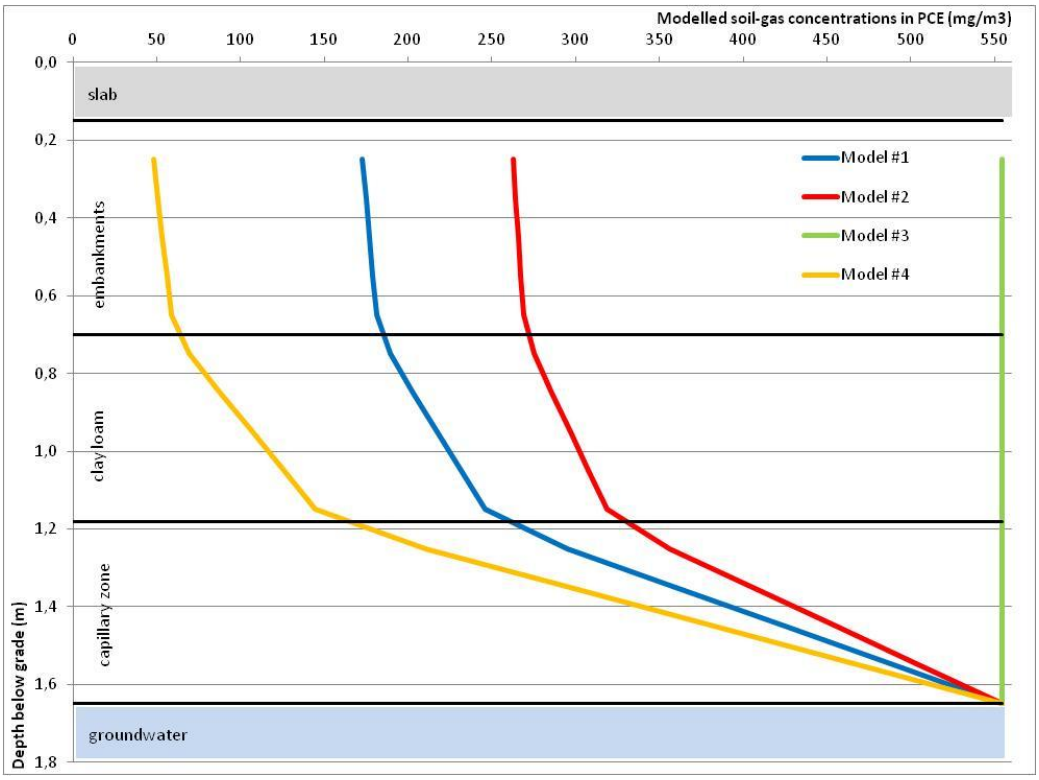
Models for predicting transfers to indoor air



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1 Introduction

1.1 CityChlor and integrated approach

Space is scarce in Europe. Even in the subsurface it is getting busier. Large-scale soil and groundwater contamination with chlorinated solvents are often an obstruction for urban developments. The traditional way of dealing with polluted soil and groundwater does not work in all cases and is not economically and sustainably feasible. In urban environments multiple contaminations with chlorinated solvents are often mixed with each other and spread underneath buildings. This not only leads to technical problems for remediation, but also to liability and financial discussions and hence has an impact on society. An integrated approach and area-oriented approach is needed to tackle the problems. The CityChlor project has demonstrated that remediation and sustainable development can evolve on a parallel timescale.

An integrated approach combines all aspects that are relevant to tackle the problems that pollution with VOC in urban environment causes. Depending on area, site and context, different aspects together or parallel to each other can be used. Not only technical solutions are included, but also socio-economical aspects as urban development, communication, financial and legal aspects, time, space, environment and actors (active & passive) have to be handled.

CityChlor did not remain at single case remediation, but looked at the area as a whole in a bigger context: the area-oriented approach. A technical approach that makes it possible to remediate, monitor and control multiple groundwater sources and plumes within a fixed area.

1.2 CityChlor and technical innovations

The managing of knowledge is one of the key to achieve a sustainable city development. A development project has to cope with loads of information coming from different disciplines in different (technical) languages and with different uncertainties. With chlorinated solvents in particular, the knowledge about the pollution will always have a certain uncertainty that can have an impact on the course and the costs of the remediation. An efficient 'managing of knowledge' will try to decrease this degree of uncertainty.

CityChlor therefore also worked on the technical aspects of characterization and remediation. The conventional techniques that are applied for investigation and remediation have their limitations when dealing with chlorinated solvents. Promising innovative techniques exist, but do not easily find their way to current application. This barrier is often caused by lack of knowledge on different levels. Experts and contractors do not always have the means to invest in experiments with new techniques, authorities are reluctant to accept techniques of which the results may be uncertain and clients aren't eager to pay for experimental techniques.

Dissemination of knowledge can break this deadlock. CityChlor therefore collected experiences from field application of innovative techniques and implemented itself a number of techniques in pilot projects. For the detailed outcomes, the reader is referred to the specific reports.

CityChlor - “new solutions for complex pollutions” **http://www.citychlor.eu/**

2 Introduction to model prediction

2.1 Main contexts for modelling transfers to indoor air

Several contexts exist for modelling transfers to indoor air:

- to characterize some transfers from soil to building,
- to estimate the indoor concentrations resulting in a future building from a soil contamination,
- to help to define some remediation operations.

Models need several input parameters related to soil and buildings characteristics, and to substances properties and location.

2.2 Analytical models

2.2.1 Model of Johnson and Ettinger [1991]

Johnson and Ettinger [1991] have developed a one-dimensional analytical model, of which the concept is based on:

- a building with a slab on grade,
- a diffusive transfer from soil to a “zone of influence of the building”,
- a convective transfer through cracks between the foundation and the basement slab floor,
- the assumption that cracks are located at the perimeter of the slab.

The authors proposed a global equation for the transfer corresponding to equation 1:

Equation 1

$$\alpha = \frac{C_{building}}{C_{source}} = \frac{\dfrac{D_{soil}^{eff} A_B}{Q_{building} L_{soil}} \exp\left(\dfrac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right)}{\exp\left(\dfrac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) + \dfrac{D_{soil}^{eff} A_B}{Q_{building} L_{soil}} + \dfrac{D_{soil}^{eff} A_B}{Q_{soil} L_{soil}}\left[\exp\left(\dfrac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) - 1\right]}$$

$C_{building}$	concentration resulting in the building (µg/m3)
C_{source}	concentration at the source (µg/m3)
Q_{soil}	volumetric flow rate of soil gas into enclosed space (m3/s)
L_{crack}	enclosed space foundation or slab thickness (m)
D_{crack}	effective diffusion coefficient through cracks (m2/s)
A_{crack}	area of total cracks (m2)
D_{soil}^{eff}	total overall effective diffusion coefficient in soil layers (m2/s)
A_B	area of the enclosed space below grade (m2)
$Q_{building}$	building ventilation rate (m3/s)
L_{soil}	source/building separation (m)

For the volumetric flow rate of soil gas into enclosed space Q_{soil}, Johnson and Ettinger [1991] have chosen to apply the analytical solution of Nazaroff [1988] given by equation 2.

Equation 2

$$Q_{soil} = \frac{2\pi k_v \Delta P X_{eq}}{\mu_a \ln\left(2Z_{eq}/r_{eq}\right)}$$

Q_{soil}	volumetric flow rate of soil gas into enclosed space (m^3/s)
k_v	air permeability of soil (m^2)
ΔP	pressure differential between the soil surface and the enclosed space (Pa)
X_{eq}	building floor-wall seam perimeter (m)
μ_a	dynamic viscosity of air (kg/m.s)
Z_{eq}	crack depth below grade (m)
r_{eq}	equivalent crack radius (m)

Some authors have proposed other formulation for the volumetric flow rate of soil gas into enclosed space. According to Yao *et al.* [2011], the equation 3 would be more appropriated for homogeneous soils.

Equation 3

$$Q_{soil} = \frac{\pi k_v \Delta P X_{eq}}{\mu_a \ln\left(4Z_{eq}/r_{eq}\right)}$$

2.2.2 Model of VolaSoil [Waitz *et al*., 1996]

In the VolaSoil model, Waitz *et al*. [1996] have adopted the following concepts:

- a building with a crawl space,
- a diffusive and convective transfer from soil to the crawl space,
- a convective transfer from the crawl space to the indoor air,
- gaps and holes are regularly distributed in the slab in the form of cylindrical tubes.

The authors proposed a global equation for the transfer corresponding to equation 4.

Equation 4

$$\alpha = \frac{C_{building}}{C_{source}} = \frac{A_{floor}^2 K_{floor} \Delta P_{indoor/crawl}}{Q_{indoor} L_{floor} Q_{crawl}} \frac{K_{soil} \frac{\Delta P_{crawl/soil}}{L_{soil}}}{1 - \exp\left(-\frac{K_{soil} \Delta P_{crawl/soil}}{D_{soil}^{eff}}\right)}$$

A_{floor}	surface area of floor (m^2)
Q_{indoor}	indoor ventilation rate (m^3/s)
Q_{crawl}	crawl space ventilation rate (m^3/s)
L_{floor}	slab thickness (m)
L_{soil}	source/building separation (m)
K_{floor}	air conductivity of floor (m^2/Pa.s)
K_{soil}	air conductivity of soil (m^2/Pa.s)
D_{soil}^{eff}	total overall effective diffusion coefficient in soil layers (m^2/s)
$\Delta P_{indoor/crawl}$	air pressure difference between indoor air and crawl space (Pa)
$\Delta P_{crawl/soil}$	air pressure difference between crawl space and soil (Pa)

With the assumptions made on the gaps and holes, the air conductivity of floor is described by equation 5.

Equation 5

$$K_{floor} = \frac{f_{of}^2}{n 8 \pi \mu_a}$$

K_{floor}	air conductivity of floor (m^2/Pa.s)
f_{of}	fraction of openings in floor (-)
n	number of openings per floor area (m^{-2})
μ_a	dynamic viscosity of air (kg/m.s)

2.2.3 The "capillary" approach for a building floor

Bakker *et al*. [2008] have proposed to extend the concept of the "capillary" approach of VolaSoil to the case of a building floor. In this approach, the defaults of the slab are supposed to be regularly distributed in the slab in the form of cylindrical tubes. This approach leads to the global equation 6.

Equation 6

$$\alpha = \frac{C_{building}}{C_{source}} = \frac{A_{floor}}{Q_{indoor}} \frac{K_T \frac{\Delta P}{L_T}}{1 - \exp\left(-\frac{K_T \Delta P\, L_{soil}}{D_{soil}^{eff} L_T}\right) \exp\left(-\frac{K_T \Delta P\, L_{floor}}{f_{of} D_{floor} L_T}\right)}$$

A_{floor}	surface area of floor (m^2)
Q_{indoor}	indoor ventilation rate (m^3/s)
L_{floor}	slab thickness (m)
L_{soil}	source/building separation (m)
L_T	source/building separation and slab thickness (m)
K_T	total overall effective air conductivity of soil and floor (m^2/Pa.s)
D_{soil}^{eff}	total overall effective diffusion coefficient in soil layers (m^2/s)
D_{floor}	effective diffusion coefficient through gaps and holes (m2/s)
ΔP	air pressure difference between indoor air and soil (Pa)
f_{of}	fraction of openings in floor (-)

2.2.4 The concept of the intact slab, or "porous medium" approach

Bakker *et al*. [2008] have also proposed to consider the case of an intact slab and its conceptualisation as a porous medium. In this approach, slab is considered as an additional layer which is integrated with the other soil layers in global parameters (total overall effective diffusion coefficient and total overall effective air conductivity). Such an approach needs to have some specific parameters for the slab due to its micro-porosity.

With this concept, the global transfer to indoor air is given by equation 7.

Equation 7

$$\alpha = \frac{C_{building}}{C_{source}} = \frac{A_{floor}}{Q_{indoor}} \frac{K_T \frac{\Delta P}{L_T}}{1 - \exp\left(-\frac{K_T \Delta P}{D_T^{eff}}\right)}$$

A_{floor}	surface area of floor (m^2)
Q_{indoor}	indoor ventilation rate (m^3/s)
L_T	source/building separation and slab thickness (m)
K_T	total overall effective air conductivity of soil and slab (m^2/Pa.s)
D_T^{eff}	total overall effective diffusion coefficient of soil and slab (m^2/s)
ΔP	air pressure difference between indoor air and soil (Pa)

These various analytical models consider a homogeneous air pressure difference over all the soil layers and the slab. In a realistic approach, the air pressure difference decreases with depth below grade. Some authors proposed an analytical model in which specific air pressure differences are consider for each layer (soil layers and slab which is considered as a porous medium). According to Thiam and Gay [2013], the global equation for such an approach is given by in the equation 8 in the case of n layers (including slab as layer n°0).

Equation 8

$$\alpha = \frac{C_{building}}{C_{source}} = \left[\frac{Q_{indoor}}{A_{floor}} \sum_{i=1}^{n} \left(\frac{1 - \exp\left(-\frac{K_i \Delta P_i}{D_i^{eff}}\right)}{\frac{K_i \Delta P_i}{L_i}} \exp\left(-\sum_{j=i-1}^{n} \frac{K_j \Delta P_j}{D_j^{eff}}\right) \right) + \exp\left(-\sum_{i=1}^{n} \frac{K_i \Delta P_i}{D_i^{eff}}\right) \right]^{-1}$$

A_{floor}	surface area of floor (m^2)
Q_{indoor}	indoor ventilation rate (m^3/s)
L_i	thickness of layer i (m)
K_i	effective air conductivity of layer i (m^2/Pa.s)
D_i^{eff}	effective diffusion coefficient of layer i (m^2/s)
ΔP_i	air pressure difference in the layer i (Pa)

3 CityChlor pilot project Ile de France

3.1 Presentation of the project

This pilot project was an in-service facility located near Paris, France in an urban area. The site area was 6 700 m^2. Industrial activities started around 1926 and today the main activity is the production of door locks, metal fittings and their surface coatings. An aerial view of the site is presented in figure 1. On site, soils were composed of 50 cm to 1 m of embankments, then about 3 m of clay/sandy-clay and finally fine sand to 10 m deep. The alluvial aquifer was studied during the project: on site, the mean depth of the water table was 1.5 to 2 m below the ground surface and the groundwater was about 10 m deep. The groundwater flow direction was monitored during the project and two main flow directions were identified: direction n°1 from north to south (during high water periods) and direction n°2 from east to west (during low water periods).

Figure 1: CityChlor pilot project Ile de France *(source: INERIS).*

Different painting, electroplating, polishing and assembly shops succeed each other at various locations during its business activity as shown in figure 2. Among others, perchloroethylene (PCE) and trichloroethylene (TCE) were used and are still used. Soils and groundwater are polluted with chlorinated solvents (perchloroethylene, trichloroethylene, dichloroethylene and vinyl chloride): source zones are identified with red dots in figure 1.

In 2006, because the electroplating shop came to an end, a diagnosis of soil and groundwater quality assessment was carried out (2007). These investigations have demonstrated that the activities have an impact on soil and groundwater quality. Then, a management plant had been created in 2010. Finely, it suggested natural attenuation as a measure of pollution management. However, because of the current French regulation about natural attenuation, the authorities required biannual monitoring of groundwater on site and off site, since 2011.

CityChlor pilot project Ile de France presentation and the whole tests and measurements carried out at this pilot site are detailed in the pilot project Ile de France report.

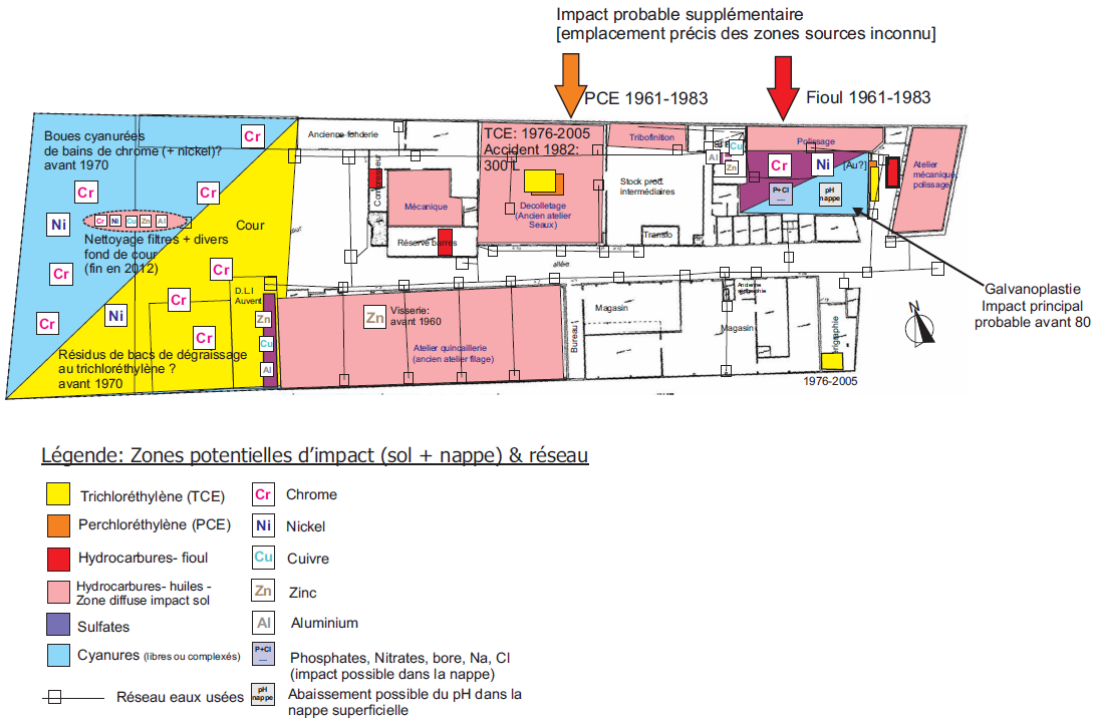

Figure 2: shop historical locations of CityChlor pilot project Ile de France.

3.2 Aims of the modelling conducted on the project

CityChlor pilot project Ile de France was characterised for several parameters:

- building parameters: dimensions, air change rate, outside/inside difference of pressure...
- soil parameters: local geology, dry bulk density, total porosity, water content...
- groundwater parameters: depth of the water table, flow direction...
- pollution concentrations: in soils, in groundwater, in soil-gas, in indoor air...

This characterisation allows comparing measured values with modelled values, in particular the indoor concentrations. In consequence, the aim of the modelling conducted on the project is to compare:

- the measured values of indoor concentrations with
- the modelled values of indoor concentrations obtained from the measured values of groundwater or soil-gas concentrations.

4 Input parameters

4.1 Perimeter of the modelling: location and period

4.1.1 Location selection

Because of the configuration of buildings, modelling was restricted to the workshop n°19 located at the South-East corner of the CityChlor pilot project Ile de France. This workshop presents several advantages:

- a piezometer (n°1) is located near the workshop and allows to estimate the quality of the groundwater;
- some soil-gas wells have been installed in the workshop in order to characterize the soil-gas concentrations;
- the workshop is one of the best closed parts of the CityChlor pilot project Ile de France (small volume, weak use, and effective door), which allows to obtain indoor air concentrations representative of the soil and groundwater pollution.

Characteristic properties of the workshop n°19 are given in table 1.

Table 1: main characteristics of the workshop n°19.

Parameter	Value and unit	Justification
Length	10.5 m	measured value
Width	5.0 m	measured value
Height	3.0 m	measured value
Perimeter	31.0 m	calculated value
Floor surface	52.5 m^2	calculated value
Volume	157.5 m^3	calculated value
Thickness of the concrete slab	0.15 m	measured value

4.1.2 Period selection

Several campaigns have been carried out on the CityChlor project Ile de France in order to characterise regularly different media: groundwater, soil-gas, and indoor air. Among these, the campaign of June 2012 has been chosen because that is the only one for which all the media have been simultaneously characterised. As possible, the time-dependent input parameters will be chosen among those which were determined in June 2012.

4.2 Input parameters for the building

4.2.1 Air change rate

The air change rate has been measured in the workshop n°19 in October 2011, in wintry conditions in the absence of heating, by recording the diminution of a tracer gas: the sulphur

hexafluoride SF_6 (see details in the CityChlor report “Pilot project: Ile de France”). This is the only measure carried out at this location. Even if this measure is not representative of summery conditions, the obtained value will be retained for the modelling.

In October 2011, air change rate has been measured at two different heights from the floor: 0.1 and 0.5 m. The diminution curves of SF_6 are illustrated in figure 3a and figure 3b respectively.

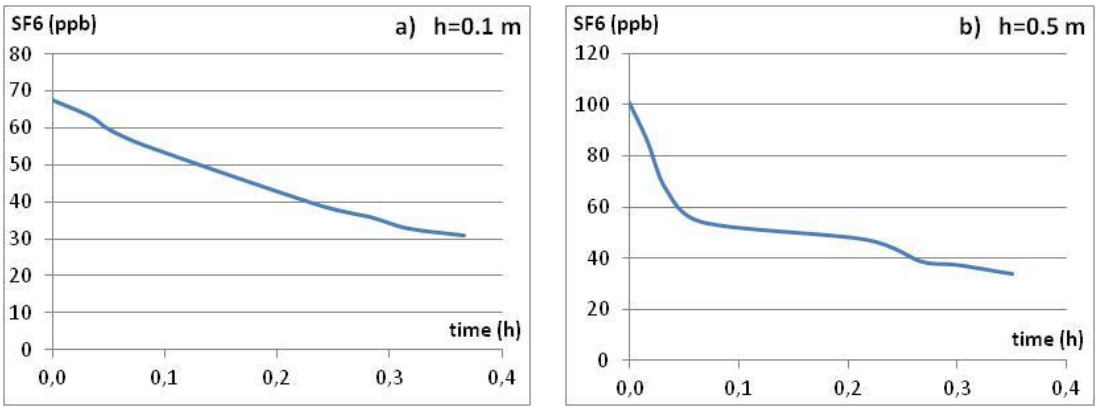

Figure 3: diminution curves of SF6 in workshop n°19 in October 2011 at 0.1 m high (a) and 0.5 m high (b).

The air change rate is determined thanks the diminution of $\log(C/C_0)$ during time, which is supposed to be linear. The measured air change rate is 2.17 volumes per hour at 0.1 m high, and 2.68 volumes per hour at 0.5 m high. The mean value is retained for the modelling: 2.4 volumes per hour. It is applied for the whole workshop n°19.

4.2.2 Outside/inside difference of pressure

The difference of pressure between outside and inside has been measured in the workshop n°19 in February 2013, in wintry conditions in the absence of heating. A continuous recording of differential pressures has been performed over four days, at the same time as inside and outside temperatures and barometric pressure (see details in the CityChlor report “Pilot project: Ile de France”). All these records are represented at the figure 4.

Outside/inside difference of pressure varies with time and alternates periods of important fluctuations and periods of relative stability. For the modelling, the mean value is retained: +0.1 Pa. It is applied for the whole workshop n°19. It is about a rather low value, in coherence with the weak difference of temperature between outside and inside.

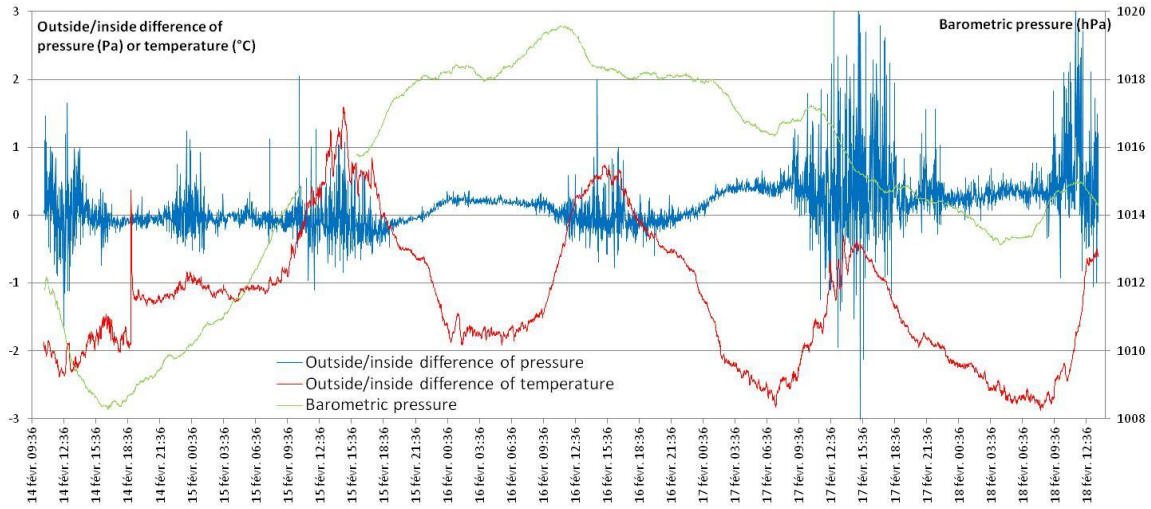

Figure 4: recording of outside/inside difference of pressure, outside/inside difference of temperature and barometric pressure at the workshop n°19.

4.2.3 Modelling of the concrete slab

There are actually three manners to model the slab of a building [Bakker *et al*., 2008].

- The "perimeter seam gap" approach assumes that gaps are located on the perimeter of the slab, due to drying shrinkage [Johnson and Ettinger, 1991].
- The "capillary" approach considers that holes are regularly distributed on the surface of the slab, and constitute tubes [Waitz *et al*., 1996].
- The "porous medium" approach consists in considering slab like a porous medium and in applying the same transfer equations that for a soil layer [Krylov and Ferguson, 1998].

These three approaches have been considered in the present report. Each approach needs some specific parameters, as resumed in table 2.

Table 2: specific parameters for concrete slab modelling.

Parameter	Value and unit	Justification
"Perimeter seam gap" approach		
Crack width	0.001 m	default value [US EPA, 2004]
Crack depth below grade	0.15 m	linked to slab thickness
"Capillary" approach		
Number of openings	10 m^{-2}	default value [Waitz *et al*., 1996]
Fraction of openings in floor	$1x10^{-5}$	default value [Waitz *et al*., 1996]
"Porous medium" approach		
Total porosity	0.165	estimated value
Tortuosity	0.0333	estimated value
Air-filled porosity	0.0497	calculated value [Millington and Quirck, 1961]
Intrinsic air permeability	$5x10^{-17}$ m^2	measured value (*)

(*) The measure has been performed on a core sample of the concrete slab of the workshop n°19.

4.3 Physico-chemical properties of the substance

4.3.1 Selection of perchloroethylene

As enlightened in the CityChlor report “Pilot project: Ile de France”, the analytical results show that many chlorinated solvents are present in the groundwater, the soils and the soil-gas. Trichloroethylene and perchloroethylene are the most frequently detected substances in soil-gas, and perchloroethylene is the most frequently detected substances in indoor air.

In order to compare modelled and measured indoor concentrations, the present modelling has to focus on perchloroethylene. The interactions with the others compounds will not be taken into account.

4.3.2 Intrinsic physico-chemical properties of perchloroethylene

The main physico-chemical properties of perchloroethylene have been looked for in the “toxicological and environmental data sheet” relative on perchloroethylene and edited by INERIS [2012]. From this data sheet, some properties of perchloroethylene are given in table 3.

Table 3: Intrinsic physico-chemical properties of perchloroethylene at 25 °C.

Parameter	Value and unit
Molar mass	165.80 $g.mol^{-1}$
Vapour pressure	2,462 Pa
Solubility	150 $mg.l^{-1}$
Organic carbon partition coefficient	247 $l.kg^{-1}$
Henry’s law constant	1,844 $Pa.m^3.mol^{-1}$
Diffusion coefficient in pure water	$8.20x10^{-10}$ $m^2.s^{-1}$
Diffusion coefficient in pure air	$7.20x10^{-6}$ $m^2.s^{-1}$

According to these data, the dimensionless Henry’s law constant is equal to 0.744 for perchloroethylene at 25 °C.

4.3.3 Influence of the temperature on parameters

Many properties of perchloroethylene depend on the temperature. As the temperature of the soil-gas may be very different of the reference temperature used for the determination of these properties, some corrections may be taken into account.

As a first approach, an uniform temperature of 15 °C is considered in the soil column. This is a typical temperature for the June period.

To apply the correction due to the temperature on the Henry’s law constant, some specific properties of perchloroethylene are needed. The corresponding values are given in a fact sheet of the US EPA [2001], and are presented in table 4.

Table 4: specific properties of perchloroethylene.

Parameter	Value and unit
Enthalpy of vaporization at the normal boiling point	8,288 cal.mol^{-1}
Normal boiling point T_B	394 °K
Critical temperature T_C	620 °K
Constant n depending on the ratio T_B/T_C	0.355

According to these data and to the equations developed in the fact sheet of the US EPA [2001], the enthalpy of vaporization at the soil temperature is equal to 9,400 cal.mol^{-1}, and the dimensionless Henry's law constant is equal to 0.426 for perchloroethylene at soil temperature.
Diffusion coefficients also depend on the temperature, according to the following equation [Pauling *et al*., 2000]:

Equation 9

$$D_{soil} = D_{ref} \times \left(\frac{T_{soil}}{T_{ref}} \right)^{2.01}$$

where T_{soil} and T_{ref}, in °K, are respectively the soil temperature and the reference temperature.
For the chosen soil temperature of 15 °C, this correction leads to:

- a diffusion coefficient in pure water equal to 7.66x10^{-10} m^2.s^{-1},
- a diffusion coefficient in pure air equal to 6.72x10^{-6} m^2.s^{-1}.

4.4 Description of soil layers

4.4.1 Local geology at the CityChlor pilot project Ile de France

As described previously, soils were globally composed:

- of 0.5 to 1 m of embankments,
- then about 3 m of clay/sandy-clay,
- and finally fine sand to 10 m deep.

The mean depth of the water table was 1.5 to 2 m below the ground surface and the groundwater was about 10 m deep.
In June 2012, near the workshop n°19 (at the piezometer n°1), the mean depth of the water table was 1.65 m below the ground surface. At the location of the workshop n°19, from grade to water table, it is possible to distinguish the following layers:

- 0.15 m of concrete slab,
- 0.55 m of embankments, which are considered as "sand" in the SCS approach,
- 0.48 m of clayey layer, which is considered as "clay loam" in the SCS approach,
- 0.47 m of clayey layer corresponding to the open capillary zone above the water table.

SCS (or soil classification system) approach is the most common engineering classification system for soils in North America, and allows to determine a textural class from the grading and to define some default values for each class. For example, the height of the open capillary zone ensues from the default value relative to "clay loam" class.

4.4.2 Properties of the soil layers

At the location of workshop n°19, two samples have been collected in the “sand” layer (Z24Bsurf and Z14subsurf) and two samples in the “clay loam” layer (Z24Bprof and Z24Cprof), in order to determine some specific soil characteristics (dry bulk density, organic carbon weight fraction, water content and total porosity). For the other characteristics (intrinsic air permeability, water-filled porosity for the open capillary zone), default values from the SCS approach were selected.

All the layers are supposed to be homogeneous within any horizontal plane. All the properties of the soil layers are resumed in the table 5.

Table 5: properties of soil layers.

Parameter	Value and unit		
	“Sand” layer	“Clay loam” layer	Open capillary zone
Dry bulk density	1,640 $kg.m^{-3}$ (a)	1,480 $kg.m^{-3}$ (c)	1,480 $kg.m^{-3}$ (c)
Organic carbon weight fraction	0.10 (a)	0.15 (a)	0.15 (a)
Total porosity	0.36 (a)	0.42 (a)	0.42 (a)
Water-filled porosity	0.197 (b)	0.320 (b)	0.356 (d)
Intrinsic air permeability	4.12×10^{-12} m^2 (d)	5.45×10^{-14} m^2 (d)	3.61×10^{-14} m^2 (d)

(a) measured value on soil samples; (b) calculated value from measurements on soil samples; (c) default value from SCS approach; (d) calculated value from default SCS values.

4.5 Depth and concentration of PCE for analytical modelling

Analytical models consider one-dimensional vertical transfer from pollution source to indoor air. In order to compare measured indoor concentrations with modelled indoor concentrations, many assumptions may be made on the depth and the concentration of PCE. In the case of the CityChlor pilot project Ile de France, three main configurations can be distinguished:

- perchloroethylene is essentially located in the groundwater: in such a case, it can be considered that groundwater is the source term of the PCE transfer, and that the depth of the source is equal to the water table, and that the vapour concentration just above the water table is in equilibrium with the groundwater concentration; this case is considered here as the baseline scenario;
- perchloroethylene is located in the “clay loam” layer: it is not strictly a source term but rather a transfer term; in this approach, specific values from soil-gas wells implanted in the “clay loam” layer will be used to determine a depth and a concentration for PCE;
- perchloroethylene is located in the embankments; as previously, it is rather a transfer term than a source term; specific values from soil-gas wells implanted in the embankments will be used to determine a depth and a concentration for PCE.

For each configuration, the selected values for the depth and the concentration of the input term of PCE are detailed in table 6.

Table 6: depth and concentration for the input term of PCE.

Parameter	Value and unit	Justification
Scenario n°1: PCE in groundwater (or "baseline scenario")		
Depth of the input term	1.65 m	mean measured water table depth in June 2012
Concentration in groundwater	1,300 $\mu g.l^{-1}$	measured value in piezometer n°1 in June 2012
Concentration in soil-gas	554.26 $mg.m^{-3}$	calculated value in equilibrium with groundwater
Scenario n°2 : PCE in "clay loam" layer		
Depth of the input term	0.90 m	mean depth of the upper part of soil-gas wells [(a)]
Concentration in soil-gas	0.46 $mg.m^{-3}$	mean measured value in soil-gas wells in June 2012
Scenario n°3 : PCE in embankments		
Depth of the input term	0.30 m	mean depth of the upper part of soil-gas wells [(b)]
Concentration in soil-gas	0.76 $mg.m^{-3}$	mean measured value in soil-gas wells in June 2012

(a) for the "clay loam" layer, concerned soil-gas wells are Pza11 and Pza13;
(b) for embankments, concerned soil-gas wells are Pza10-H, Pza12 and Pza14.

5 Results of analytical modelling

5.1 Results of the baseline scenario: PCE in groundwater

In addition to indoor concentrations, other parameters are compared between the different models and with measured values when available. Table 7 gives a synthesis of these various modelled parameters.

Table 7: comparison of the modelled results of the analytical models in the baseline scenario of a source in groundwater.

Parameter	Unit	Measured value	J&E 1991 - Perimeter cracks	Yao et al. 2011 - Perimeter cracks	RIVM 2008 - Gaps and holes	RIVM 2008 - Intact floor	Thiam & Gay - Intact floor
Attenuation coefficient α	-	/	$2.3x10^{-6}$	$1.8x10^{-6}$	$1.2x10^{-7}$	$3.0x10^{-6}$	$3.1x10^{-6}$
Indoor concentration	$mg.m^{-3}$	$1.1x10^{+0}$	$1.3x10^{-3}$	$9.7x10^{-4}$	$6.9x10^{-5}$	$1.7x10^{-3}$	$1.7x10^{-3}$
Mass flow at the floor surface	$mg.m^{-2}.s^{-1}$	/	$2.5x10^{-6}$	$1.9x10^{-6}$	$1.4x10^{-7}$	$3.4x10^{-6}$	$3.4x10^{-6}$
intermediate concentration at 0.45 m [(a)]	$mg.m^{-3}$	$7.6x10^{-1}$	$1.8x10^{+2}$	$2.7x10^{+2}$	$5.5x10^{+2}$	$5.4x10^{+1}$	$5.3x10^{+1}$
intermediate concentration at 1.10 m [(b)]	$mg.m^{-3}$	$4.6x10^{-1}$	$2.4x10^{+2}$	$3.1x10^{+2}$	$5.5x10^{+2}$	$1.4x10^{+2}$	$1.4x10^{+2}$

(a) mean value of the measured concentrations in soil-gas wells Pza11 and Pza13
(b) mean value of the measured concentrations in soil-gas wells Pza10-H, Pza12 and Pza14

Except for the capillary approach, the other models give results relatively similar. For instance, the attenuation coefficient α is comprised between $1.8x10^{-6}$ and $3.1x10^{-6}$ (instead of $1.2x10^{-7}$ for the capillary approach). This remark is also available for the other parameters.

In this particular case of modelling, all the modelled indoor concentrations are under the measured value. There are substantial differences.

Concerning the comparison with the measured soil-gas concentrations at intermediate depths, the modelled values over-estimate the measured values.

All these observations lead to the conclusion that the modelled mass flow is to weak in comparison with the reality.

Vertical profiles for soil-gas concentrations may be extracted from these models. The five profiles are compared in figure 5.

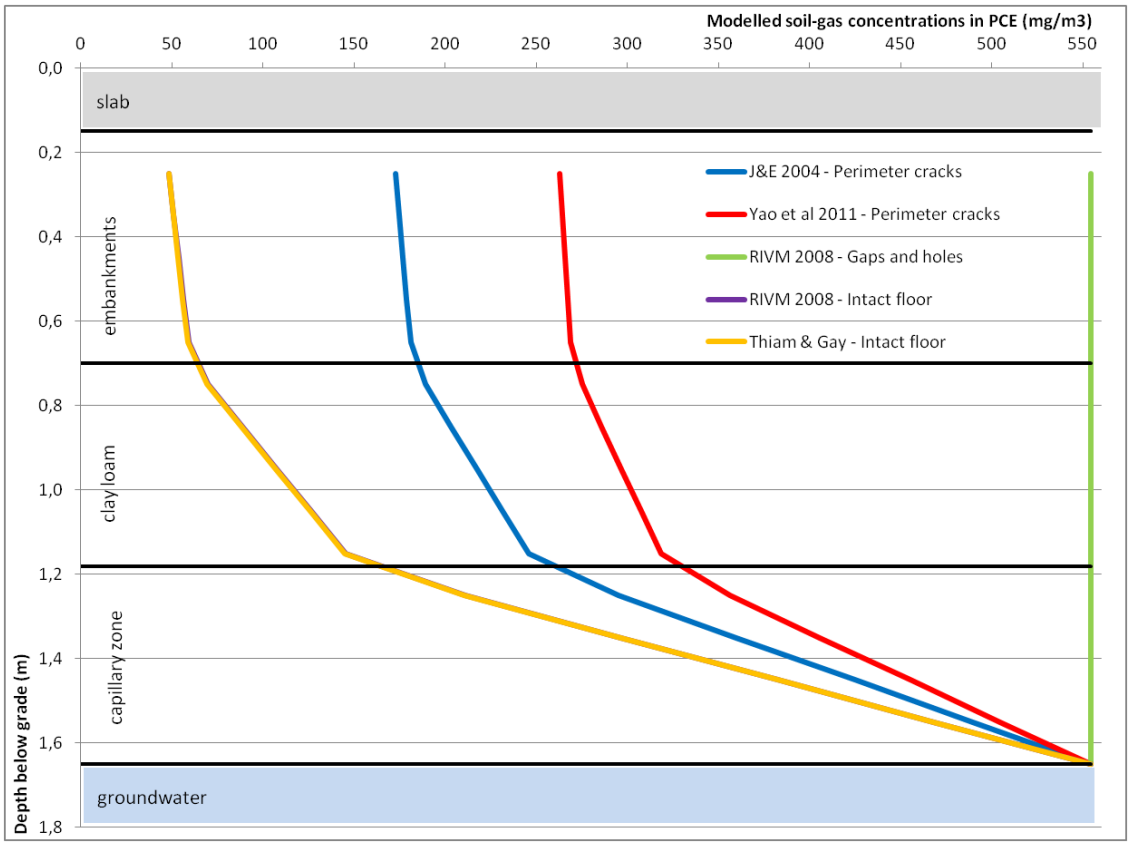

Figure 5: vertical profiles of soil-gas concentrations in PCE from the analytical models.

5.2 Comparison of different source assumptions

5.2.1 Source in clayey layer

With the assumption of a source in the clayey layer, the gaps between measured and modelled values for indoor concentrations are even more important. Table 8 details the modelled parameters.

Table 8: comparison of the modelled results of the analytical models for the scenario with a source in clayey layer.

Parameter	Unit	J&E 1991 - Perimeter cracks	Yao et al. 2011 - Perimeter cracks	RIVM 2008 - Gaps and holes	RIVM 2008 - Intact floor	Thiam & Gay - Intact floor
Attenuation coefficient α	-	6.0×10^{-6}	3.3×10^{-6}	6.6×10^{-7}	1.7×10^{-5}	1.7×10^{-5}
Indoor concentration	$mg.m^{-3}$	2.7×10^{-6}	1.5×10^{-6}	3.0×10^{-7}	7.8×10^{-6}	7.9×10^{-6}
Mass flow at the floor surface	$mg.m^{-2}.s^{-1}$	5.5×10^{-9}	3.0×10^{-9}	6.0×10^{-10}	1.6×10^{-8}	1.6×10^{-8}

5.2.2 Source in embankments

The observations are the same with the assumption of a source in embankments. Table 9 details the modelled parameters.

Table 9: comparison of the modelled results of the analytical models for the scenario with a source in embankments.

Parameter	Unit	J&E 1991 - Perimeter cracks	Yao et al. 2011 - Perimeter cracks	RIVM 2008 - Gaps and holes	RIVM 2008 - Intact floor	Thiam & Gay - Intact floor
Attenuation coefficient α	-	7.3×10^{-6}	3.7×10^{-6}	6.7×10^{-7}	2.3×10^{-5}	2.3×10^{-5}
Indoor concentration	$mg.m^{-3}$	5.5×10^{-6}	2.8×10^{-6}	5.1×10^{-6}	1.7×10^{-5}	1.8×10^{-5}
Mass flow at the floor surface	$mg.m^{-2}.s^{-1}$	1.1×10^{-8}	5.6×10^{-9}	1.0×10^{-8}	3.5×10^{-8}	3.5×10^{-8}

5.2.3 Synthesis

The figure 6 gives the ratios between modelled values and measured values for all the analytical models and all the source scenarios.

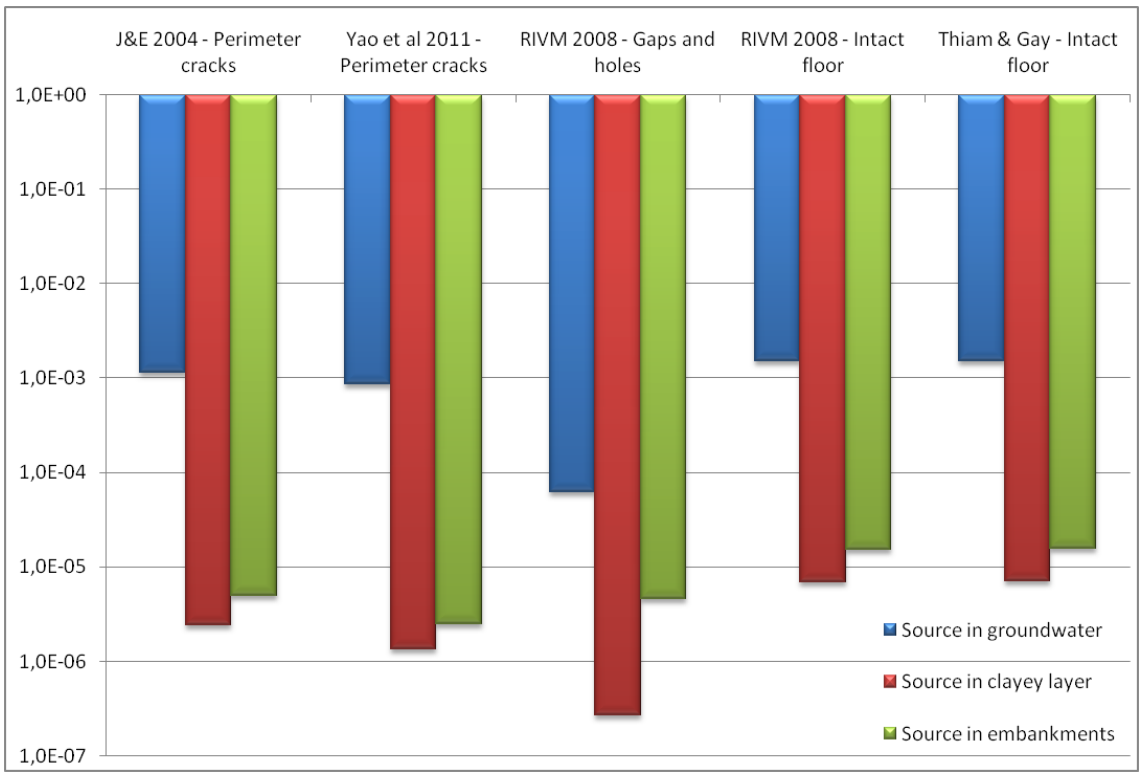

Figure 6: ratios of modelled values on measured values for indoor concentrations for all the analytical models and all the source scenarios.

It appears that the baseline scenario with a source in groundwater is the more appropriate: the other scenarios lead to important under-estimations of the indoor concentrations. Nevertheless, the modelled indoor concentrations with a source in groundwater are not satisfactory.

5.3 Sensitivity study on selected parameters

A sensitivity study has been carried out by studying the influence of several parameters on the attenuation coefficient α, which is the ratio between the modelled indoor concentration and the measured source concentration.

5.3.1 Influence of the outside/inside difference of pressure

Figure 7 shows the influence of the outside/inside difference of pressure on the attenuation coefficient.

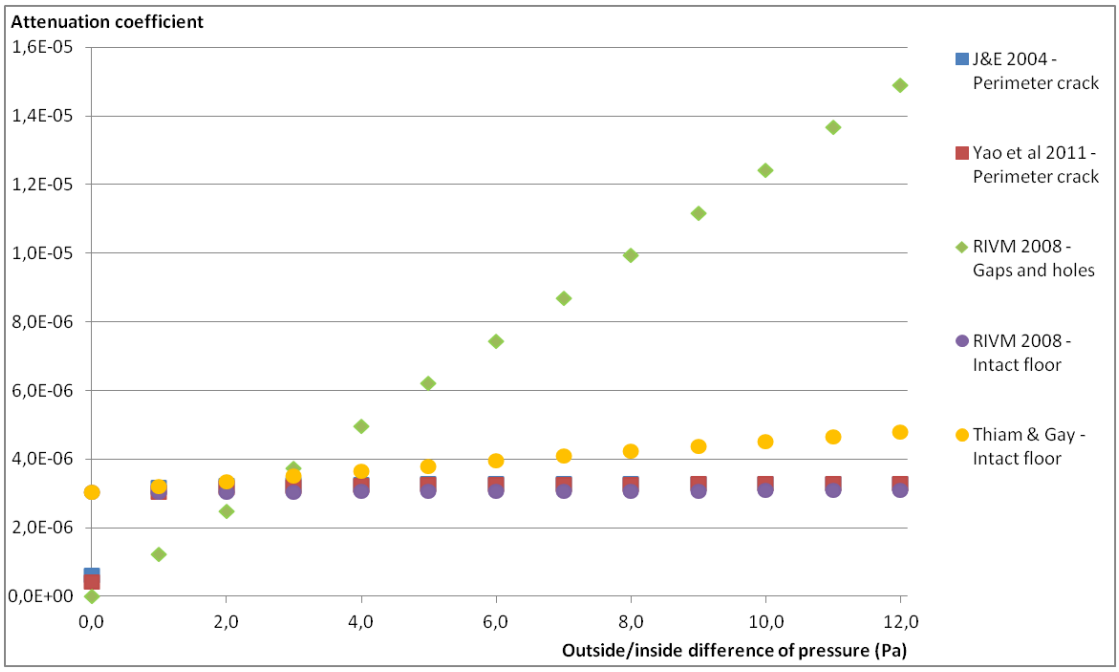

Figure 7: influence of the outside/inside difference of pressure on the attenuation coefficient.

As outside/inside difference of pressure increases, convective transfer is supposed to increase too. Nevertheless, the influence of this parameter depends on the importance of the convective transfer, in comparison with the diffusive one, in the model. Except for the capillary approach, for which the influence is linear, the convective transfer seems to play a minor role in the global transfer for the analytical models.

5.3.2 Influence of the height of the open capillary zone

Figure 8 shows the influence of the height of the open capillary zone on the attenuation coefficient (the global height of the clayey layer staying constant).

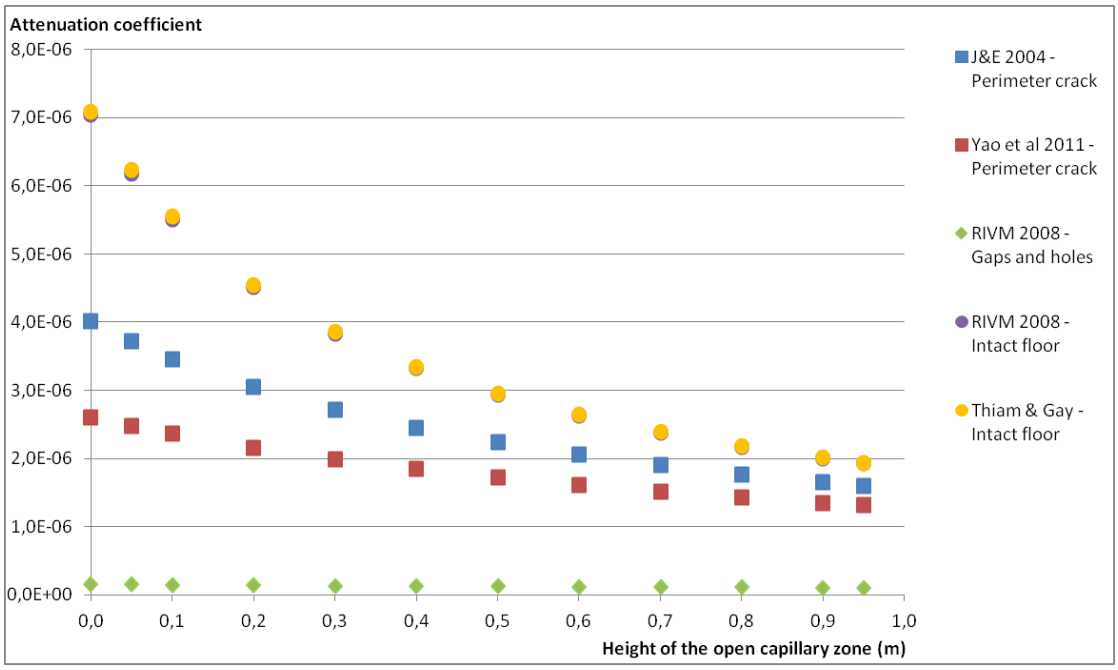

Figure 8: influence of the height of the open capillary zone on the attenuation coefficient.

The open capillary zone is characterised by a lower air-filled porosity than the bulk clayey layer. When the height of the open capillary zone increases, the height of the rest of the clayey layer decreases, and the global diffusion coefficient in soil-gas decreases too because the porosity is globally more filled with water.

This influence is only valuable for models for which the diffusive transfer is dominant. This is the case for all analytical models, except the capillary approach.

5.3.3 Influence of the water-filled porosity of the clayey layer

The figure 9 shows the influence of the water-filled porosity of the clayey layer on the attenuation coefficient. The water-filled porosity varies between the residual water content and the saturation of the porosity with water.

This parameter influences the global diffusion coefficient in soil-gas: when the porosity is filled with water, there is no more place for gas transfer.

This influence is only valuable for models for which the diffusive transfer is dominant. This is the case for all analytical models, except the capillary approach

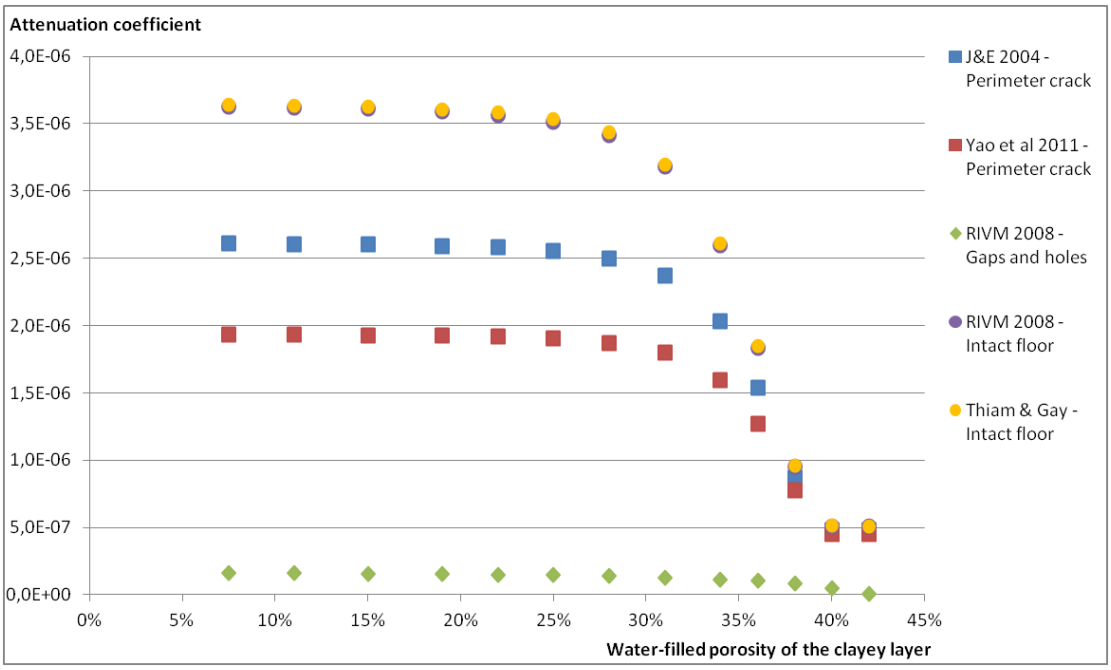

Figure 9: influence of the water-filled porosity of the clayey layer on the attenuation coefficient.

5.3.4 Influence of the water-filled porosity of the embankments

Figure 10 shows the influence of the water-filled porosity of the embankments on the attenuation coefficient. The evolutions are the same as previously.

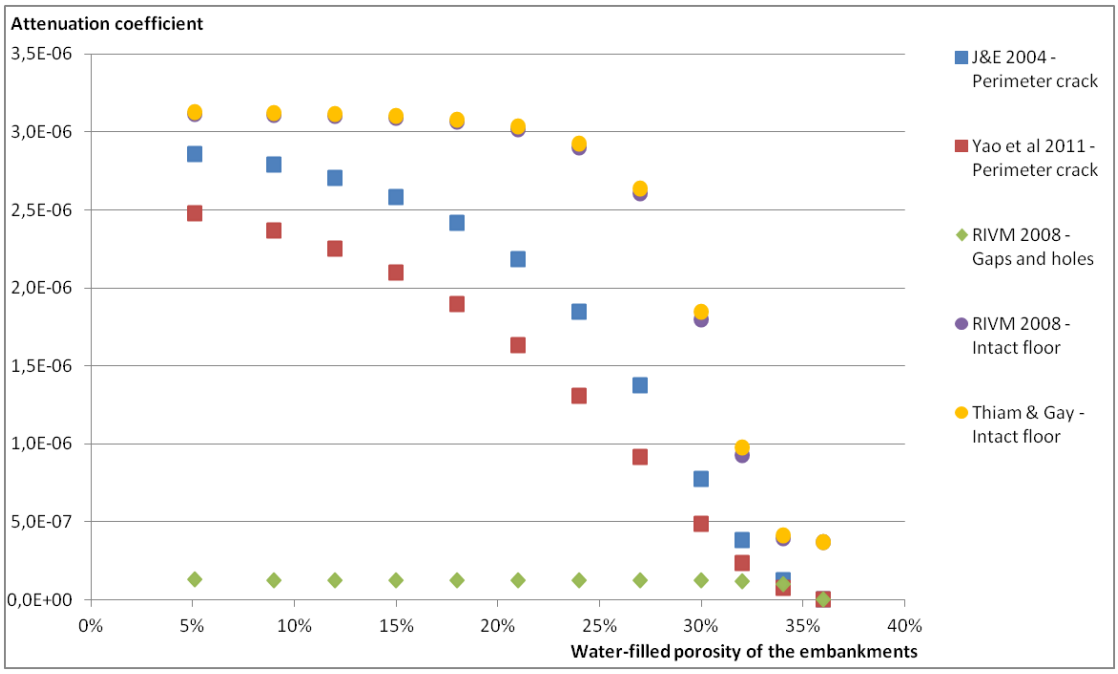

Figure 10: influence of the water-filled porosity of the embankments on the attenuation coefficient.

5.3.5 Influence of the air permeability of the embankments

Figure 11 shows the influence of the air permeability of the embankments on the attenuation coefficient.

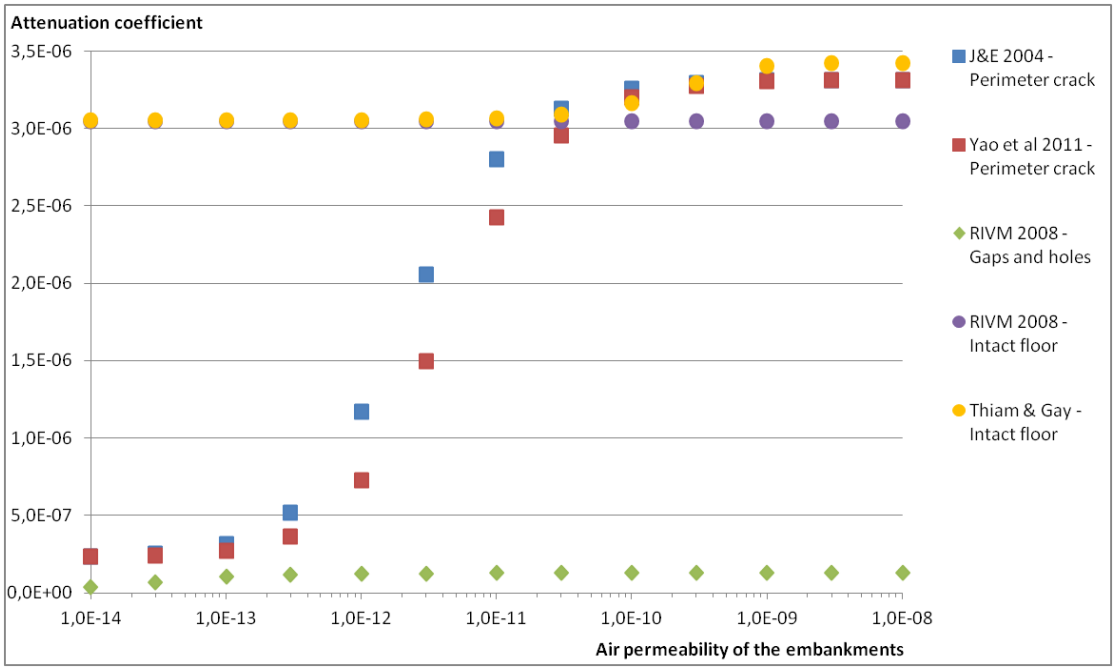

Figure 11: influence of the air permeability of the embankments on the attenuation coefficient.

The air permeability of embankments plays a role in the convective transfer.

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