

Istituto superiore per la Ricerca e la
Protezione Ambientale



Ministero del Lavoro, Salute e
Politiche Sociali

In collaborazione con:

Ministero dell'Ambiente e della Tutela del Territorio e del Mare

Ministero dello Sviluppo Economico

Istituto Superiore di Sanità

STRUMENTI INFORMATICI A SUPPORTO DELLE VALUTAZIONI

Leonello Attias

Istituto Superiore di Sanità

RISK ASSESSMENT

EFFECT ASSESSMENT

- “Hazard identification”
- dose-response assessment (concentration-effect)

RISK ASSESSMENT

EXPOSURE ASSESSMENT

- Human exposure assessment (workers, consumers, via the environment)
- Environmental exposure assessment (water, soil, air)

RISK ASSESSMENT

- Human health (evaluation of effects data and comparison with exposure data)
- Environment (evaluation of effects data and comparison with exposure data)

HUMAN HEALTH

- Hazard identification
- Dose (concentration)-response(effect) assessment
- Exposure assessment
- Risk characterisation

Human exposure assessment is based on representative monitoring data and/or model calculations. If appropriate, available information on substances with analogous use and exposure patterns or analogous properties is taken into account.

Il rischio delle sostanze chimiche e il regolamento REACH

http://webdomino1.oecd.org/comm/chem/models.nsf... Internet Explorer

http://webdomino1.oecd.org/comm/chem/models.nsf

OECD's Database on Chemical Risk Assessment Models

View by [Models Listed By All Countries](#) [Models Listed By Country](#) [Models Listed By Property / Effect](#) [Contact Names Listed Per Model](#)

Contents:

This searchable database includes information on models (computerised or capable of being computerised) that are used by OECD Member governments and industry to predict health or environmental effects (e.g., QSARs), exposure potential and possible risks. **The methods described here have not been evaluated or validated by OECD, and no endorsement of the methods by OECD should be inferred by the inclusion of certain methods in this database (Disclaimer).**


To add Information on Models Not in the Database:

Complete the appropriate survey(s) and submit to the OECD Secretariat for that survey:

- For health or environmental effects models predicting physical / chemical properties, chemical and fate properties, and human and aquatic hazard effects, complete [Survey A](#) and send to env.riskassessment@oecd.org.
- For models predicting human health or environmental exposure potential and potential environmental, worker or consumer risk, complete [Survey B](#) and send to env.riskassessment@oecd.org.

If the model predicts health or environmental effects AND exposure potential and possible risk, complete BOTH [Survey A](#) and [Survey B](#) and send to env.riskassessment@oecd.org.

Surveys submitted to the Secretariat will be reviewed by OECD's Issue Team on Tools for R&D Screening and/or OECD's Task Force on Environmental Exposure Assessment Task Force before the information is added to the database.

The surveys are available in WORD97 and/or in PDF. In order to read the PDF file, you will need to have an Acrobat Reader. If you do not have the programme, you can download it for free by clicking here: 

Comments, questions or corrections:

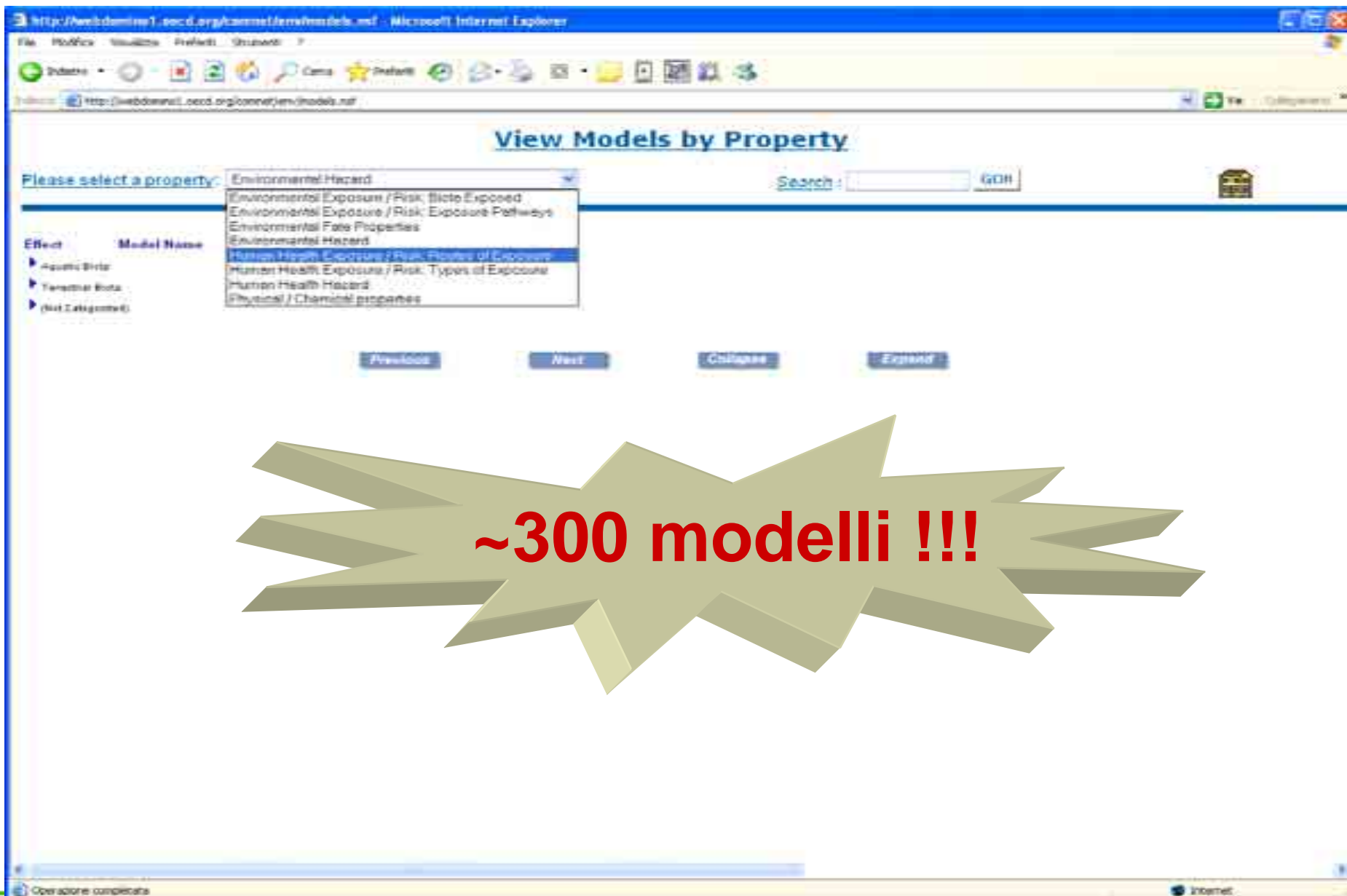
If you would like to suggest a correction to the database, or if you have any questions or comments, please contact the project leader, [Maggie Wilson](#).

Disclaimer:

This database is intended as an information resource only, and is not intended to present a comprehensive evaluation of these methods. OECD is not recommending these methods as being the best or only methods available. The users should conduct their own investigation of the methods to determine if the

Internet

Il rischio delle sostanze chimiche e il regolamento REACH



The screenshot shows a web browser window with the address bar displaying <http://webdamine1.eccd.org/connet/en/models.nsf>. The page title is "View Models by Property". Below the title, there is a search bar and a "GO!" button. A dropdown menu is open, showing a list of model categories. The categories are:

- Environmental Hazard
- Environmental Exposure / Risk: Biota Exposed
- Environmental Exposure / Risk: Exposure Pathways
- Environmental Fate Properties
- Environmental Hazard
- Human Health Exposure / Risk: Routes of Exposure
- Human Health Exposure / Risk: Types of Exposure
- Human Health Hazard
- Physical / Chemical properties

Below the dropdown menu, there are four buttons: "Previous", "Next", "Collapse", and "Expand".

~300 modelli !!!

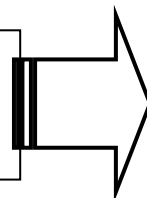
Modelli per la valutazione dell'esposizione (... e degli effetti)

EASE

Stima dell'esposizione
lavoratori *nei siti industriali*

CONSEXPO

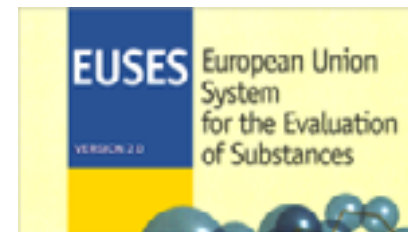
Stima dell'esposizione
consumatori



EUSES

Mackay

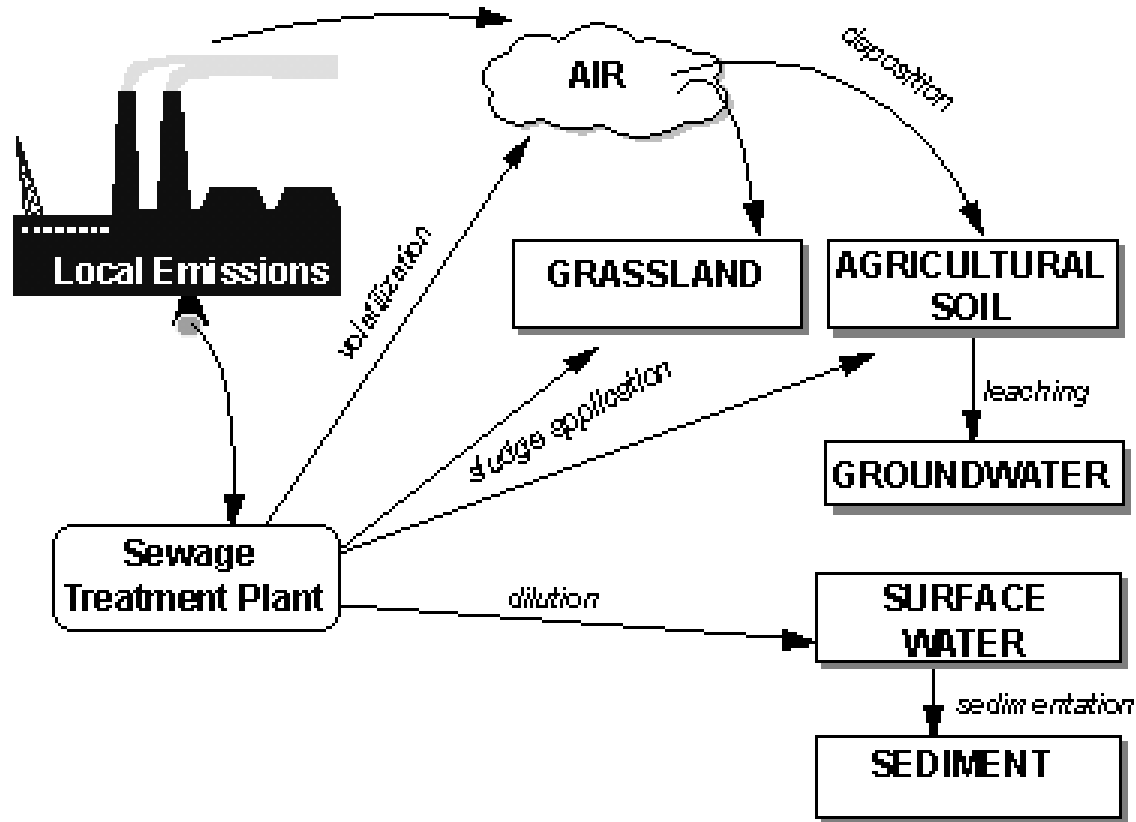
Stima dell'esposizione
ambientale



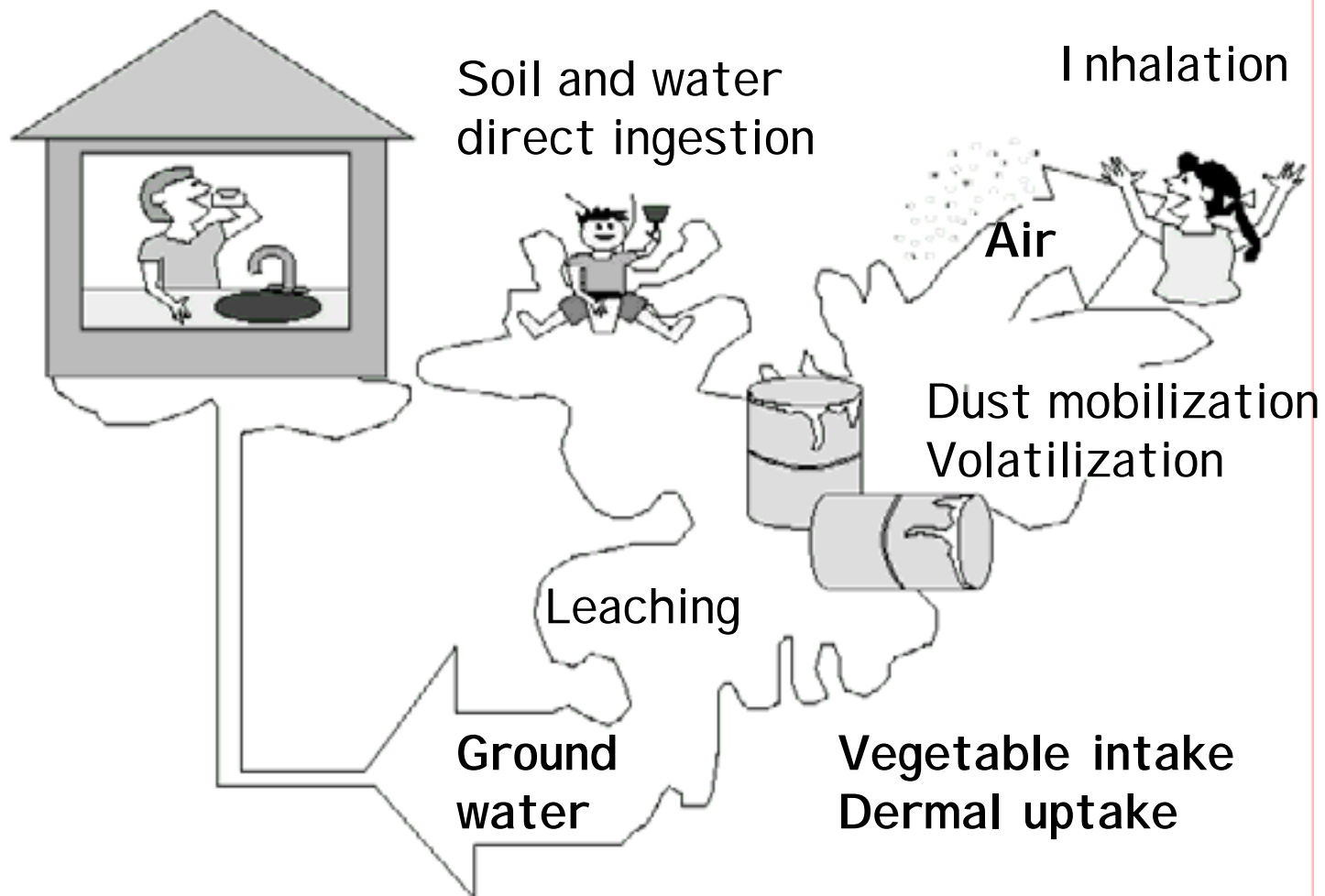
QSAR

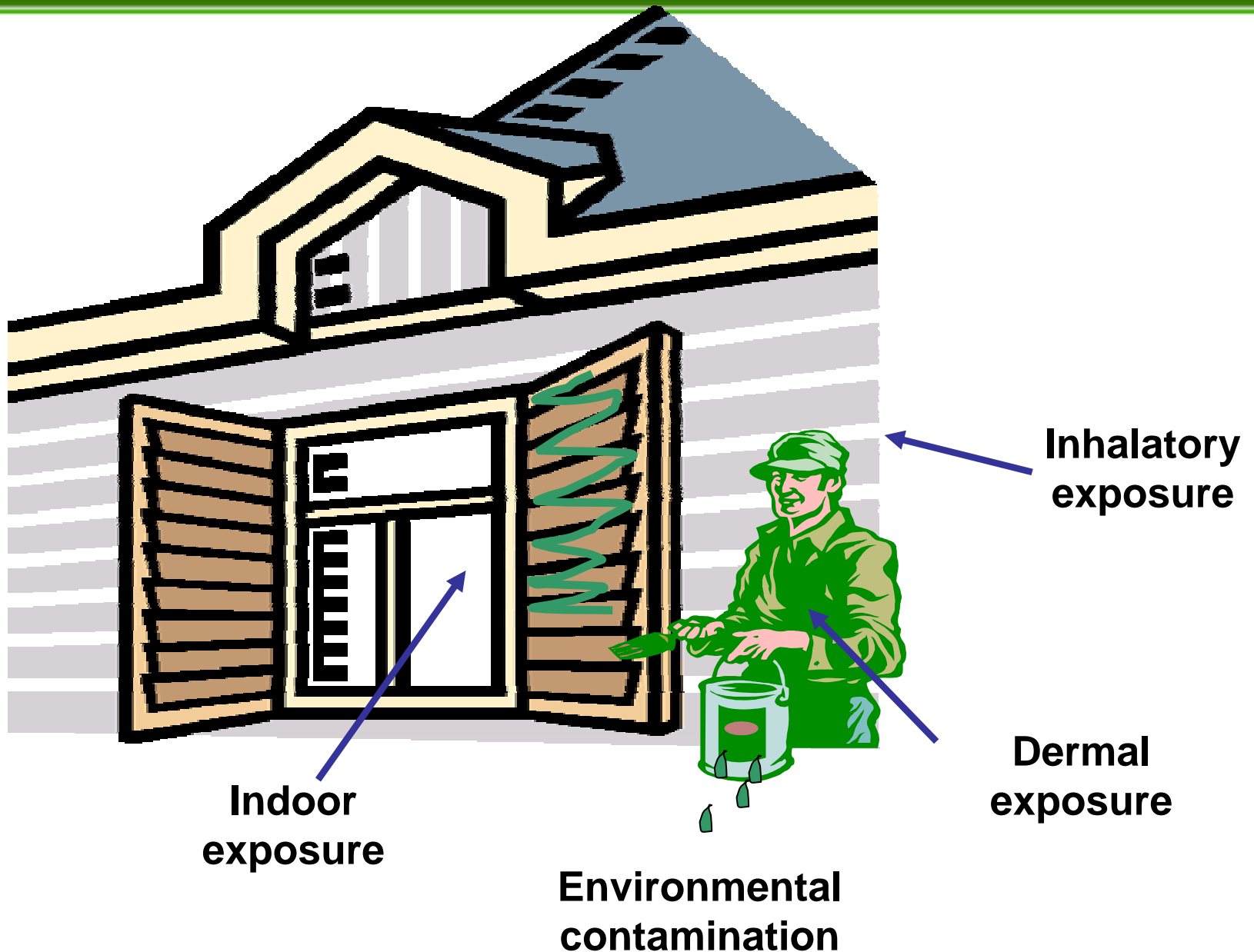
Stima
dell'esposizione
dei downstream users

Emission scenario

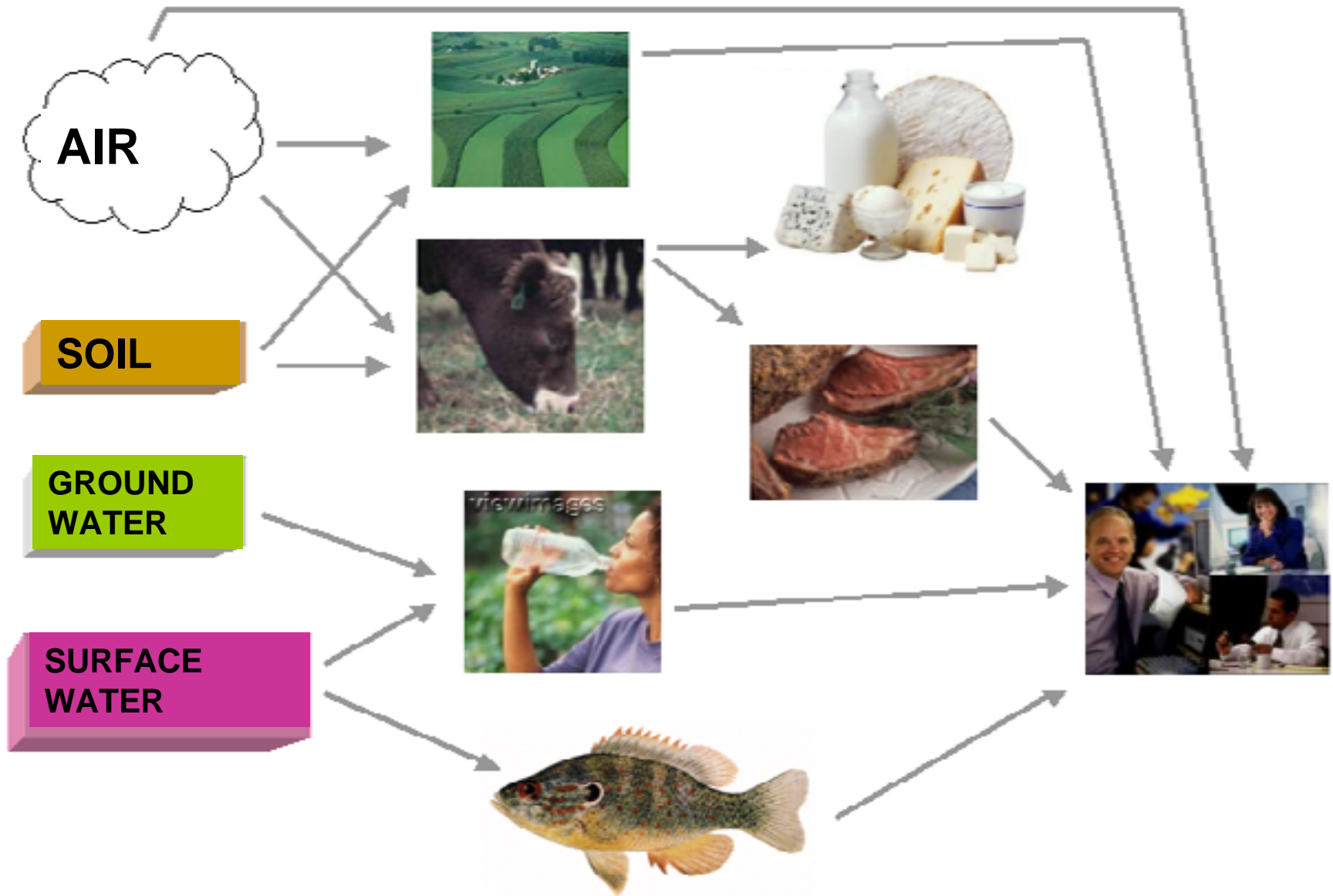


Exposure routes in relation to soil pollution





Il rischio delle sostanze chimiche e il regolamento REACH



Il rischio delle sostanze chimiche e il regolamento REACH

LEVEL 1B

Compartimento	Volume (m3) standard	Densità (kg/m3)	Concentrazioni (g/m3)		Quantità (g)	%	Z
ACQUA	7.00E+06	1.00E+03	4.78E-04	4.78E-04	3.35E+03	17.61	0.105263158
ARIA	6.00E+09	1.18E+00	1.76E-06	1.49E-03	1.05E+04	55.45	0.000386749
SEDIMENTO	2.10E+04	1.50E+03	1.18E-01	7.84E-02	2.47E+03	12.99	25.89473684
PESCE	7.00E+00	1.00E+03	2.39E-01	2.39E-01	1.67E+00	0.01	52.63157895
SUSP SED	3.50E+01	1.50E+03	1.18E-01	7.84E-02	4.11E+00	0.02	25.89473684
SUOLO	4.50E+04	1.50E+03	5.88E-02	3.92E-02	2.65E+03	13.92	12.94736842



D. Mackay (1991). Multimedia Environmental Models. The Fugacity Approach. Lewis Publishers.

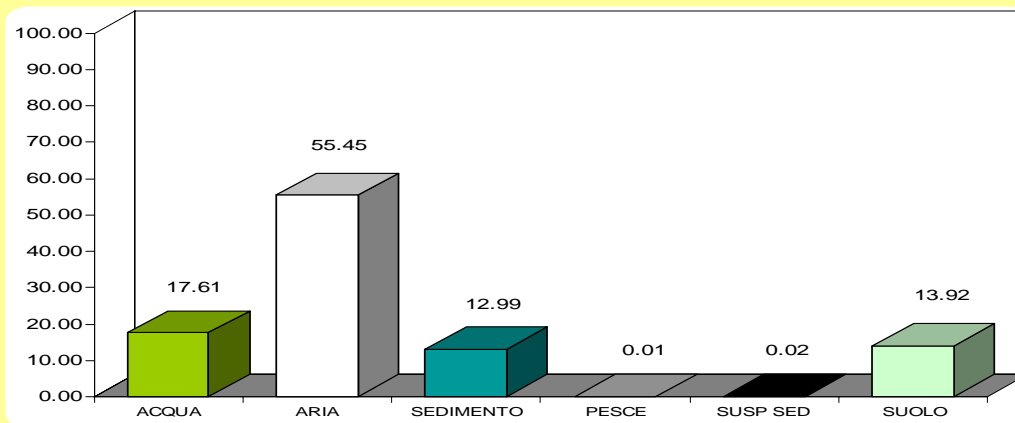
S (mol/m3):	0.105263158	Kbw:	5.00E+02
Koc:	4100	Ksed	1.49354E-05
Kow:	10000	BCF	500
f(Pa):	2.38947E-05	Henry Co:	9.37577E-05
Kaw:	3.67E-03	VP (atm)	9.86923E-06
Ksedw:	2.46E+02	peso (Kg)	19

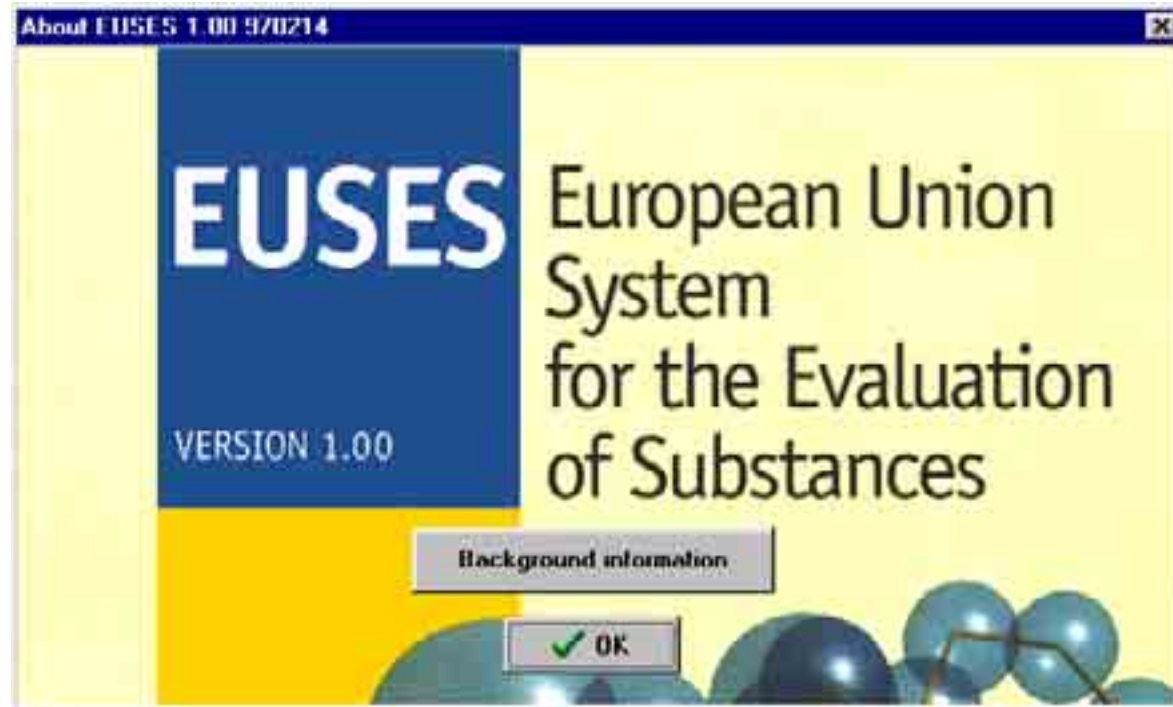
Hypothene

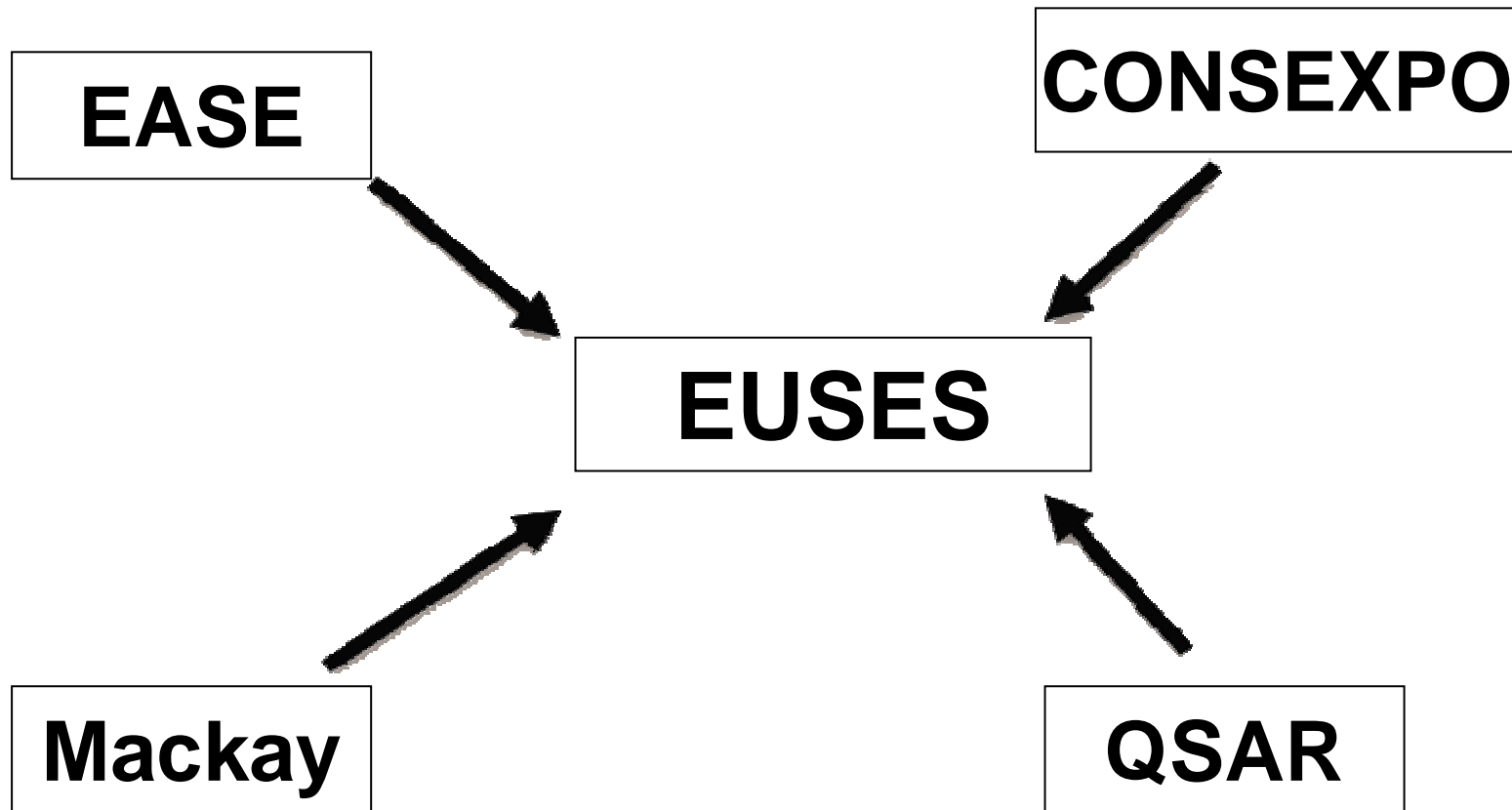
Standard
 Continental
 Default/Mackay

Sostanza:	Hypothene
VP (Pa):	1.0.E+00
T (K)	311
S (g/m3):	2.0.E+01
log(10) Kow	4
P.M. (g/mol):	190
n. moli:	1.0.E+02
T (C°)	38

VP T S log Kow PM





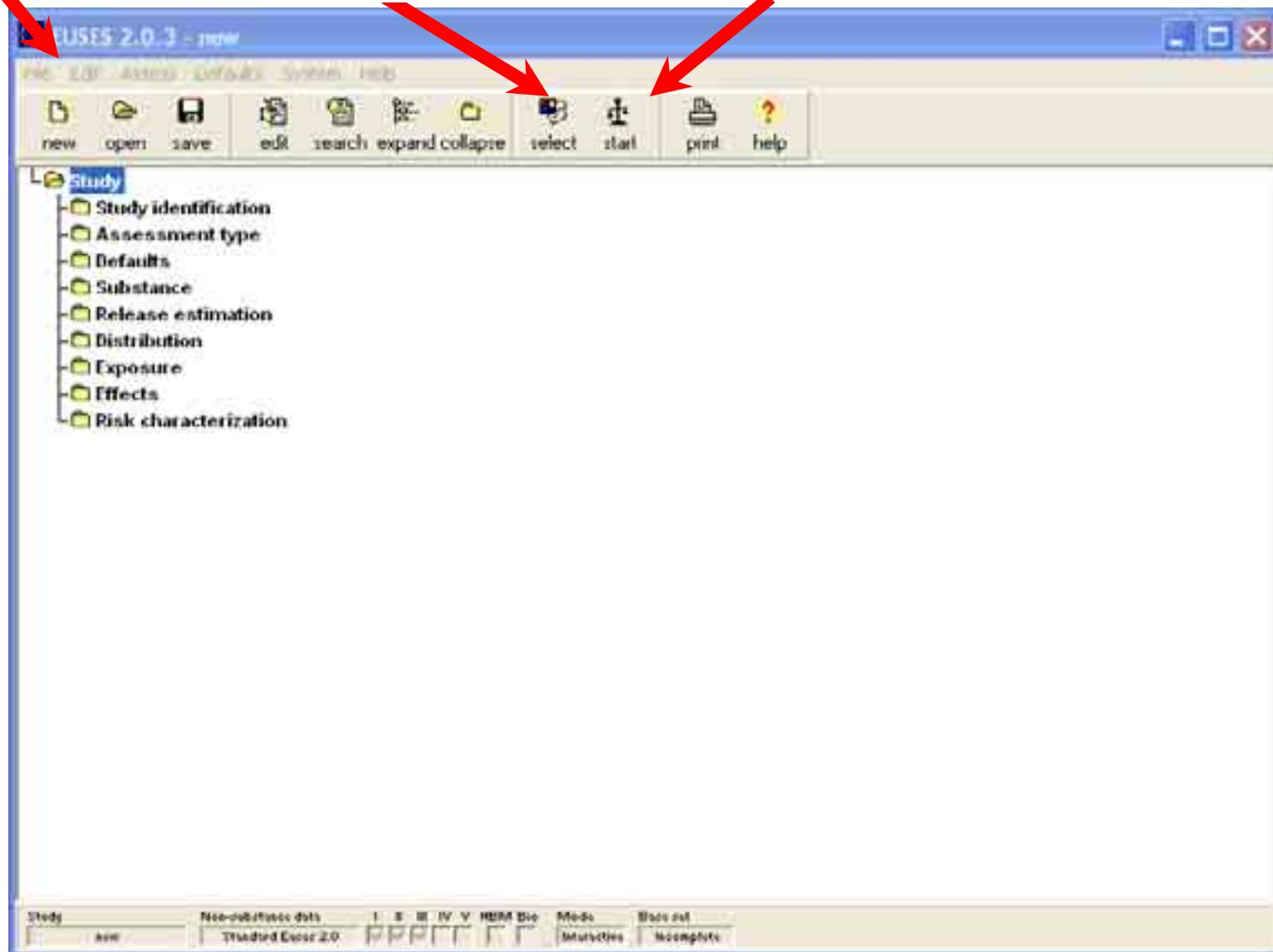


Il rischio delle sostanze chimiche e il regolamento REACH

Menu

Assessment type

START



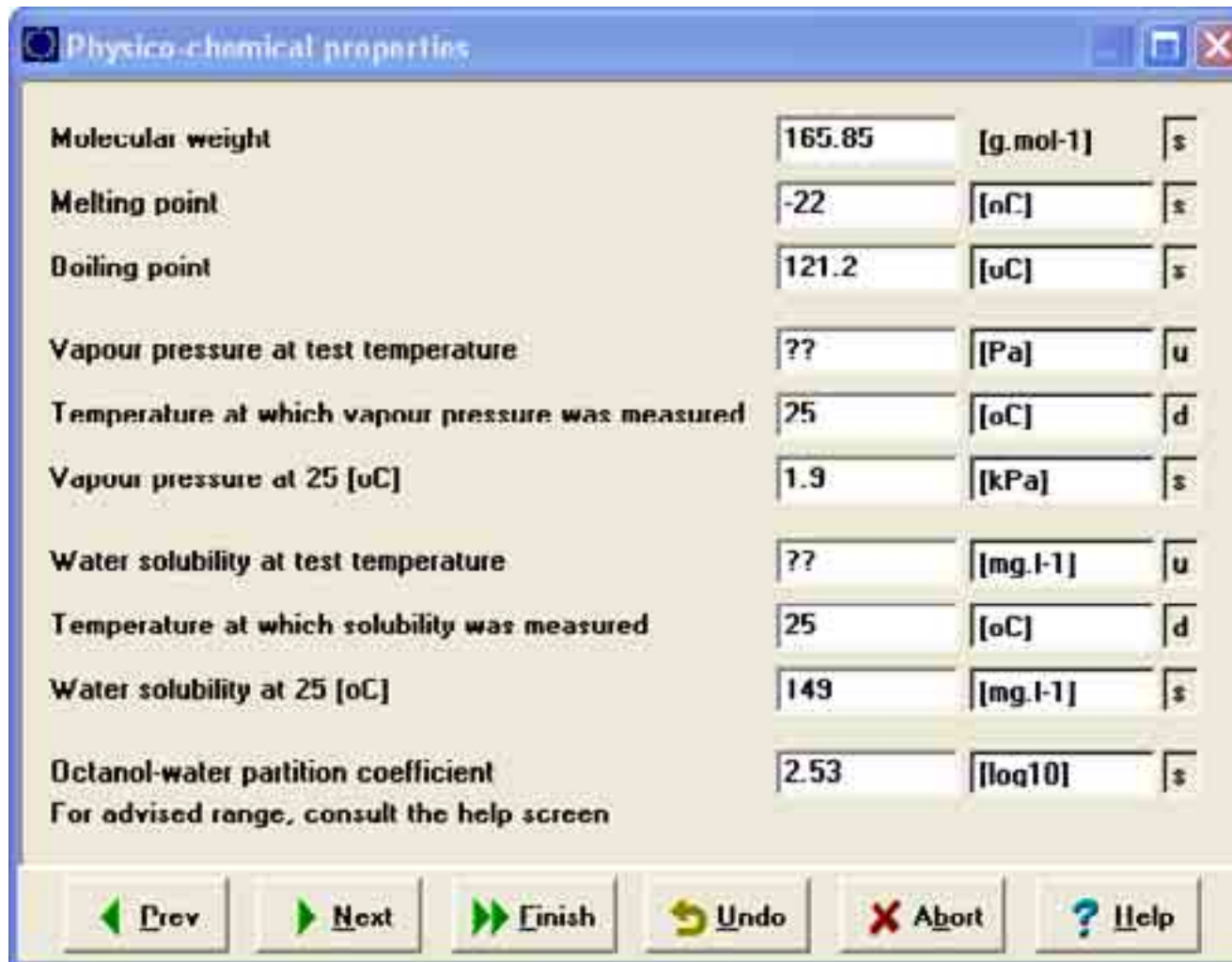
Dati iniziali di input

The image shows a software dialog box titled "Substance identification". It contains several input fields for chemical data. The "General name" field is filled with "Tetrachloroethylene". The "CAS-No" field is filled with "127-18-4". The "EINECS no." field is filled with "204-825-9". The "Description" field is empty. At the bottom of the dialog, there are six buttons: "Prev", "Next", "Finish", "Undo", "Abort", and "Help".

General name	Tetrachloroethylene
Description	
CAS-No	127-18-4
EC-notification no.	
EINECS no.	204-825-9

Navigation buttons: **Prev**, **Next**, **Finish**, **Undo**, **Abort**, **Help**

Dati iniziali di input



The screenshot shows a software window titled "Physico-chemical properties" with a list of input fields for various chemical properties. The fields are arranged in a table-like structure with three columns: the property name, the numerical value, the unit, and a selection box.

Property	Value	Unit	Selection
Molecular weight	165.85	[g.mol-1]	s
Melting point	-22	[oC]	s
Boiling point	121.2	[oC]	s
Vapour pressure at test temperature	??	[Pa]	u
Temperature at which vapour pressure was measured	25	[oC]	d
Vapour pressure at 25 [oC]	1.9	[kPa]	s
Water solubility at test temperature	??	[mg.l-1]	u
Temperature at which solubility was measured	25	[oC]	d
Water solubility at 25 [oC]	149	[mg.l-1]	s
Octanol-water partition coefficient	2.53	[log10]	s

For advised range, consult the help screen

Navigation buttons: Prev, Next, Finish, Undo, Abort, Help

Uso della sostanza

15/0 Others	▼
55/0 Others	▼
31 Impregnation agents	▲
32 Insulating materials	
33 Intermediates	
34 Laboratory chemicals	
35 Lubricants and additives	
36 Odour agents	
37 Oxidizing agents	
38 Plant protection products, agricultural	
39 Biocides, non-agricultural	
40 PH-regulating agents	
41 Pharmaceuticals	
42 Photochemicals	
43 Process regulators	
44 Reducing agents	
45 Reprographic agents	
46 Semiconductors	▼
III Non-dispersive use	▼

Uso della sostanza

Emission input data

Usage/production title

Use pattern | Tonnages |

Industry category

Use category

Extra details on use category

Extra details on use category

Production

Formulation

Industrial use

Private use

Service life

Waste treatment

Industrial Use |

Use specific emission scenario

Emission tables

Emission scenario

Main category industrial use

Scenario choice for biocides

Additional scenario information

OK Cancel Help

Calcolo delle emissioni locali



Usage	Step	Emis. Air	Emis. Water	Show	Intermittent
1 "" (13/48)	3 Indus	421.201 [kg.d-1]	2.106E+03 [kg.d-1]	Yes	No

Buttons: Edit, Prev, Next, Finish, Abort, Help

Calcolo dei coefficienti di ripartizione

Partition coefficients and bioconcentration factors

Solids-water | Air-water | Bioconcentration factors | Biotin-water

Chemical class for Koc-QSAR: Non-hydrophobics (default QSAR) [d]

Organic carbon-water partition coefficient	141.147	[L.kg-1]	[r]
Solids-water partition coefficient in soil	2.02	[L.kg-1]	[u]
Solids-water partition coefficient in sediment	7.06	[L.kg-1]	[o]
Solids-water partition coefficient suspended matter	14.1	[L.kg-1]	[o]
Solids-water partition coefficient in raw sewage sludge	42.3	[L.kg-1]	[n]
Solids-water partition coefficient in settled sewage sludge	42.3	[L.kg-1]	[o]
Solids-water partition coefficient in activated sewage sludge	52.2	[L.kg-1]	[o]
Solids-water partition coefficient in effluent sewage sludge	52.2	[L.kg-1]	[o]
Soil-water partition coefficient	4.61	[m3.m-3]	[u]
Suspended matter water partition coefficient	4.43	[m3.m-3]	[o]
Sediment-water partition coefficient	4.33	[m3.m-3]	[o]

◀ Prev ▶ Next ▶▶ Finish ↶ Undo ✖ Abort ? Help

Concentrazioni locali nei vari comparti

Compartment	Local PEC	Unit	Control
Annual average local PEC in air (total)	0.446	[mg m-3]	o
Local PEC in surface water during emission episode (dissolved)	6.99	[mg.l-1]	o
Qualitative assessment might be needed (TGD Part II, 5.6)	No		o
Annual average local PEC in surface water (dissolved)	5.76	[mg.l-1]	o
Local PEC in fresh-water sediment during emission episode	26.9	[mg.kgwwt-1]	o
Local PEC in sea water during emission episode (dissolved)	10.5	[mg.l-1]	o
Qualitative assessment might be needed (TGD Part II, 5.6)	No		o
Annual average local PEC in sea water (dissolved)	8.66	[mg.l-1]	o
Local PEC in marine sediment during emission episode	40.6	[mg.kgwwt-1]	o
Local PEC in agric. soil (total) averaged over 30 days	3.54	[mg.kgwwt-1]	o
Local PEC in agric. soil (total) averaged over 180 days	0.593	[mg.kgwwt-1]	o
Local PEC in grassland (total) averaged over 100 days	0.122	[mg.kgwwt-1]	o
Local PEC in pore water of agricultural soil	0.219	[mg.l-1]	o
Local PEC in pore water of grassland	0.0451	[mg.l-1]	o
Local PEC in groundwater under agricultural soil	0.219	[mg.l-1]	o

I valori di esposizione per l'uomo vengono calcolati a partire da . . .

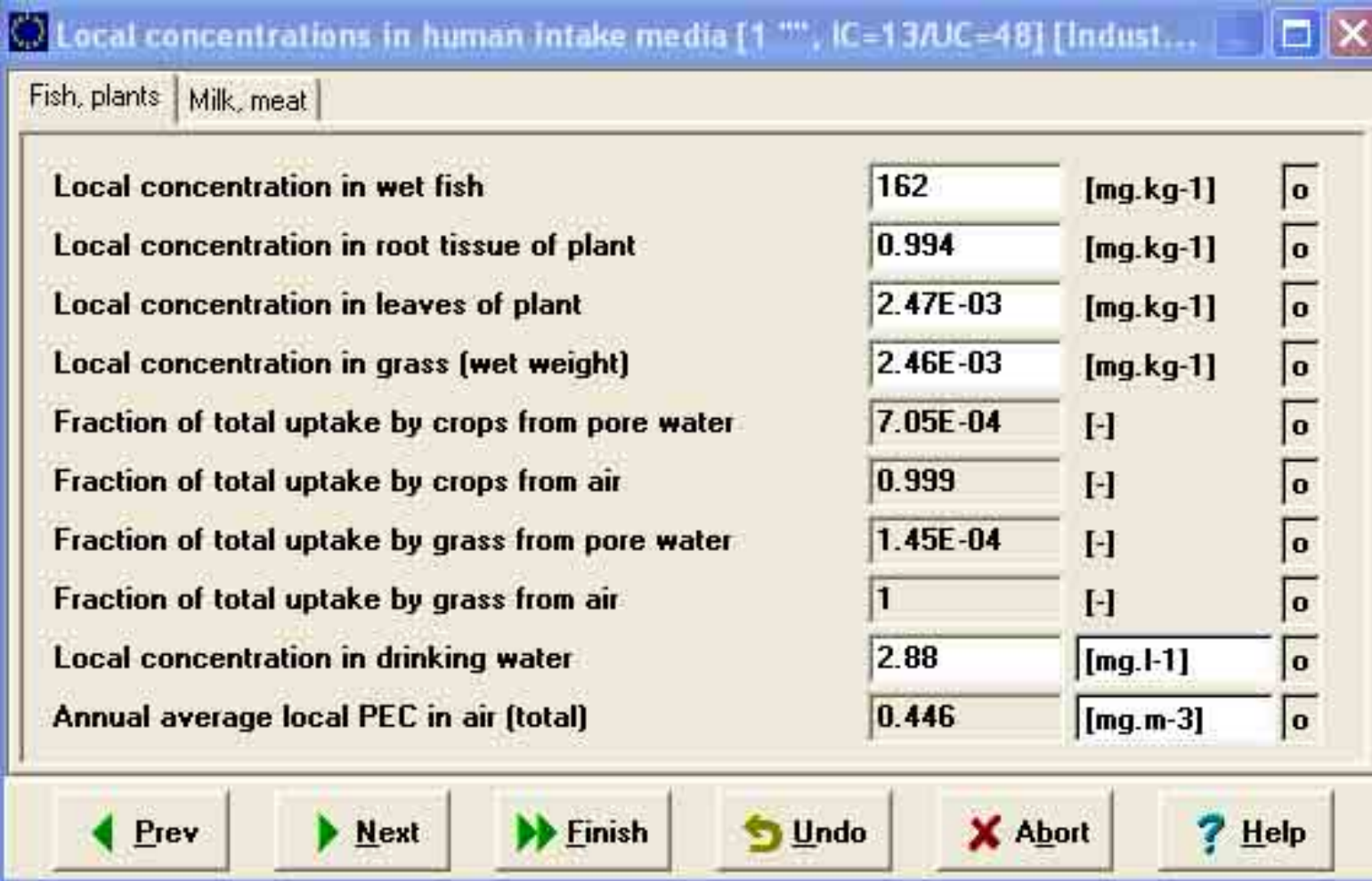


Local exposure - daily human doses [1 "", IC=13/UC=48] [Industrial use]

	Dose		Fraction
Daily dose through intake of drinking water	0.0822	[mg.kg-1.d-1] o	0.171
Daily dose through intake of fish	0.267	[mg.kg-1.d-1] o	0.553
Daily dose through intake of leaf crops	4.23E-05	[mg.kg-1.d-1] o	8.77E-05
Daily dose through intake of root crops	5.45E-03	[mg.kg-1.d-1] o	0.0113
Daily dose through intake of meat	7.79E-06	[mg.kg-1.d-1] o	1.62E-05
Daily dose through intake of milk	1.36E-05	[mg.kg-1.d-1] o	2.81E-05
Daily dose through intake of air	0.128	[mg.kg-1.d-1] o	0.265
Local total daily intake for humans	0.482	[mg.kg-1.d-1] o	

◀ Prev ▶ Next ▶▶ Finish ↶ Undo ✖ Abort ? Help

.....valori di concentrazione negli alimenti



Media	Concentration	Units	Icon
Local concentration in wet fish	162	[mg.kg-1]	o
Local concentration in root tissue of plant	0.994	[mg.kg-1]	o
Local concentration in leaves of plant	2.47E-03	[mg.kg-1]	o
Local concentration in grass (wet weight)	2.46E-03	[mg.kg-1]	o
Fraction of total uptake by crops from pore water	7.05E-04	[-]	o
Fraction of total uptake by crops from air	0.999	[-]	o
Fraction of total uptake by grass from pore water	1.45E-04	[-]	o
Fraction of total uptake by grass from air	1	[-]	o
Local concentration in drinking water	2.88	[mg.l-1]	o
Annual average local PEC in air (total)	0.446	[mg.m-3]	o

I dati ecotossicologici . . .

Aquatic effects input

Fresh water | Marine | Fresh water sediment | Marine sediment

L(E)C50 short term tests

LC50 for fish	5	[mg.l-1]	s
L(E)C50 for Daphnia	8.5	[mg.l-1]	s
EC50 for algae	3.64	[mg.l-1]	s
LC50 for additional taxonomic group	??	[mg.l-1]	u

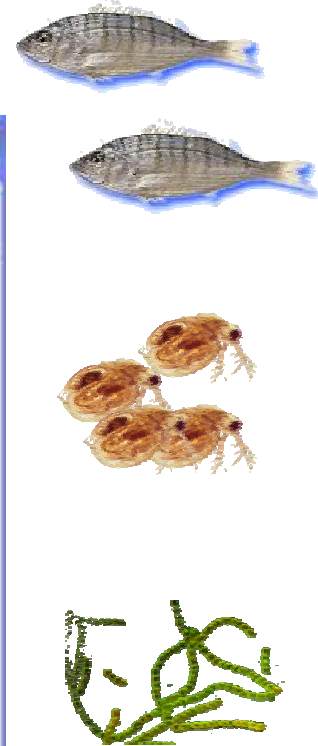
Aquatic species: other

NOEC long-term tests

NOEC for fish	1.99	[mg.l-1]	s
NOEC for Daphnia	0.51	[mg.l-1]	s
NOEC for algae	16	[mg.l-1]	s
NOEC for additional taxonomic group	??	[mg.l-1]	u
NOEC for additional taxonomic group	??	[mg.l-1]	u
NOEC for additional taxonomic group	??	[mg.l-1]	u
NOEC for additional taxonomic group	??	[mg.l-1]	u

◀ Prev ▶ Next ▶▶ Finish ↶ Undo ✖ Abort ? Help

.. con l'utilizzo degli appropriati "Assessment Factors" ..



Environmental PNECs

Fresh water | Marine | Fresh water sediment | Marine sediment | Terrestrial | Secondary poisoning | STP

Same taxonomic group for LC50 and NOEC	Yes	<input type="radio"/>
Toxicological data used for extrapolation to PNEC Aqua	0.51	[mg.l-1] <input type="radio"/>
Assessment factor applied in extrapolation to PNEC Aqua	10	[-] <input type="radio"/>
PNEC for aquatic organisms	0.051	[mg.l-1] <input type="radio"/>
Intermittent releases		
Toxicological data used for extrapolation to PNEC Aqua	3.64	[mg.l-1] <input type="radio"/>
Assessment factor applied in extrapolation to PNEC Aqua	100	[-] <input type="radio"/>
PNEC for aquatic organisms, intermittent releases	0.0364	[mg.l-1] <input type="radio"/>
Statistical		
PNEC for aquatic organisms with statistical method	??	[mg.l-1] <input type="radio"/>

◀ Prev ▶ Next ▶▶ Finish ↶ Undo ✖ Abort ? Help

.. permettono di calcolare le PNECs

Category	Value	Unit	Radio
PNEC for aquatic organisms	0.051	[mg.l-1]	<input type="radio"/>
PNEC for aquatic organisms, intermittent releases	0.0364	[mg.l-1]	<input type="radio"/>
PNEC for micro-organisms in a STP	10	[mg.l-1]	<input type="radio"/>
PNEC for secondary poisoning of birds and mammals	10	[mg.kg-1]	<input type="radio"/>
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	<input type="radio"/>

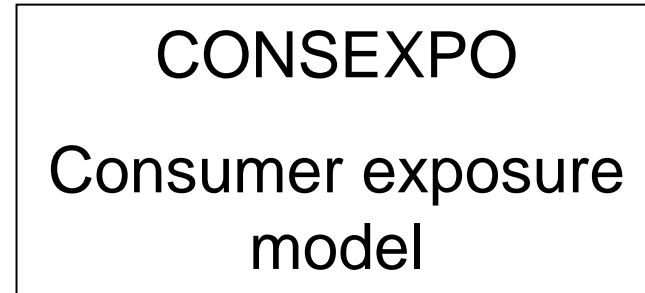
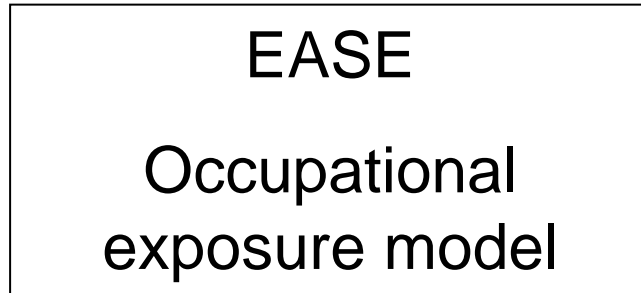
Navigation buttons:

... ed effettuare la caratterizzazione del rischio per l'ambiente e per la popolazione esposta indirettamente attraverso l'ambiente

Usage/step	Report	Fr water	IM	Marine	Fr soil	*10	Mar soil	*10	Soil	*10	STP	Fish	Mar fish	Mar top	Worm
1. Indus	Yes	1.07		0.000+00	1.13		0.000+00		0.00		0.00	??	??	??	??
Regional	Yes	1.07		0.900	1.13		0.912		0.033						

I dati tossicologici confrontati con i valori di esposizione umana permettono la caratterizzazione del rischio per i lavoratori e i consumatori

Parameter	Value	Unit	Icon
Oral NOAEL	100	[mg.kg-1.d-1]	x
Oral LOAEL	??	[mg.kg-1.d-1]	o
Inhalatory NOAEL	75	[mg.m-3]	v
Inhalatory LOAEL	??	[mg.m-3]	o
Dermal NOAEL	100	[mg.kg-1.d-1]	o
Dermal LOAEL	??	[mg.kg-1.d-1]	o
NOEC via food	1E+03	[mg.kg-1]	o
LOEC via food	??	[mg.kg-1]	d
Duration of (sub-)chronic oral test	28 days		d
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<6 weeks)		x
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	o
Fibres			
Inhalatory (fibre) NOAEL	??	[fibres.m-3]	d
Inhalatory (fibre) LOAEL	??	[fibres.m-3]	d



- Vapor pressure
- Physical state
- Process temperature
- Segregation
- Ventilation systems

- Number and duration of events
- Exposure days
- Fraction of the substance in preparation
- Exposed body surface
- Indoor volume

Estimation and Assessment of Substance Exposure

L'EASE è stato sviluppato dall'HSE (UK) per calcolare l'esposizione inalatoria e cutanea in ambiente di lavoro in varie circostanze.

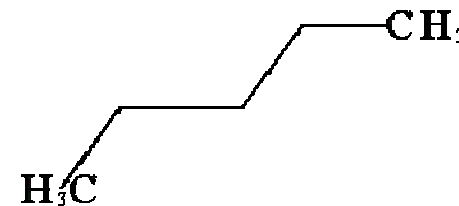
E' un modello analogico basato su dati misurati relativi a scenari specifici; si può scegliere attraverso diverse opzioni di parametri come le proprietà chimico fisiche durante durante la lavorazione (tendenza a migrare al comparto aria, potenziale contatto cutaneo), pattern di utilizzo e di controllo.

La combinazione delle variabili scelte è associata a degli intervalli di valori misurati che sono compresi nel "UK National Exposure Database"

I dati utilizzati dal modello per derivare gli intervalli di esposizione corrispondono a valori TWA 8h

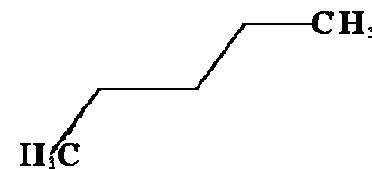
I valori calcolati verranno utilizzati come input per la caratterizzazione del rischio e comparati con i valori derivati dalla valutazione degli effetti per la salute umana.

n-pentane



Uso
Schiumogeno per Polistirene
Schiumogeno per Poliuretano
Diluyente di processo / carrier per la polimerizzazione
Solvente nella formulazione di Aerosol
Solvente nella formulazione di Adesivi
Sostanza chimica di Laboratorio
Altri usi

Occupational exposure



Scenario 1 Production of n-pentane

Scenario 2 Industrial use of products containing n-pentane
Scenario 2A: Production of polystyrene granulates (formulation)

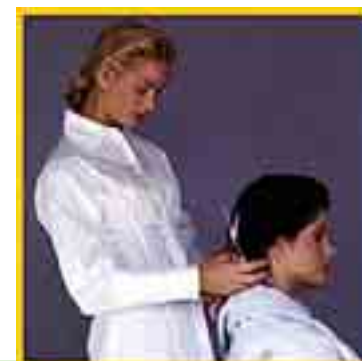
Scenario 2B: EPS manufacturing (processing)

Scenario 2C: Production of rigid polyurethane foam

Scenario 2D: Manufacturing of aerosol-containers

Professional end use of products containing n-pentane

Scenario 3A: Hair salons



Calcolo empirico

Parametro	Valore	Commento
Volume stanza	50 m³	Piccola sala
Ricambio aria	3 ricambi aria per ora	Ventilazione naturale
Quantità aerosol usata	1.15 g/sec	
Frazione in peso dell'n-pentano	40 %	Limite superiore
Durata tipica	3 secondi	
Numero clienti/giorno	60	
Percentuale richiedente hairspray (%)	50	

Calcolo empirico

$1.15 \text{ g/sec} \times 1000 \text{ mg/g} \times 0.4 \text{ (frazione pentano)} \times 3 \text{ sec (durata)} \times (60 \times 0.5) \text{ numero di clienti} = 41400 \text{ mg n-pentano}$

Assumendo una distribuzione uniforme nell'aria che passa nella sala in un giorno ($50 \times 3 \text{ m}^3/\text{h} \times 8\text{h}$), il pentano emesso corrisponde a una 8h TWA di 35 mg/m^3 (104 ppm)

Calcolo EASE

Assumendo una sala di 50 m³ and 3 ricambi aria per ora, e che le stime EASE sono 8h TWA, la stima EASE corrisponde a un consumo di 1800- 3600 g n-pentano per giorno che corrispondono a una 8h TWA di 3000 mg/m³

Calcolo EASE

Physico-chemical properties [X]

Molecular weight	<input type="text" value="72.15"/>	[g.mol ⁻¹]	<input type="text" value="\$"/>
Melting point	<input type="text" value="-130"/>	[oC]	<input type="text" value="\$"/>
Boiling point	<input type="text" value="36.15"/>	[oC]	<input type="text" value="\$"/>
Vapour pressure at 25 [oC]	<input type="text" value="5.656E+04"/>	[Pa]	<input type="text" value="\$"/>
Octanol-water partition coefficient.	<input type="text" value="3.45"/>	[log10]	<input type="text" value="\$"/>
Water solubility	<input type="text" value="38.5"/>	[mg.l ⁻¹]	<input type="text" value="\$"/>

Calcolo EASE

Worker exposure input

Substance	Pattern of use	Dermal
Process temperature	??	[oC] d
Boiling point	36.15	[oC] s
Melting point	-130	[oC] s
Physical state of a substance	Liquid	s
Vapour pressure at 25 [oC]	5.656E+04	[Pa] s
Vapour pressure at the process temperature	??	[Pa] u
Aerosol formed	No	d
Inhalation exposure to dust particles	No	o
Particle size of the substance	Granular	d
Type of dust	Non-Fibrous	d
Ability of fibrous dust to become airborne	High	d
Dust particles aggregates readily	No	d

◀ Prev ▶ Next ✓ Finish ✗ Abort ? Help

Calcolo EASE

Worker exposure input

Substance	Pattern of use	Dermal
Pattern of use	<input type="text" value="Non-dispersive use"/>	<input type="button" value="\$"/>
Is closed system (considered to be) breached	<input type="text" value="Closed system"/>	<input type="button" value="d"/>
Pattern of control applied to the process	<input type="text" value="Non-dispersive use"/>	<input type="button" value="\$"/>
	<input type="text" value="Wide dispersive use"/>	<input type="button" value="\$"/>
Dust exposure		
Type of process operations	<input type="text" value="Dry crushing & grinding"/>	<input type="button" value="d"/>
Local Exhaust Ventilation (LEV) present	<input type="text" value="No"/>	<input type="button" value="d"/>

Calcolo EASE

The screenshot shows a software window titled "Worker exposure input" with three tabs: "Substance", "Pattern of use", and "Dermal". The "Pattern of use" tab is active and contains the following fields and options:

Field	Value	Unit
Pattern of use	Non-dispersive use	s
Is closed system (considered to be) breached	No	d
Pattern of control applied to the process	Direct handling & dilution ventilation	s
Dust exposure	Full Containment	
Type of process operations	Local Exhaust Ventilation (LEV)	d
Local Exhaust Ventilation (LEV) present	Segregation	
	Direct handling	
	Direct handling & dilution ventilation	d
	No	

At the bottom of the window, there are five buttons: "Prev", "Next", "Finish", "Abort", and "Help".

Calcolo EASE

Worker exposure input

Substance Pattern of use **Dermal**

Amount of dermal contact between worker and substance Incidental \$


Exposed body part Hands (fronts and backs) \$

Area of contact between substance and skin 420 [cm2] \$

Thickness of layer of product on skin 0.01 [cm] d

Mean number of events 10 [d-1] \$

Pattern of control applied to the process Direct handling \$



◀ Prev ▶ Next ✓ Finish ✗ Abort ? Help

Calcolo EASE

Worker exposure - intermediate results

Inhalation Dermal

	range			
Vapour concentration in air for workers	500	1000	[ppm]	<input type="radio"/>
Vapour concentration in air for workers	1.5E+03	3E+03	[mq.m-3]	<input type="radio"/>
Fibre concentration in air for workers	0	0	[fibres.m-3]	<input type="radio"/>
Dust concentration in air for workers	0	0	[mg.m-3]	<input type="radio"/>

Concentrazione in aria

◀ Prev ▶ Next ✓ Finish ✗ Abort ? Help

Calcolo EASE

The screenshot shows a software window titled "Worker exposure - intermediate results" with a blue title bar. It has two tabs: "Inhalation" and "Dermal", with "Dermal" being the active tab. The main area contains two rows of input fields under the heading "range". The first row is "Dermal weight of substance on the skin of workers" with input boxes for "0" and "0.1" and a unit "[mg.cm-2.d-1] o". The second row is "Potential dermal uptake for workers" with input boxes for "0" and "0.6" and a unit "[mq.kq-1.d-1] o". A large white arrow points from a box below to the "0.6" input field. The box below contains the text "Potenziale assunzione". At the bottom of the window are five buttons: "Prev", "Next", "Finish" (with a green checkmark), "Abort" (with a red X), and "Help" (with a blue question mark).

Il rischio delle sostanze chimiche e il regolamento REACH

<https://www.ecetoc-tra.org/index.asp>

Units	LEV	Fugacity	Predicted EASE Exposure (95th%)	Exposure Prediction Adopted by ECETOC	Comments	Rationale for Deviation from EASE Prediction
Exposure category						
Use in a continuous process (with no process sampling)						
Solids mg/m ³	Yes	High	1	0.01	Assumes respirable, low dust technique, non-fibrous and readily aggregating dust	The EASE prediction is plainly wrong for a totally enclosed system. Revision consistent with EASE range
	No		1	0.01		
	Yes	Moderate	1	0.01	Assumes inhalable, low dust technique, non-fibrous readily aggregating dust	
	No		1	0.01		
	Yes	Low	0.1	0.01	EASE predicts zero based on granular	
	No		0.1	0.01		
Use in a continuous process (with process sampling)						
Volatiles (ppm)	Yes	High	0.1	0.01	Assumes no aerosols, 500 hPa vapour pressure and full containment	The EASE prediction is plainly wrong for a totally enclosed system. Zero exposure foreseen which should equate to no >0.01 ppm
	No		0.1	0.01		
	Yes	Moderate	0.1	0.01	Ditto, 150 hPa vapour pressure	
	No		0.1	0.01		
	Yes	Low	0.1	0.01	10 hPa vapour pressure	
	No		0.1	0.01		
Use in a continuous process (with process sampling)						
g/m ³	Yes	High	1	1	Assumes respirable, low dust technique, non-fibrous non-readily	

Il rischio delle sostanze chimiche e il regolamento REACH

The screenshot shows the ECCIOC Targeted Risk Assessment web tool interface. The browser title is "ECCIOC: Windows Internet Explorer" and the address bar shows "https://www.eurochem.org/ra/ra.asp". The page has a green header with the text "ECCIOC Targeted Risk Assessment". Below the header, there is a navigation menu on the left with sections: "General Menu" (Welcome, Add new substance, Search substances), "Process" (Start, Chemical identity, Health, Workers, Consumer, Environment), and "Contact" (ECCIOC ANEL, Via E. Van Meeuwenstraat 4, Ste 0, B-1100 Brussels, Belgium). The main content area is titled "Welcome to the ECCIOC Targeted Risk Assessment Web Tool" and contains several sections: "Introduction" (describing the tool as an initial electronic implementation of ECETOC proposals), "The basic principles and flow of the Tiered and Targeted Risk Assessment approach", "Instructions for data input and risk assessment" (describing the logic steps and data entry), "Data input requirements" (linking to a list of required data), "Confidentiality" (describing access control and data storage), "What information is stored?", and "Members" (listing ECETOC Task Force members). A disclaimer at the top of the page states: "THIS TOOL IS UNDER DEVELOPMENT AND IS NOT A FINAL VERSION. THIS SITE WILL SOON BE UPDATED TO REFLECT DIFFERENCES BETWEEN IT AND THE PUBLISHED FINAL TIA REPORT."

Calcolo CONSEXPO

Consumer exposure input

Inhalation Dermal Ural

Time scale of inhalatory exposure: Acute [v] \$

Number of events: 1 [d-1] \$

Duration of contact per event: 50 [min] \$

Amount of product released: 3E+03 [mg] \$

Weight fraction of substance in product: 0.4 [-] \$

Room volume: 50 [m3] \$



◀ Prev ▶ Next ✓ Finish ✗ Abort ? Help

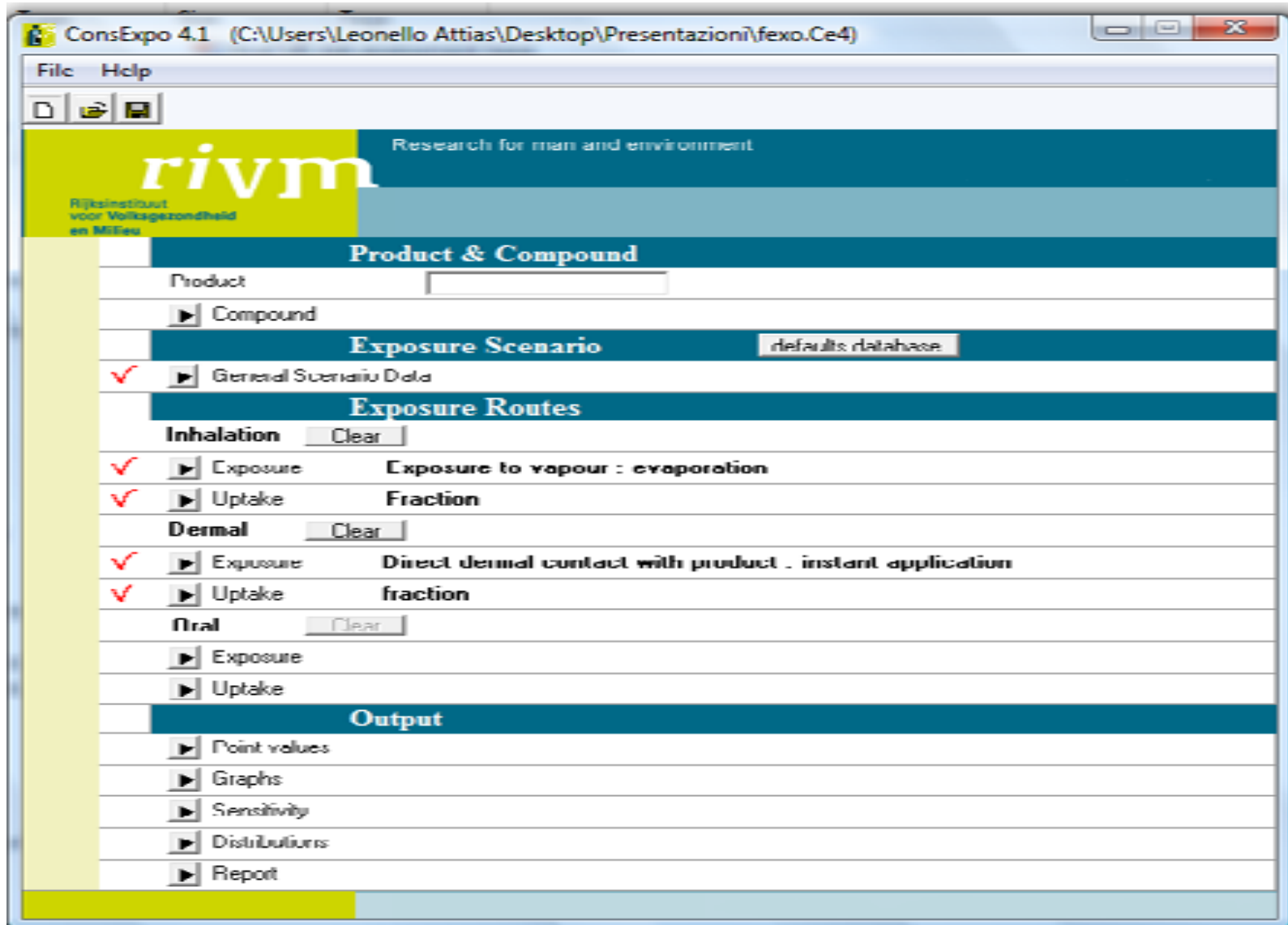
Calcolo CONSEXPO

The screenshot shows a software window titled "Consumer exposure - intermediate results". The window has a tabbed interface with five tabs: "Inhalation" (selected), "Dermal", "Oral", "Chronic exposure", and "Total exposure". The main area displays two rows of data:

Parameter	Value	Unit	Control
Concentration in air of room	24	[mg.m-3]	o
Inhalatory intake	0.238	[mg.kgbw-1.d-1]	o

At the bottom of the window, there are five buttons: "Prev" (with a left arrow), "Next" (with a right arrow), "Finish" (with a green checkmark), "Abort" (with a red X), and "Help" (with a blue question mark).

Calcolo CONSEXPO



Calcolo CONSEXPO

Inhalation: evaporation model

general

exposure duration	minute	D	5
product amount	gram	D	1E3
weight fraction compound	fraction	D	0,5
room volume	m3	D	40
ventilation rate	1/hr	D	1,25

mode of release

instantaneous release

All of the chemical is released at once into the room.
Use as a first tier approach

constant rate

The chemical is released with a constant rate in a certain time.
Use when details of evaporation are not exactly known

evaporation

The chemical is released by evaporation.
Use when details of evaporation are known

release area

release area	m2	D	1
application duration	hour	D	1

release area is constant (i.e. from a can or treated wall)
 the area of release increases over time (i.e. in case of painting a surface)

release rate

Note: all data at application temperature

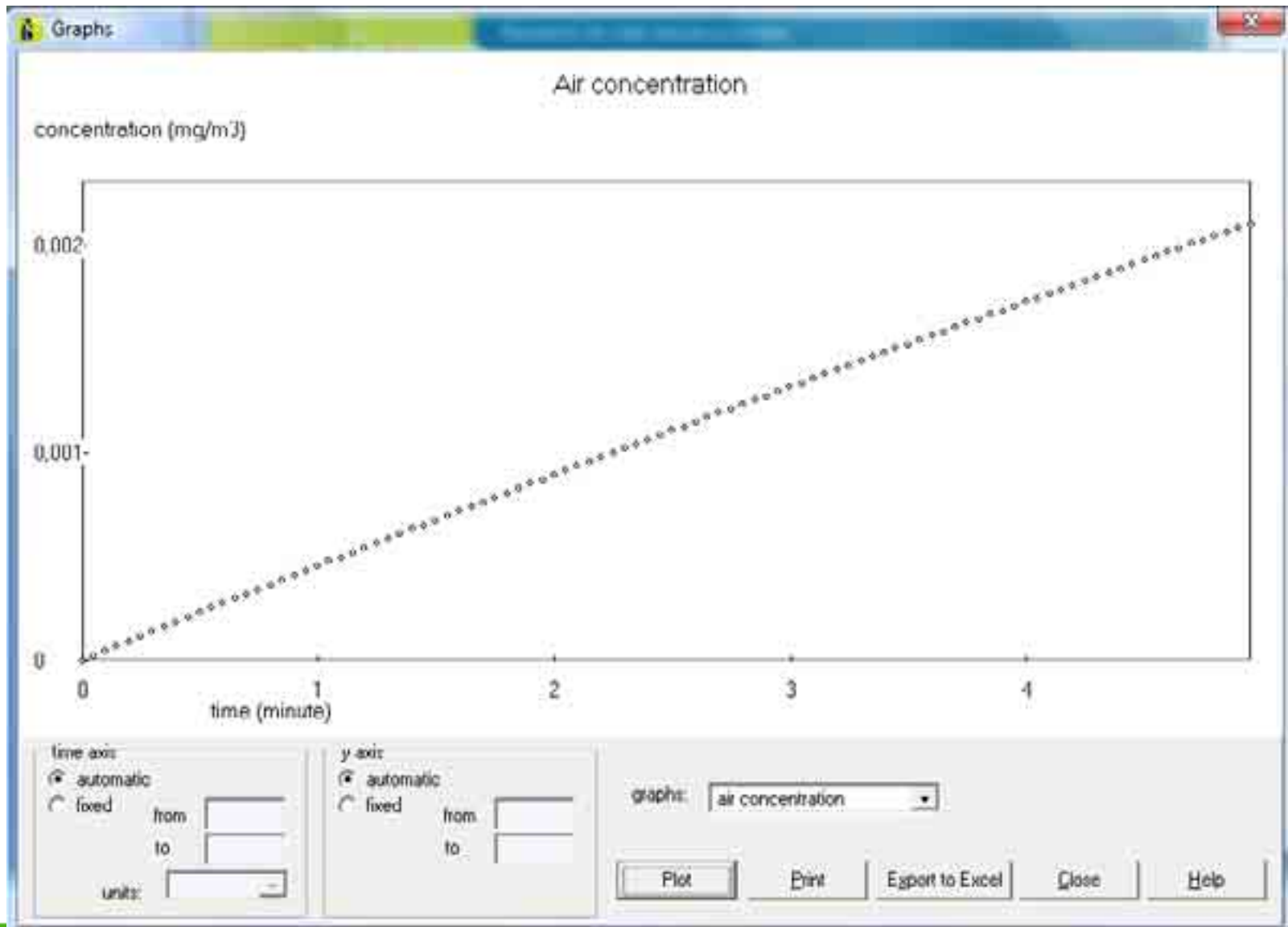
temperature	Celsius	D	25	
molecular weight	g/mol	D	482	
vapour pressure	Pascal	D	0,00021	
mass transfer rate	m/min	D	0,45	default

the product is the compound in pure form

mol weight matrix	g/mol	D	
-------------------	-------	---	--

OK Cancel Help

Calcolo CONSEXPO

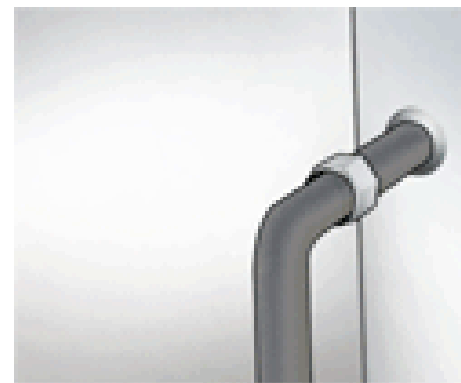


Scenario “Evaporazione da sostanza pura”

Modo a rilascio per evaporazione

Descrive il rilascio di un composto in aria per evaporazione dalla superficie del prodotto (es. vasca, secchio, contenitore). Durante questo tempo il composto viene simultaneamente rimosso dall'aria della stanza mediante ventilazione.

Il tasso di evaporazione è legato alla differenza di tensione di vapore nell'aria della stanza e la tensione di vapor saturo del composto. Il tasso di evaporazione è proporzionale a questa differenza di pressione e dipende dalla superficie del prodotto e dal tasso di trasferimento di massa. Quest'ultimo è una misura della velocità di rimozione della sostanza evaporata dalla superficie del prodotto.

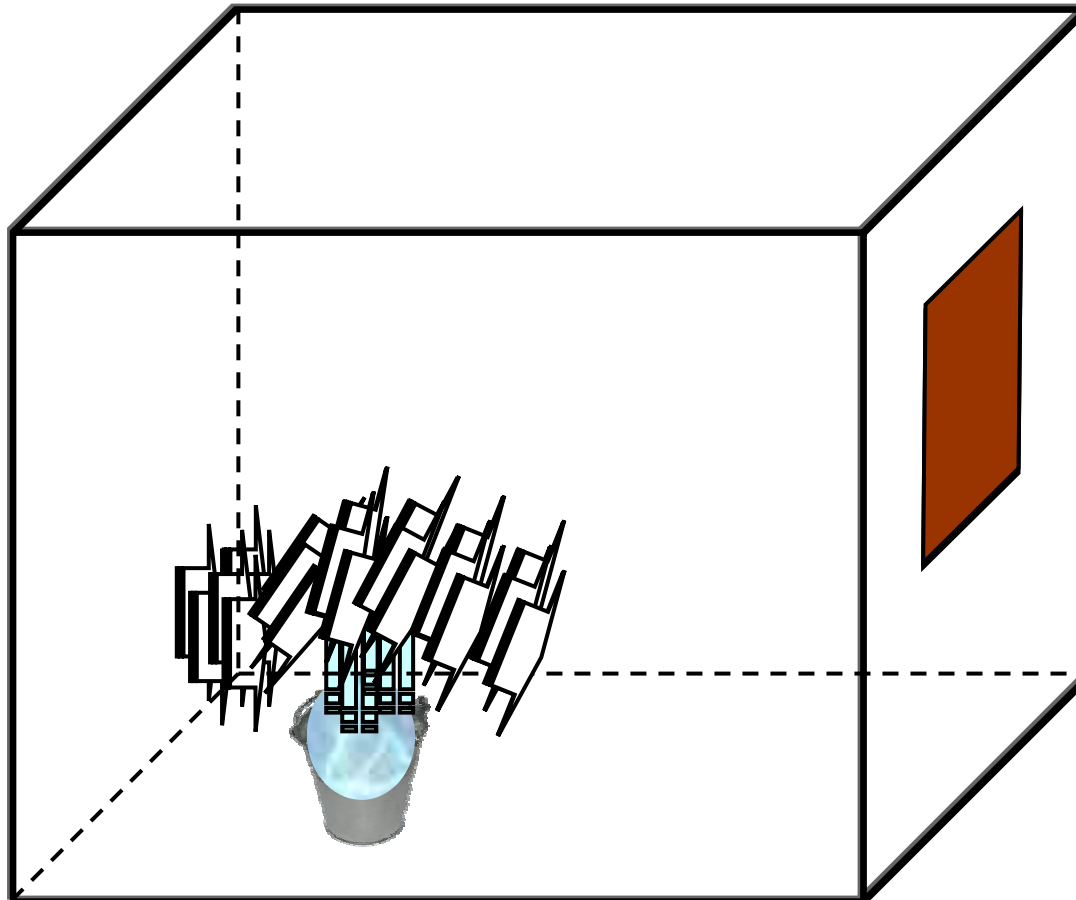


$$C_{\text{sat}} = \frac{10^6 \cdot VP_T \cdot MW}{24.45 \cdot (298.15 / T_{\text{air}})}$$

Scenario “Evaporazione da sostanza pura”

PARAMETRI DI INPUT	
Tasso di ventilazione del locale	m ³ /min
Concentrazione ambientale (esterna)	mg/m ³
Superficie di rilascio	m ²
Volume del locale	m ³
Tempo di esposizione	min
Conc. Iniziale	mg/m ³
Peso Molecolare della sostanza	g/mole
Pressione di vapore a 25 °C	Pa
Temperatura di utilizzo del locale	K

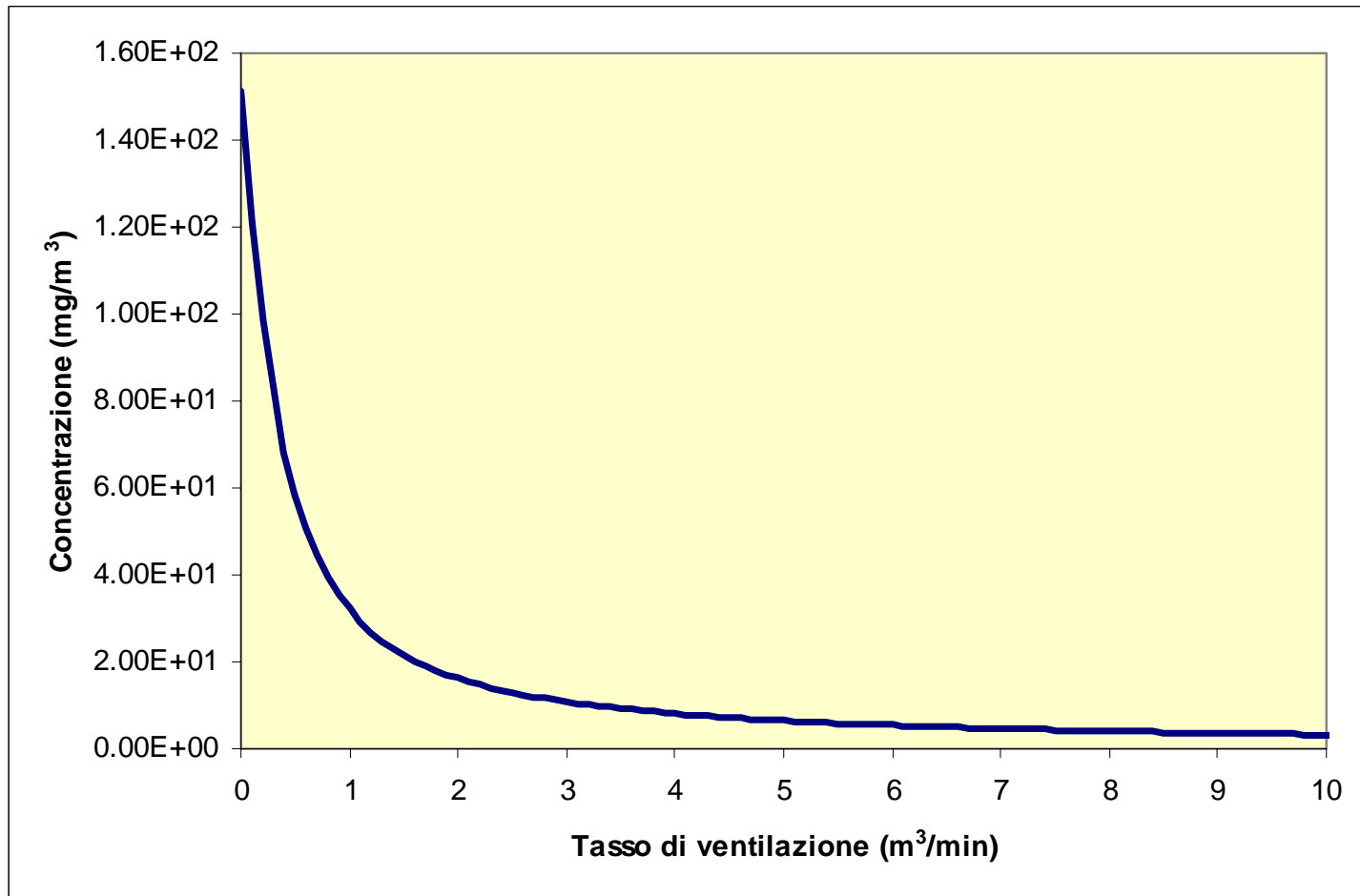
INTERMEDI DI CALCOLO	
Coefficiente di trasferimento di massa K_t	m/min
Entalpia di vaporizzazione a 25°C	kJ mol^{-1}
Entalpia di vaporizzazione alla temperatura di utilizzo	J mol^{-1}
Pressione di vapore alla temperatura di utilizzo	Pa



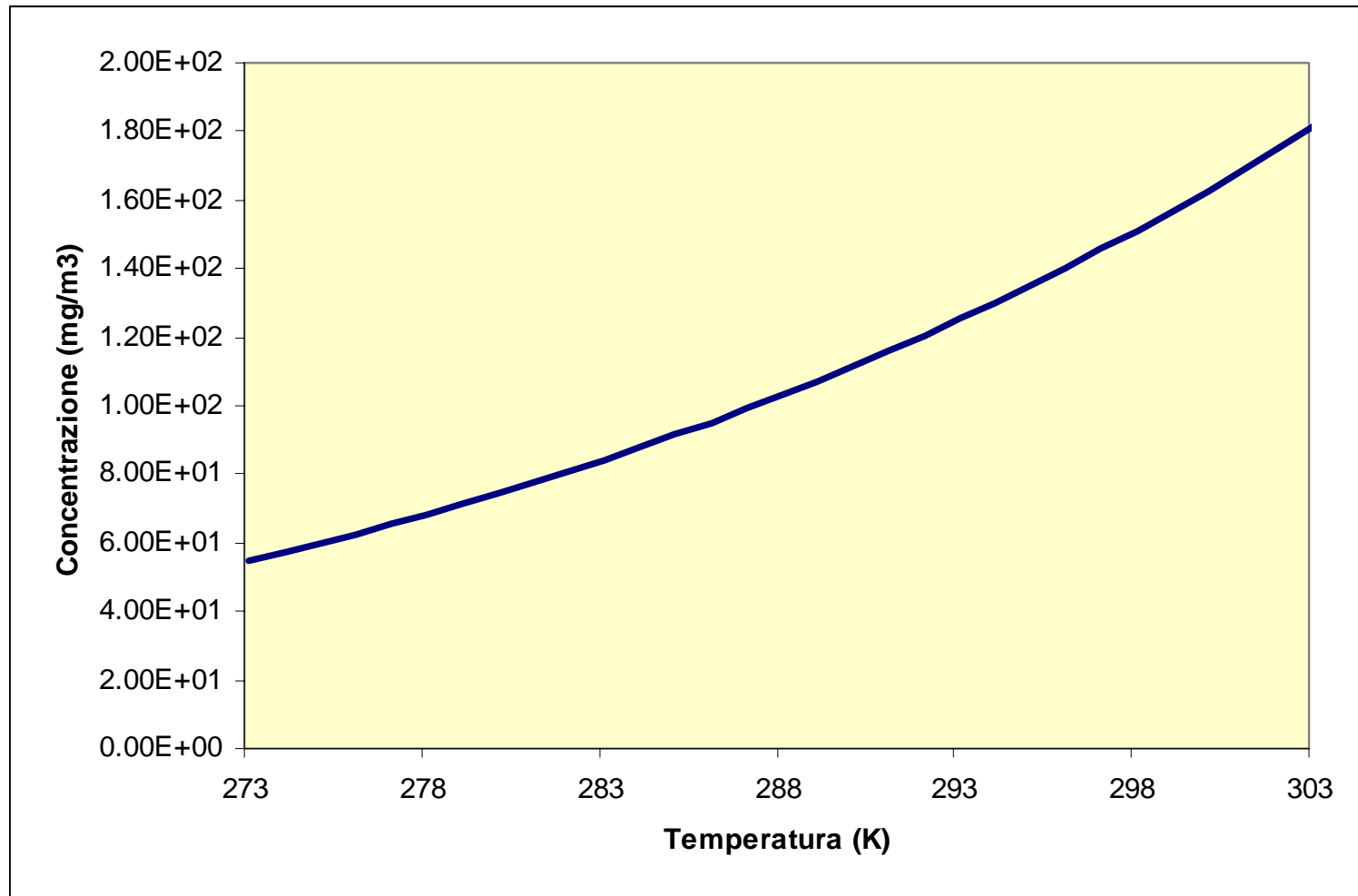
Per il tasso di ventilazione indoor è stato preso come riferimento il lavoro pubblicato dall' US Environmental Protection Agency, Exposure Factors Handbook (USEPA, 1989), dove sulla base di statistiche regionali combinate, gli autori suggeriscono un valore per il tasso di ricambio di aria per ora (ACH) di 0.18 e 0.45 rispettivamente come 10mo e 50mo percentile

OUTPUT PER TUTTI GLI SCENARI

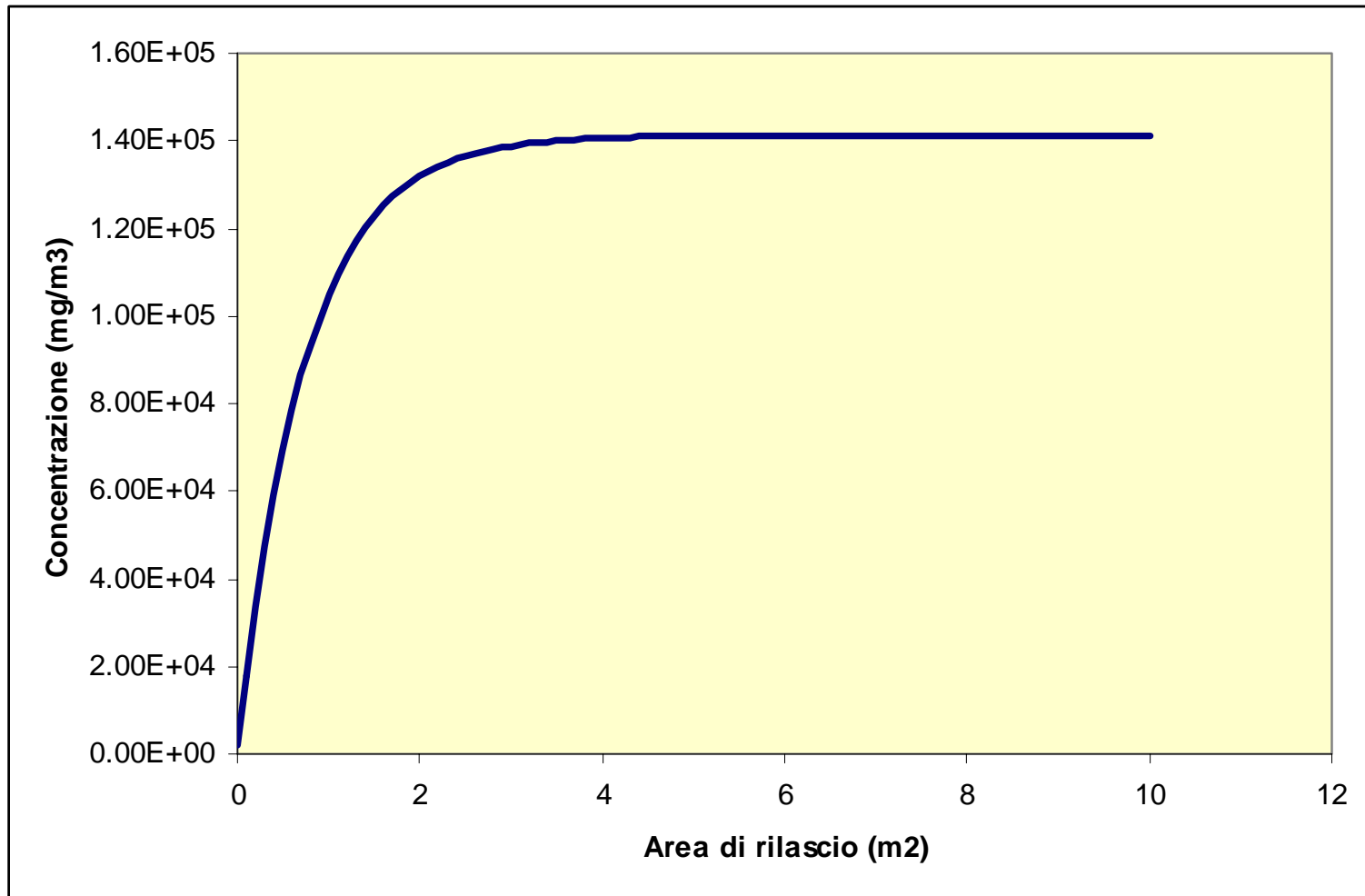
<i>Esposizione inalatoria</i>	mg/m^3
Dose inalatoria	$mg\ kg^{-1}\ gg^{-1}$
<i>Esposizione Cutanea indiretta</i>	mg/cm^3
<i>Dose Cutanea indiretta</i>	$mg\ kg^{-1}\ gg^{-1}$
<i>Esposizione Orale indiretta</i>	mg/cm^3
<i>Dose Orale indiretta</i>	$mg\ kg^{-1}\ gg^{-1}$



Tasso di ventilazione



Temperatura



Area di rilascio

Il rischio delle sostanze chimiche e il regolamento REACH

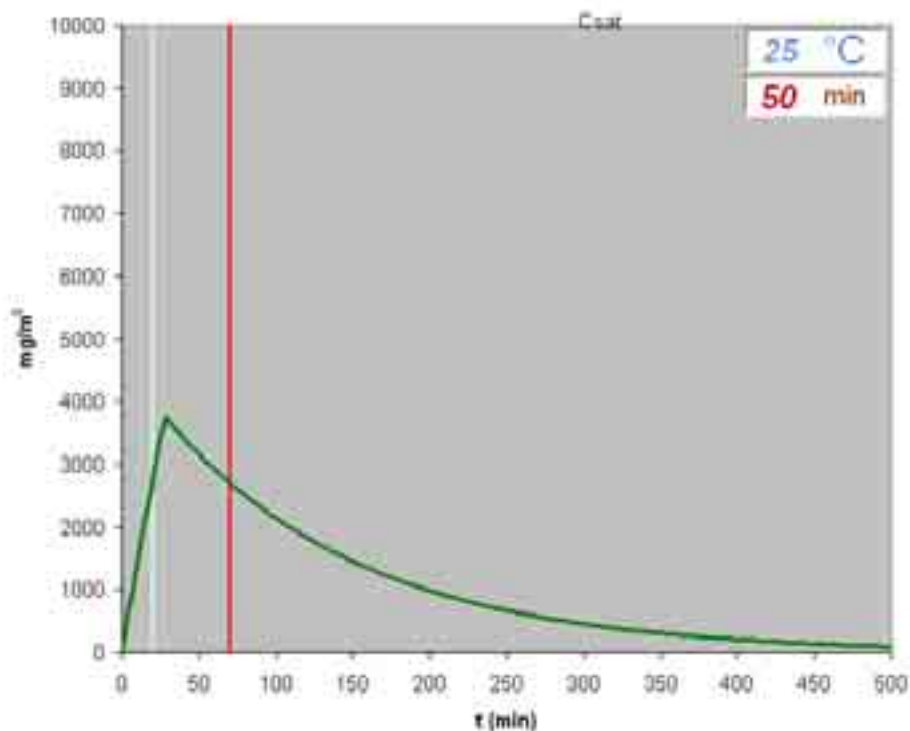
inputs

Toluene	
MW (g/mole)	92.15
VP 25 °C (Pa)	3.80E+03
Volume locale (m³)	0.214
Tasso vent. locale (m³/min)	0.001666667
Quantità di prodotto rilasciata (mg)	1.00E+03
Concentrazione sostanza (%)	100.000000
Densità prodotto (mg/cm³)	1
Area di rilascio (m²)	0.00
Temperatura locale (K)	298.15
Concentrazione iniziale (mg/m³)	0
Tempo inizio esp. I (min)	20
Durata evento (min)	50
Peso molecolare matrice (g/mole)	18
Csat (mg/m³)	141345.9797
Tasso vent. locale (m³/min) 0°	0.001666667
Temperatura locale (°C)	25
Concentrazione matrice (mg/kg)	0.00E+00
Tensione di vapore parziale 25 °C (Pa)	3.80E+03
Tensione di vapore parziale a T (Pa)	3.80E+03
Kt (m/min) (idrodraus)	2.90E-01
Entalpia di vaporizzazione (kJ/mol)	2.98E+01
Entalpia di vaporizzazione a T (kJ/mol)	2.98E+04
Tensione di vapore a T (Pa)	3.80E+03
Quantità di prodotto (kg)	1.00E-03
Concentrazione sostanza mg/kg	1.00E+06
Quantità sostanza (mg)	1.00E+03
Tasso di ventilazione (l/s)	1.30E-04
Tasso di ventilazione (l/h) - ACH	4.67E-01
Esposizione inalatoria media (mg/m³)	3.21E+03
Esposizione inalatoria media (ug/m³)	3.21E+06

Evaporazione da sostanza pura

intermedi

outputs



Emission Scenario Documents:

EU, 2003	Technical Guidance Document on Risk Assessment in support of Directive 93/67/EEC on risk assessment for new notified substances, Commission Regulation (EC) No. 1488/94 on risk assessment for existing substances (Parts I, II, III and IV) and Directive 98/8/EC of the European Parliament and the Council concerning the placing of biocidal products on the market. European Chemicals Bureau, Ispra (It.), 2003
OECD, 2001	Use and Release of Industrial Chemicals, OECD's Database on Use and release of Industrial Chemicals http://appli1.oecd.org/ehs/urchem.nsf

Il rischio delle sostanze chimiche e il regolamento REACH

Application of OPPT's Exposure Assessment Tools and Models

Model	Consumer		General Population			Workers	Environmental	Download Availability
	Dermal	Inhalation	Drinking Water	Fish Ingestion	Inhalation			
<u>Specialized Priority Setting Tools</u>								
SRD		✓						v4.0 4/2004
UCSS						✓	✓	
<u>Screening Level Tools</u>								
*ChemSTEER						✓	✓	Beta 5/2004
E-FAST	✓	✓	✓	✓	✓		✓	V2.0 3/2007
**EPI Suite								v.1.2 02/2007
PIRAT	✓	✓						Beta 12/2003
ReachScan			✓	✓			✓	
<u>Higher Tier Tools</u>								
AMEM								AMEM v. 1.0
IGEMS			✓	✓	✓		✓	Beta Test 10/2002
MCCEM		✓						v 1.2 2/2001
WPEM		✓				✓		v 3.2 4/2001

<http://www.epa.gov/oppt/exposure/index.htm>

Il rischio delle sostanze chimiche e il regolamento REACH

http://ecb.jrc.it/

Toxicology and Chemical Substances European Chemicals Bureau

ECB Activities

- Bioassays
- Classification & Labeling
- Computational Toxicology
- Identifying Chemicals
- Exposure-assess
- New Chemicals
- REACH
- Testing strategies

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ECB

The Toxicology and Chemical Substances (TCS) Unit, widely known as European Chemicals Bureau (ECB), is part of the Institute for Health and Consumer Protection (IHCP), which is one of the seven scientific institutes in the European Commission's Joint Research Centre (JRC).

Our mission is to provide scientific and technical support to the conception, development, implementation and monitoring of EU policies on dangerous chemicals. This includes managing the risk assessment process for New and Existing Chemicals, the authorisation process for PBTs, and the classification and labeling of hazardous chemicals. Our work also focuses on the development and harmonisation of testing methods and non-testing methods (e.g. QSARs), and the development of guidance documents and tools in support of the REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) regulation.

For any information concerning the ECB, please contact the Head of Unit: [Stefano.Scorchi](mailto:Stefano.Scorchi@ecb.jrc.it); the ECB Website, please contact the IT Manager: [Stefano.Artusi](mailto:Stefano.Artusi@ecb.jrc.it)

Il rischio delle sostanze chimiche e il regolamento REACH

ECB Existing Chemicals

ihp EUROPEAN COMMISSION and Commission Joint Research Centre

ECB Home Page | Documents | Data Collection | Priority Setting | Risk Assessment | EUSES | HEDSET | IUCLID

ECB Activities

- Biocides
- Classification & Labelling
- Computational Toxicology
- Existing Chemicals
- Export-Import
- New Chemicals
- REACH
- Testing Methods

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The Existing Chemicals Work Area provides technical and scientific support to the Commission concerning the:

- Data Collection
- Priority Setting
- Risk Assessment

steps of Council Regulation (EEC) No 793/93.

Contact Person: [Sazan PAKALJI](#)



[Overview](#) | [EINECS Information System](#) | [ESR Evaluation Report](#)
[Existing Substances Regulation Results](#) | [HPV-LPV Chemicals Information System](#)
[Online EURATS \(Online European Risk Assessment Tracking System\)](#)
[Public Availability of Data on EU High Production Volume Chemicals](#) | [TGD \(Technical Guidance Document\)](#)
[Council Regulation \(EEC\) No 793/93](#) | [Commission Regulation \(EC\) No 1488/94](#)

Overview

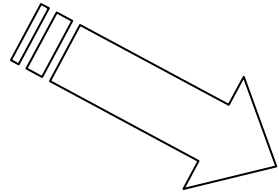
1 Background

The Existing Chemicals work area provides technical and scientific support to the Commission Services ([DG Environment](#)) and Member State Authorities concerning the implementation of the data collection, priority setting and risk assessment activities required under Council Regulation (EEC) No 793/93 on the Control and Evaluation of the Risks of Existing Substances.

The concern regarding the potential risks of chemicals and in particular existing chemicals, was already a policy priority in the late 1980s. The Council of the European Communities, in approving the Fourth Community Action Programme on the Environment (1987-1992), stated that one of the priority areas was the evaluation of the risks to the environment and human health posed by chemical substances [1]. This Action Programme underlined the need for a legislative instrument, which would provide a comprehensive structure for the evaluation of the risks posed by "existing" chemicals. In particular, the Action Programme stated that such a legislative instrument "will establish a procedure for treating priority lists of chemicals for immediate attention, as well as setting out the means for gathering information, requiring testing and evaluating the risks to people and the environment". Consequently, the European Commission proposed a series of legal instruments, which were aimed at meeting the objectives outlined in the Action Programme. One of these instruments was the Existing Substances Regulation.

IC - 12 Pulp, paper and board industry

Emissions calculation



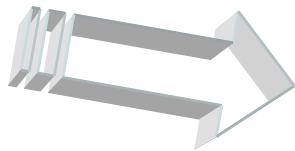
$$E = W_s \cdot Q \cdot \frac{(100 - F)}{100} \cdot \frac{(100 - C)}{100} \cdot \frac{G}{100}$$

dove:

E	emission per day	kg/d
W_s	substance specific consumption	kg/t paper
Q	paper produced in 1 site per day	t/d
F	fixation degree	%
C	aquatic system closure degree	%
G	fraction of the substance in preparation	%

IC - 12 Pulp, paper and board industry

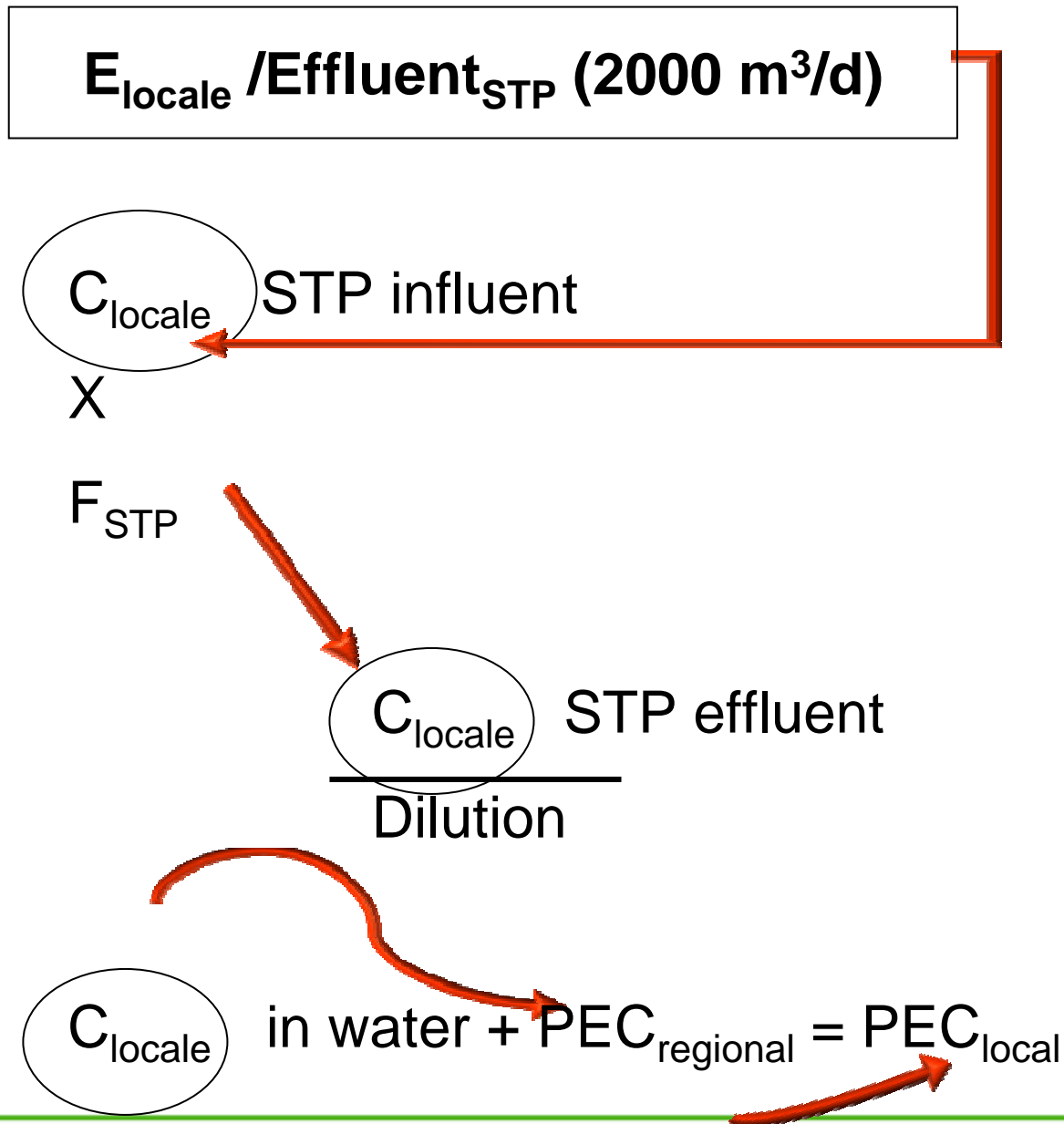
Emissions calculation knowing water conc.



$$E = C_s \cdot A_s \cdot Q \cdot \frac{(100 - F)}{100}$$

dove:

E	kg/d	emission per day
C _s	kg/m ³	concentration in water
A _s		water consumption per tonn. of paper produced m ³ /t
Q	t/d	paper produced in 1 site per day
F		fixation degree
		%



DNEL

$$\text{DNEL} = \frac{\text{N(L)OAEL}}{\text{AF}_{\text{inter}} * \text{AF}_{\text{allom}} * \text{AF}_{\text{intra}} * \text{AF}_{\text{expdur}} * \text{AF}_{\text{exprt}} * \text{AF}_{\text{dose-resp}}}$$

AF_{inter} = interspecies differences

AF_{allom} = allometric factors

AF_{intra} = intraspecies differences

$\text{AF}_{\text{expdur}}$ = exposure duration

AF_{exprt} = route of exposure

$\text{AF}_{\text{dose-resp}}$ = uncertainties nature of effects/quality of data

Needs for Consumer Exposure Estimation

- **Antropometric data**

- total population
- subpopulations

Behaviour data (e.g.)

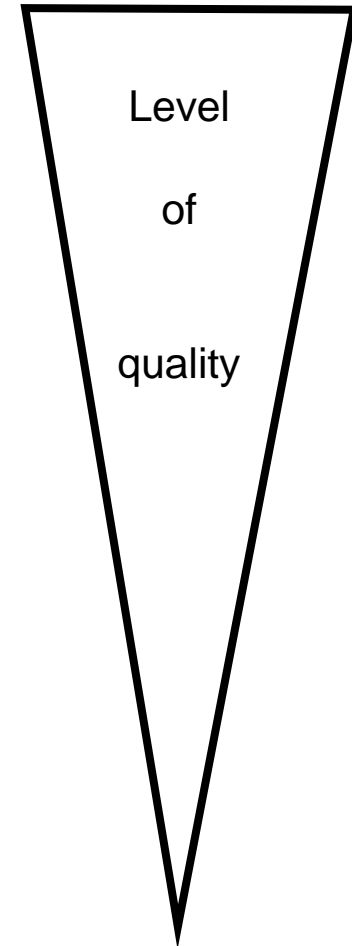
- staying inhouse
- staying outside
- staying at workplace
- certain behaviours of subpopulations (focus on children, e.g. playing with toys, sucking)

What about secondary literature - body weight

• Albania	61,07	
• Bosnia-Herzegovina	61,70	
• Croatia	61,70	
• Macedonia	61,07	
• Malta	61,07	
• Portugal	61,07	
• Slovenia	61,07	
• Italy	73,23	Source: WHO, cited in ECETOC Technical Report
• Spain	73,23	
• Yugoslavia	75,28	
• Greece	76,13	

Data quality of some exposure factors

Body weight and height
formulations
physiologic data
use descriptions
food consumption
time patterns
house and room characteristics
room ventilation
dermal uptake data
dust and soil uptake
hand to mouth
emission rates
migration of substances in material
etc.



Comparison with screening criteria



Type of data	Criterion	Screening assignment
Persistence		
Ready biodegradability test	Readily biodegradable	Not P and not vP
Enhanced ready biodegradability test	Readily biodegradable	Not P and not vP
Specified tests on inherent biodegradability Zahn-Wellens (OECD 302B)	$\geq 70\%$ mineralisation (DOC removal) within 7 d, log phase no longer than 3d, removal before degradation occurs below 15%, no pre-adapted inoculum	Not P
MITI II test (OECD 302C)	$\geq 70\%$ mineralisation (O ₂ uptake) within 14 days, log phase no longer than 3d, no pre-adapted inoculum	Not P
Biowin 2 (non-linear model prediction) and Biowin 3 (ultimate biodegradation time) or Biowin 6 (MITI non-linear model prediction) and Biowin 3 (ultimate biodegradation time)	Does not biodegrade fast (probability < 0.5), and ultimate biodegradation timeframe prediction: \geq months (value < 2.2) or Does not biodegrade fast (probability < 0.5) and ultimate biodegradation timeframe prediction: \geq months (value < 2.2)	P
Bioaccumulation		
Convincing evidence that a substance can biomagnify in the food chain (e.g. field data)	e.g. BMF > 1	B or vB, definitive assignment possible
Octanol-water partitioning coefficient (experimentally determined or estimated by QSAR)	Log Kow ≤ 4.5	not B and not vB
Toxicity		
Short-term aquatic toxicity	EC ₅₀ or LC ₅₀ < 0.01 mg/L	T, criterion considered to be definitely fulfilled
Short-term aquatic toxicity	EC ₅₀ or LC ₅₀ < 0.1 mg/L	T
Avian toxicity (subchronic or chronic toxicity or toxic for reproduction)	NOEC < 30 mg/kg food	T

Il rischio delle sostanze chimiche e il regolamento REACH

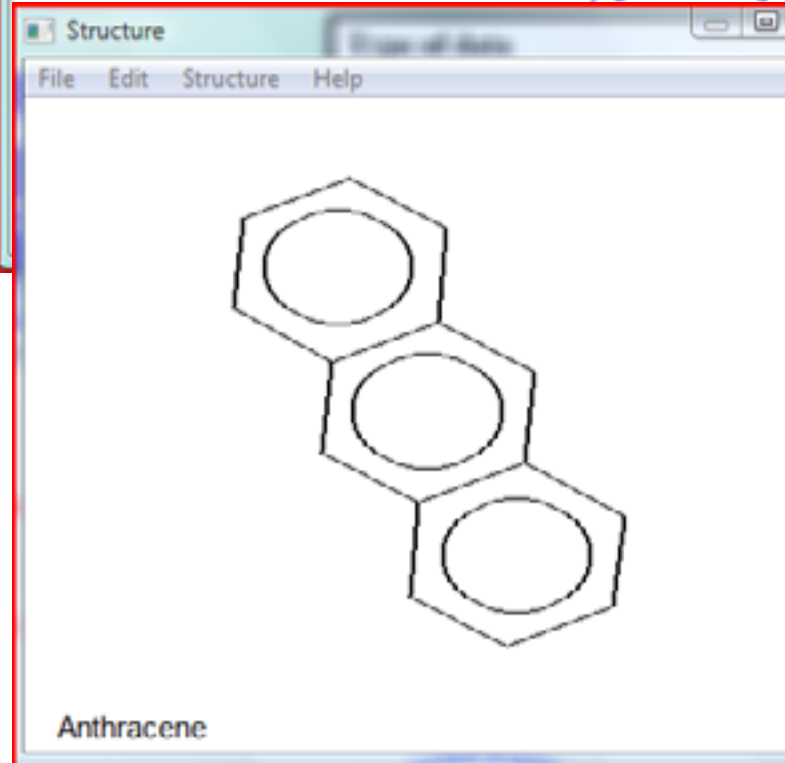
BioWin v4.10

File Edit Functions BatchInput ShowStructure Quit Help

Previous Get User Save User CA

Enter SMILES: c(c(ccc1)cc(c2ccc3)c3)(c1)c2

Enter NAME: Anthracene



Bio Results

Print Save Results Copy Remove Window Help

SMILES : c(c(ccc1)cc(c2ccc3)c3)(c1)c2
 CHEN : Anthracene
 MOL FOR: C14 H10
 MOL WT : 178.24

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Biodegrades Fast
 Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
 Biowin3 (Ultimate Biodegradation Timeframe): Months
 Biowin4 (Primary Biodegradation Timeframe): Weeks
 Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable
 Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable
 Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
 Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Unsubstituted aromatic (3 or less rings)	0.3192	0.3192
MolWt	*	Molecular Weight Parameter		-0.0849
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.9819

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Unsubstituted aromatic (3 or less rings)	7.1908	7.1908
MolWt	*	Molecular Weight Parameter		-2.5309
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.9995

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Unsubstituted aromatic (3 or less rings)	-0.5859	-0.5859
MolWt	*	Molecular Weight Parameter		-0.3939
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.2194

Il rischio delle sostanze chimiche e il regolamento REACH

The image shows two windows from the KOWWIN v1.67 software. The top window is the main interface with a menu bar (File, Edit, Functions, BatchMode, ShowStructure, Zwitterions, Help) and a toolbar with buttons: Previous, Get User, Save User, CAS Input, ExpValAdj, Calculate. It has two input fields: "Enter SMILES:" and "Enter NAME:". The bottom window is titled "Kowwin Results" and contains the following information:

Log Kow(version 1.67 estimate): 4.35

SMILES : c(c(ccc1)cc(c2ccc3)c3)(c1)c2
CHEM : Anthracene
MOL FOR: C14 H10
MOL WT : 178.24

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	14	Aromatic Carbon	0.2940	4.1160
Const		Equation Constant		0.2290
Log Kow =				4.3450