (m)	y2 (m)	Well name	Darcy velocity (m/d)
0	75	Pz A	0.06
75	85	A26	0.06
85	90	A4	0.06
90	100	A25	0.06
100	119.50	Pz A	0.06

Now in the *volatilisation and rain recharge* area, you must load the control volume shape file (*TUTOControlVolume.shp*). The surface of the control volume is then computed (the geometric surface area covered by the plume between the two sections) as well as the surface of the central area (stream tube area). Those are displayed for information.

You need also to set the following data:

- The recharge flux corresponds to the effective rainfall, it was measured at 30 mm/year on the site ($9.5 \cdot 10^{-10}$ m/s);
- The *Volatilized fluxes* were calculated beforehand from the concentration of dissolved compounds measured in the plume and the application of Henry's and Fick's laws (vapour diffusion in the vadose zone). The resulting fluxes are presented in the print screen below. Note that this fluxes can also be issued from measurements at the soil / outdoor interface or by measurements of soil gas concentrations (and application of Fick's law) (Côme et al, 2006a);
- The *Concentrations of recharge* are the concentrations of dissolved compounds resulting from vapour washout. These concentrations are assessed from soil gas measurements in piezair and the Henry's law. They are showed on the print screen below.

Finally, the volatilization and rain recharge area of the input window should look like the one below.

Volatilisation and Rain Recharge

Total control volume shape file: TUTOControlVolume.shp

Surface of total area (m²): 8912.47

Surface of central area (m²): 2744.20

Recharge flux (m/s): 9.5E-10

Contaminant	Volatilized flux (µg/m ² /d)	Concentration of recharge (µg/l)
PCE	0.3	0.009
TCE	23.3	0.173
DCE	149	24
VC	12.4	0.0736
Ethene	26.1	0.009
Ethane	54.8	0.009

Now you are ready to compute the mass balance. Click the *Compute* button at the bottom of the window and proceed to the *Results in the plume* tab.

The *Result in the plume* tab should look like the one below.

Input Results in the Plume

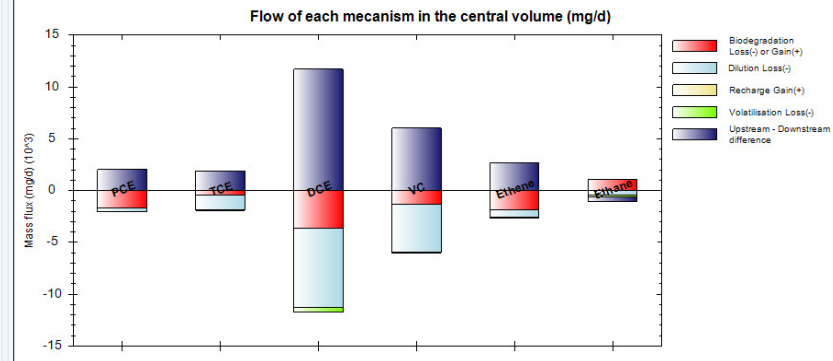
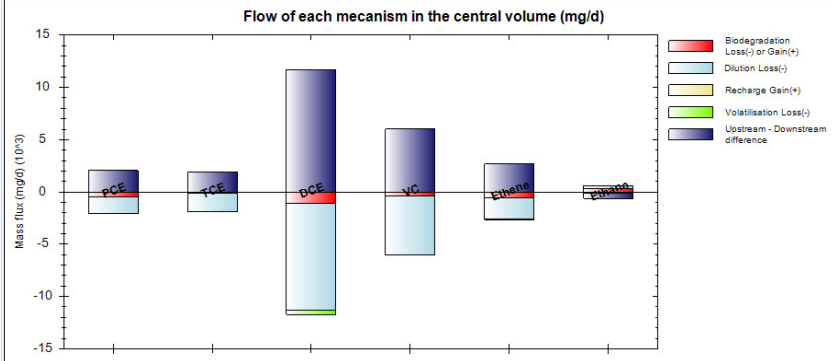
Assumption 1: the biodegradation occurs in the whole plume

	PCE	TCE	DCE	VC	Ethene	Ethane	
Residual total balance (mg/d)	1635.813	455.692	3672.666	1318.238	1880.013	-1049.92	
Apparent biodegradation rate (µg/l/d)	0.765	0.213	1.717	0.616	0.879	-0.491	
Intrinsic biodegradation rate (µg/l/d)	0.765	0.819	2.321	2.113	1.827	1.509	
1st order biodegradation constant (1/year)	0.901	0.806	0.179	0.669	1.339	3.506	
Mass balance on the central region							
INFLUX (mg/d)	(upstream) convection	2109.12	2090.626	28503.547	6599.258	2986.942	202.397
	recharge	0.002	0.039	5.406	0.017	0.002	0.002
	(downstream) convection	-61.339	-177.103	-16796.388	-585.283	-329.266	-667.692
OUTFLUX (mg/d)	volatilisation	-0.823	-63.94	-408.886	-34.028	-71.624	-150.382
	dispersion	-	-	-	-	-	-
	dilution (*)	-1543.284	-1709.311	-10172.845	-5574.071	-2007.188	292.399
%	biodegradation	-503.676	-140.31	-1130.835	-405.893	-578.867	323.276
	convection gain	100.	99.998	99.981	100.	100.	99.999
	recharge gain	9.612e-00b	0.002	0.019	2.512e-004	6.78e-00b	0.001
%	convection loss	-2.908	-8.471	-58.916	-8.869	-11.023	-329.889
	volatilisation loss	-0.039	-3.058	-1.434	-0.516	-2.398	-74.3
	dispersion loss	-	-	-	-	-	-
%	dilution loss	-73.172	-81.759	-35.683	-84.465	-67.199	144.467
	biodegradation loss	-23.881	-6.711	-3.967	-6.151	-19.38	159.722
	Mass balance on the total region						
INFLUX (mg/d)	(upstream) convection	2109.12	2090.626	28503.547	6599.258	2986.942	202.397
	recharge	0.007	0.127	17.557	0.054	0.007	0.007
	(downstream) convection	-470.64	-1427.4	-23520.48	-5170.56	-874.32	-763.92
OUTFLUX (mg/d)	volatilisation	-2.674	-207.661	-1327.958	-110.515	-232.615	-488.403
	biodegradation	-1635.813	-455.692	-3672.666	-1318.238	-1880.013	1049.92
	convection gain	100.	99.994	99.938	99.999	100.	99.997
%	recharge gain	3.122e-004	0.006	0.062	8.159e-004	2.204e-004	0.003
	convection loss	-22.314	-68.272	-82.467	-78.35	-29.271	-377.425
	volatilisation loss	-0.127	-9.932	-4.656	-1.675	-7.788	-241.302
%	biodegradation loss	-77.559	-21.796	-12.877	-19.975	-62.941	518.726

Assumption 2: the biodegradation occurs in the central region only

	PCE	TCE	DCE	VC	Ethene	Ethane	
Residual total balance (mg/d)	1635.813	455.692	3672.666	1318.238	1880.013	-1049.92	
Apparent biodegradation rate (µg/l/d)	2.484	0.692	5.576	2.002	2.855	-1.594	
Intrinsic biodegradation rate (µg/l/d)	2.484	2.66	7.538	6.863	5.935	4.901	
1st order biodegradation constant (1/year)	4.935	2.405	0.602	2.042	4.99	4.21	
Mass balance on the central region							
INFLUX (mg/d)	(upstream) convection	2109.12	2090.626	28503.547	6599.258	2986.942	202.397
	recharge	0.002	0.039	5.406	0.017	0.002	0.002
	(downstream) convection	-61.339	-177.103	-16796.388	-585.283	-329.266	-667.692
OUTFLUX (mg/d)	volatilisation	-0.823	-63.94	-408.886	-34.028	-71.624	-150.382
	dispersion	-	-	-	-	-	-
	dilution (*)	-411.147	-1393.93	-7631.013	-4661.726	-706.042	434.245
%	biodegradation	-1635.813	-455.692	-3672.666	-1318.238	-1880.013	1049.92
	convection gain	100.	99.998	99.981	100.	100.	99.999
	recharge gain	9.612e-00b	0.002	0.019	2.512e-004	6.78e-00b	0.001
%	convection loss	-2.908	-8.471	-58.916	-8.869	-11.023	-329.889
	volatilisation loss	-0.039	-3.058	-1.434	-0.516	-2.398	-74.3
	dispersion loss	-	-	-	-	-	-
%	dilution loss	-19.494	-66.674	-26.767	-70.64	-23.638	214.549
	biodegradation loss	-77.559	-21.796	-12.883	-19.975	-62.941	518.738
	Mass balance on the total region						
INFLUX (mg/d)	(upstream) convection	2109.12	2090.626	28503.547	6599.258	2986.942	202.397
	recharge	0.007	0.127	17.557	0.054	0.007	0.007
	(downstream) convection	-470.64	-1427.4	-23520.48	-5170.56	-874.32	-763.92
OUTFLUX (mg/d)	volatilisation	-2.674	-207.661	-1327.958	-110.515	-232.615	-488.403
	biodegradation	-1635.813	-455.692	-3672.666	-1318.238	-1880.013	1049.92
	convection gain	100.	99.994	99.938	99.999	100.	99.997
%	recharge gain	3.122e-004	0.006	0.062	8.159e-004	2.204e-004	0.003
	convection loss	-22.314	-68.272	-82.467	-78.35	-29.271	-377.425
	volatilisation loss	-0.127	-9.932	-4.656	-1.675	-7.788	-241.302
%	biodegradation loss	-77.559	-21.796	-12.877	-19.975	-62.941	518.726

(*) Refer to the user guide for details



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The mass fluxes of each mechanism together with residual total balance and biodegradation rates are computed by SAMBBA and showed in the resulting tables and charts. Assuming biodegradation rates are homogeneous over the whole control volume (assumption 1), the results leads to the following comments:

- all contaminants show a decrease in the convective mass fluxes of dissolved contaminant in groundwater between section 1 and section 2, except for ethane;
- "dilution" (considered here as the sum of dilution and dispersion, cf. Section 3.4.2) is the most prevalent process in the central volume for all contaminants, except for DCE (where convection is predominant) and ethane: depending on the contaminant, dilution accounts for 67 to 84 % of the flux attenuation between sections (difference between the up-gradient and down-gradient transects). The error flag shown next to the dilution flux of ethane indicates a mass balance incoherence as dilution fluxes should be negative (outfluxes sign is negative by convention);
- the second most prevalent processes, except for ethane, are convection and biodegradation, the later accounting for 4% to 24%;
- the contribution from volatilization is non-significant, while the contribution from vapour washout is nearly zero (largely due to the presence of industrial buildings and road asphalt);
- 1st order biodegradation constants given from mass balance calculations vary from 0.67 year⁻¹ for Vinyl Chloride to 1.3 year⁻¹ for Ethene (since Ethane dilution sign is positive, it is best to rule out the biodegradation constant for this contaminant);
- The mass balance for ethane is inconsistent. Indeed, the positive flux on the dilution line should mean that there is a production of ethane by dilution which is not physically possible. This problem can often be solved by changing the subsection discretisation and attributes (wells, velocity) and/or the plume geometry. This could be tested as a sensitivity analysis of these parameters.

Assuming biodegradation only occurs in the central stream tube (assumption 2), the results leads to the following comments:

- Assumption 2 allows to correctly interpret the mass balance, even for ethane. For this compound, the residual balance is negative indicating a (bio)-production of the compound in the plume. The "dilution" flux is however negative as it should be (loss of mass in the central plume due to dilution and dispersion);
- Dilution and biodegradation are the main mechanisms for all the compounds except for DCE (where convection is predominant). Moreover, biodegradation is prevalent for PCE and Ethene (77% and 62%, respectively). The high biodegradation level for Ethane comes from a counterbalance against downstream concentration rise and the loss related to volatilization, dispersion and dilution;
- The contribution from volatilization and vapour washout are still non-significant;
- The biodegradation rates are greater than in assumption 1 by a factor 3 to more than 5 (Ethane is not included in the comparison since its mass flux balance seems off). The computed biodegradation constants are between 0.60 year⁻¹ (DCE) and 5.0 year⁻¹ (Ethene).

5. References

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- [4] Côme et al, 2006b, modelling the fate of chlorinated solvents in aquifers, Technical guide, extended abstract. MACAOH R&D project, ADEME.
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