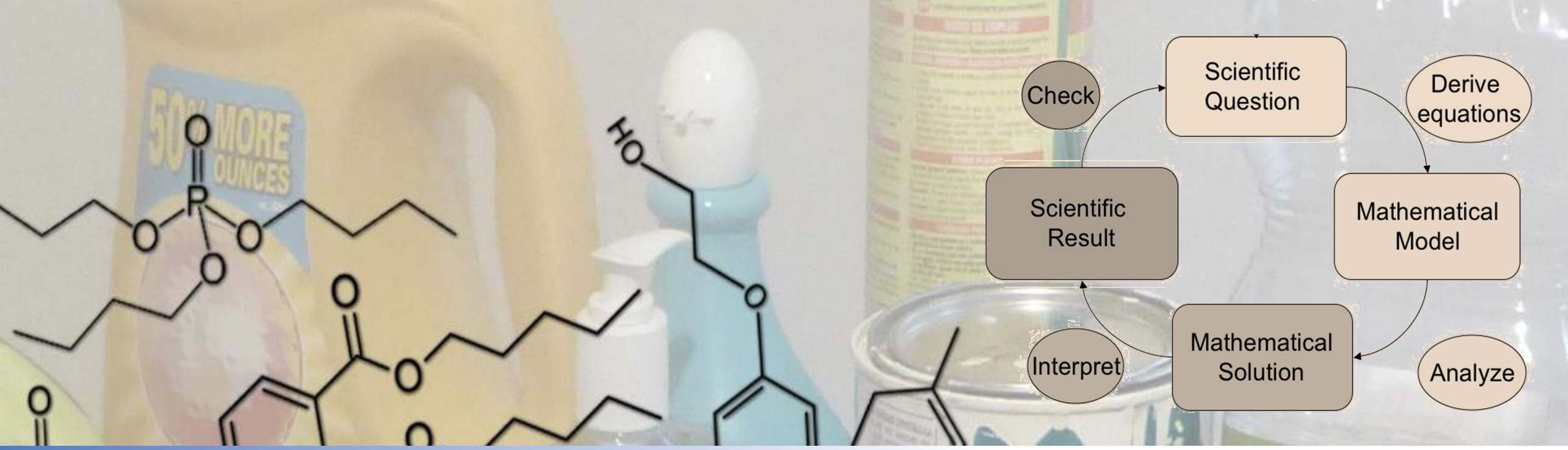


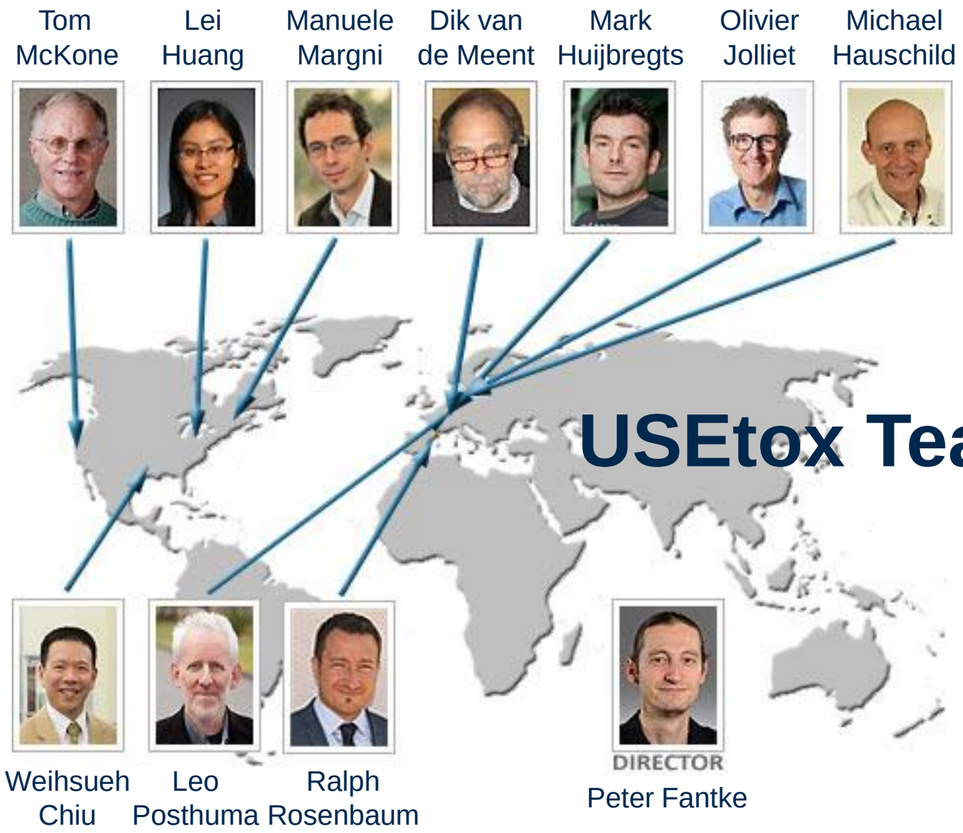
USEtox for application in building & construction

Prof. Peter Fantke, Prof. Olivier Jolliet, Dr. Lei Huang

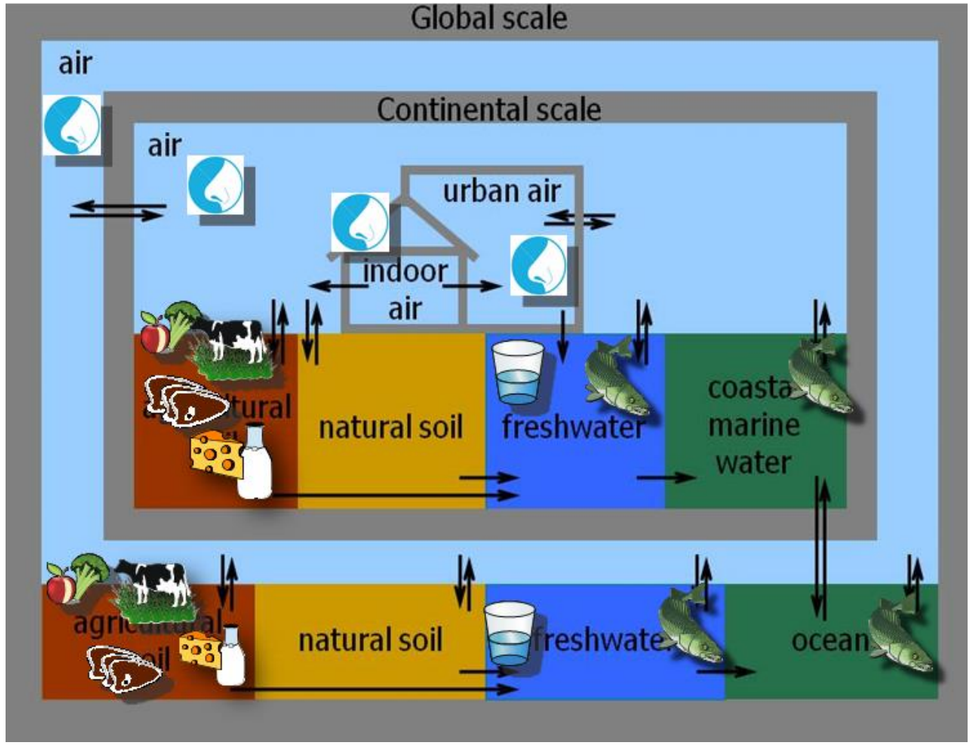
USEtox®

USEtox® – the UNEP-SETAC toxicity consensus model

USEtox: A parsimonious model to assess toxic impacts of chemicals on humans and ecosystems.
Now extended to chemicals in products



USEtox Team



USEtox® – the UNEP-SETAC toxicity consensus model

USEtox base model + six basic models applied to 10000 chemicals in 500 products

→ customized to particular applications + developed necessary QSARS for high throughput determination

→ Relevant mass balance-based models for building and materials:

- Releases from **building materials**, *with indoor sorption)*
- Releases from **object surface** (e.g. wet **paints**, cleaning agents)
- Indoor air modeling

→ USEtox determines

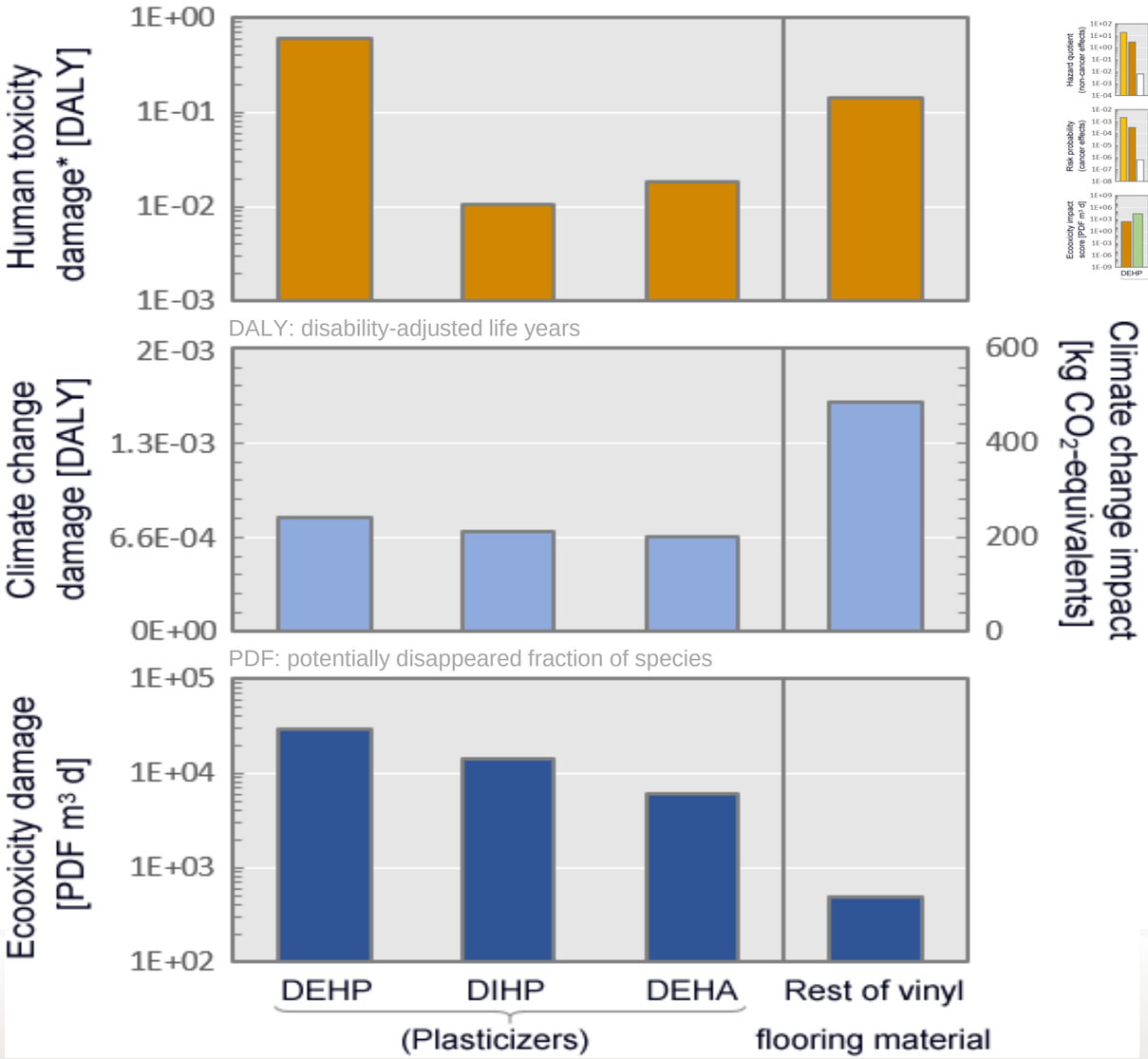
- Human exposures of the user and the general population via inhalation, ingestion incl. mouthing and dust , dermal direct contact and gaseous uptake
- Risks for cancer, developmental and other non-cancer
  Maximum chemical content for acceptable risk
  Cumulative human health and ecosystem impacts for LCA

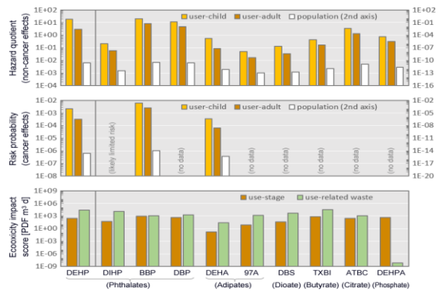
Chemicals of concern in building materials

5

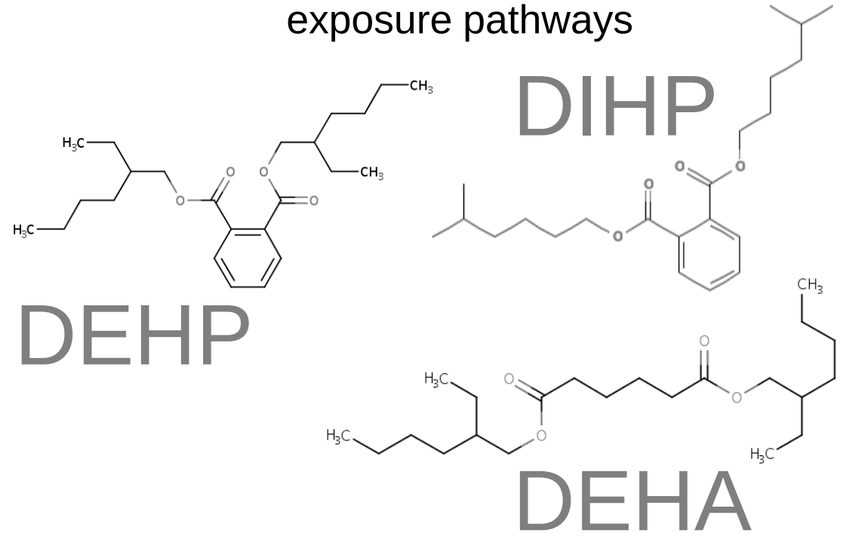
CAS	Chemical	Product categories*	Chemical function	MAC (ppm)	MAC endpoint	Actual content (ppm)	HCR
822-06-0	1,6-Hexamethylene diisocyanate (HDI)	Carpet flooring	Crosslinker	0.2	Non-cancer	48800	244000
		Acrylic flooring adhesive	Crosslinker	7	Non-cancer	13650	1950
		Flooring (wood, cork, vinyl)	Crosslinker, Residual monomer	0.1	Non-cancer	2.8 - 236	28 - 2360
51-79-6	Ethyl carbamate	Flooring (rubber, cork, wood)	Solvent	0.2	Cancer	11560 - 28800	57800 - 144000
50-00-0	Formaldehyde	Wooden furniture, Base cabinetry	Preservative, Residual monomer	0.1	Cancer	6.6 - 3102	110 - 51700
		Flooring (wood, cork, bamboo, fluid-applied)	Preservative, Residual monomer	0.1	Cancer	6.58 - 1890	94 - 27000
		Gypsum wallboard	Preservative	0.03	Cancer	1032	34400
		Foam insulation (polyurethane, spray), Gypsum ceiling	Preservative, Residual monomer	0.1	Cancer	2.8 - 236.8	35 - 2960

Substituting DEHP phthalate in flooring





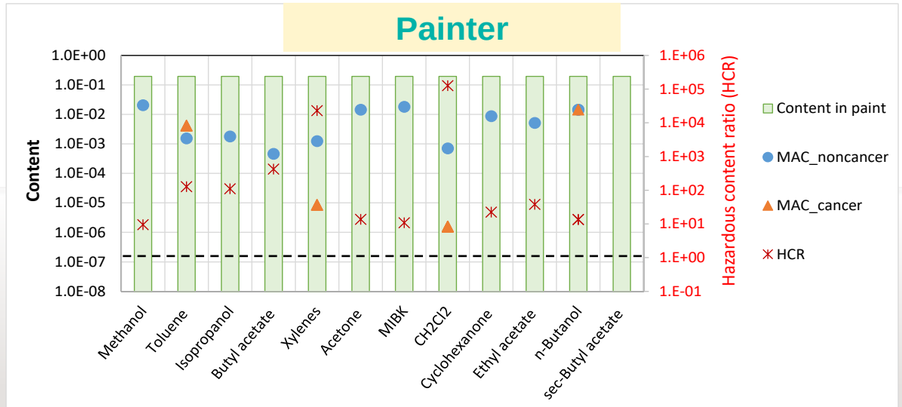
- Screen alternatives
- Impacts beyond use-stage risks: depends on chemical function and product appliation
- **Chemical function** determines weight fraction and risk potency
- **Product application** determines main direct exposure pathways



- Impacts brought to **damage level** for highest possible aggregation and evaluation of potential trade-offs

Summary – Building materials interface

- USEtox enables us to assess thousands of chemicals in 100+ different types building materials
- It combines far-field and near-field exposures, accounting for multiple exposure pathways
- Exposure in the near-field environment are usually dominant, but environmental exposures can remain high for persistent and bio-accumulating chemicals
- Enables both a risk and a damage-oriented approach
- Applied in multiple building materials and products, including
  - PU vs EPS and XPS inner and outer insulation, including indoor air quality & optimal ventilation rates
  - Chemicals in paints in Sri Lanka
  - Plasticizer substitution in flooring materials
  - High throughput screening of 400+ chemical in building materials: chemicals of concern



Main Application Areas of USEtox version 3

Near-field/far-field USEtox framework is suitable for **comparative evaluation of chemicals** emitted along product life cycles and chemicals in various product applications. Primary application areas are (model already tested):

Application area	Product types already covered in our framework (emissions already directly or indirectly included)
Product life cycle assessment (LCA)	Food contact materials
High-throughput exposure screening	Personal care products; food contact materials
High-throughput risk screening	Children toys; building materials; paints
Chemical exposure and risk prioritization	Household products (cleaning, personal care, and home maintenance products)
Chemical alternatives assessment (CAA) / chemical substitution	Building materials; personal care products; agricultural pesticides

http://doi.org/10.1007/s11367-021-01889-y

USEtox product interfaces

USEtox® – the UNEP-SETAC toxicity consensus model

USEtox base model + six basic models applied to 10000 chemicals in 500 products

→ customized to particular applications + developed necessary QSARS for high throughput determination

Life Cycle Initiative

Direct environmental emission (e.g. industrial processes)

Skin surface (e.g. cosmetics)

Article interior (e.g. building materials) *(with indoor sorption)*

Food contact materials

Object surface (e.g. wet paints, cleaning agents)

Pesticide residues

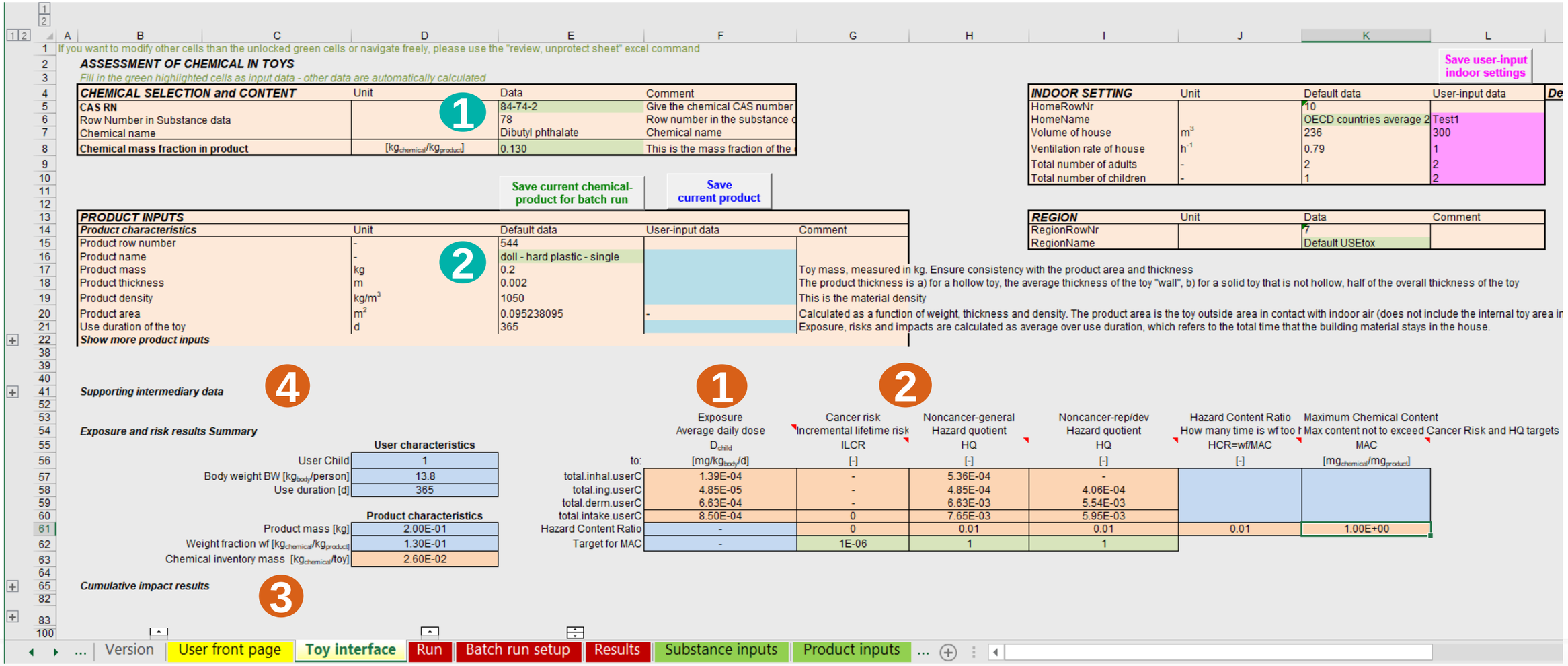
USEtox Product interfaces (https://manual.usetox.org)

1. Select your chemical among 400+ chemicals and provide the chemical mass fraction in product
2. Define your product and usage characteristics

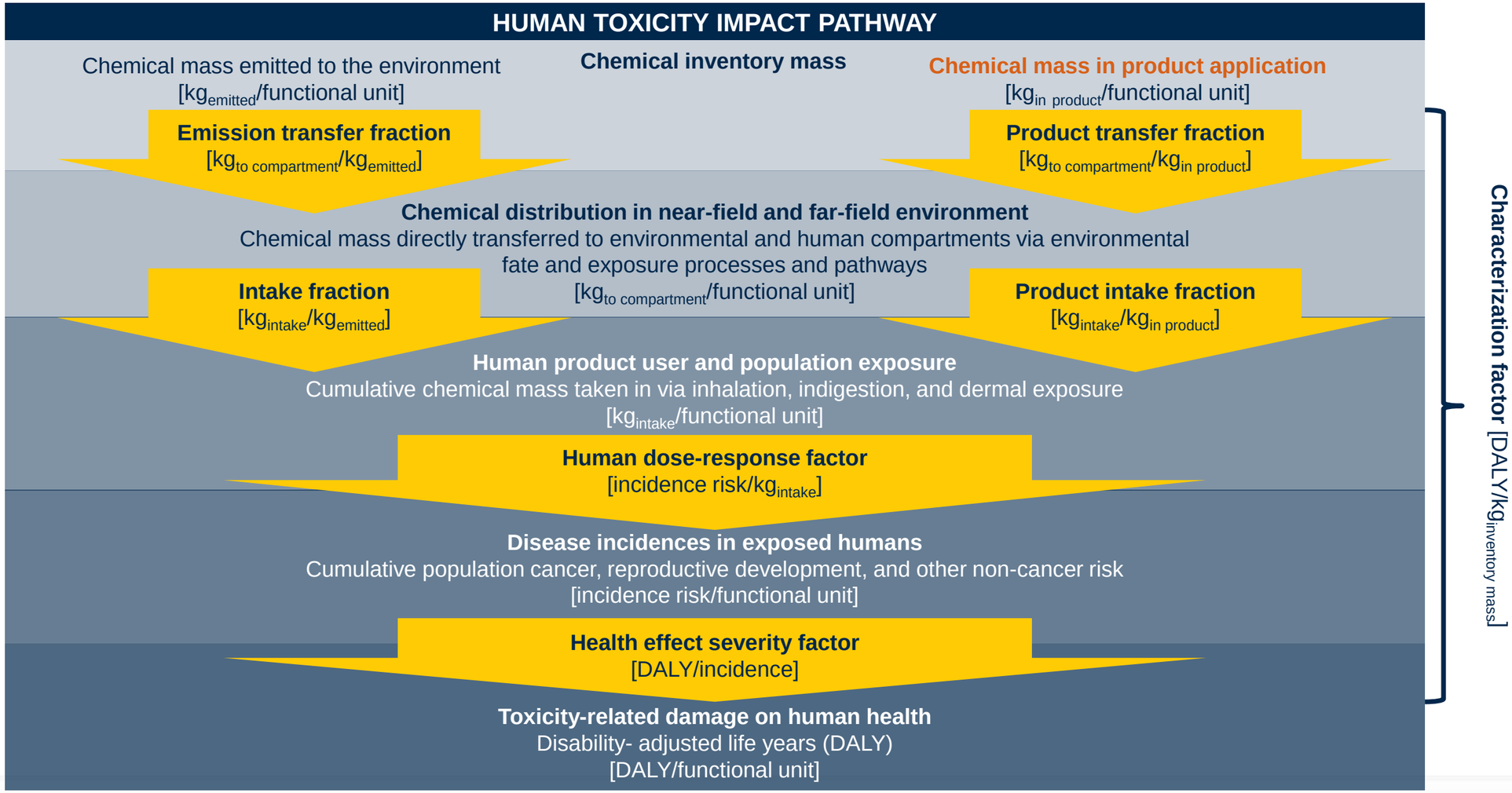
USEtox determines

1. The exposure of the user and of the general population
2. Relative measure of risks (incremental lifetime cancer risk - ILCR, hazard quotient -HQ, maximum chemical content - MAC)
3. Relative cumulative measures of impacts for LCA or alternatives assessment
4. Supporting intermediary data, such as the product intake fraction, i.e. the fraction of the chemical mass in product taken in by the user and the general population

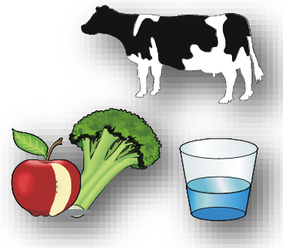
USEtox Product interfaces (https://manual.usetox.org)



Human health assessment framework



Emission to Intake



1 2 3 6

Mass emitted or in product [$kg_{emitted}$]

Transfer to environment [$kg_{to\ compartment}$]

Exposure=transfer to human [$kg_{intake\ =\ to\ human\ compartment}$]

Fraction transferred T

4

Fraction transferred to environment and to humans

[$kg_{to\ compartment\ n}/kg_{emitted\ to\ compartment\ m}$] = [-]

5

T_{cum} = T^{-1}= (Product) Intake fraction, *iF*

[$kg_{intake}/kg_{emitted}$]

Exposure Doses for Chemical *i* in Product *p*

6 Intake: $I_i = PiF_{i,p}^{tot} \cdot f_{i,p} \cdot M_p$ [kg/functional unit, FU]

$PiF_{i,p}^{tot}$ [$kg_{\text{i intake}}/kg_{\text{i in product p}}$]: Product intake fraction

$f_{i,p}$ [$kg_{\text{i in product p}}/kg_{\text{product p}}$]: Fraction of chemical *i* in product *p*

M_p [$kg_{\text{product p}}$/FU]: Mass of product p applied or used

Intake dose rate: $IR_i = \frac{PiF_{i,p}^{tot}}{BW \cdot N_{\text{pers}}} \cdot f_{i,p} \cdot \frac{M_p}{\Delta t} \cdot cf_{\text{kg to mg}}$ [mg/kg_{body}-d]

BW [kg_{body}]: Body weight (e.g 70 kg for an adult)

N_{pers} [capita]: Number of persons exposed (e.g. 2 adults for household)

Δt [d]: Exposure time considered (M_p/Δt = mass applied per day)

$cf_{\text{kg to mg}}$ = 10^6 mg/kg

Cancer and non-cancer risk characterization

End point	Chemical mass in product	Exposure dose	Dose – response metric	Assessment metric & criteria
A **Cancer**	$m_{applied\ in\ product}$ [kg/d]	Oral ingestion $D_{lifetime}$ [mg/kg-day]	Linear dose-response Cancer slope factor **CSF** [1/(mg/kg-day)]	Compare **risks** **Risk**= $D_{lifetime}$·CSF **Risk<10^{-4} to 10^{-6}**
B **Non-cancer**		Oral ingestion **D** [mg/kg-day]	Non linear dose-response Reference dose **RfD** Safe dose = PoD/UF [mg/kg-day]	Compare **doses** **Dose ratio:** **Hazard quotient** **HQ**=D/RfD**<1**

Cancer risk < 10^{-6} ?

Non cancer dose ratio:
Hazard quotient HQ < 1?
- general non cancer
- reproductive/developmental

Hazardous Content Ratio

HCR = maximum (cancer risk/10^{-6}, HQ)

How many times is the risk higher than target

Maximum Chemical Content

MAC=Actual content/HCR

Max chemical content in product not to exceed targets HQ = 1 or cancer risk = 10^{-6}

USEtox applied to assess chemicals in building materials

Illustrative example: Formaldehyde in wood flooring

Formaldehyde's main use in buildings is in resin such as urea formaldehyde, used as a binder in composite wood flooring.

CAS 50-00-0, with residual monomer of up to 0.3% in urea formaldehyde, that is itself found at 8.3% in the wood flooring, the resulting concentration of residual formaldehyde in wood flooring amounts to $2.5 \cdot 10^{-4}$.

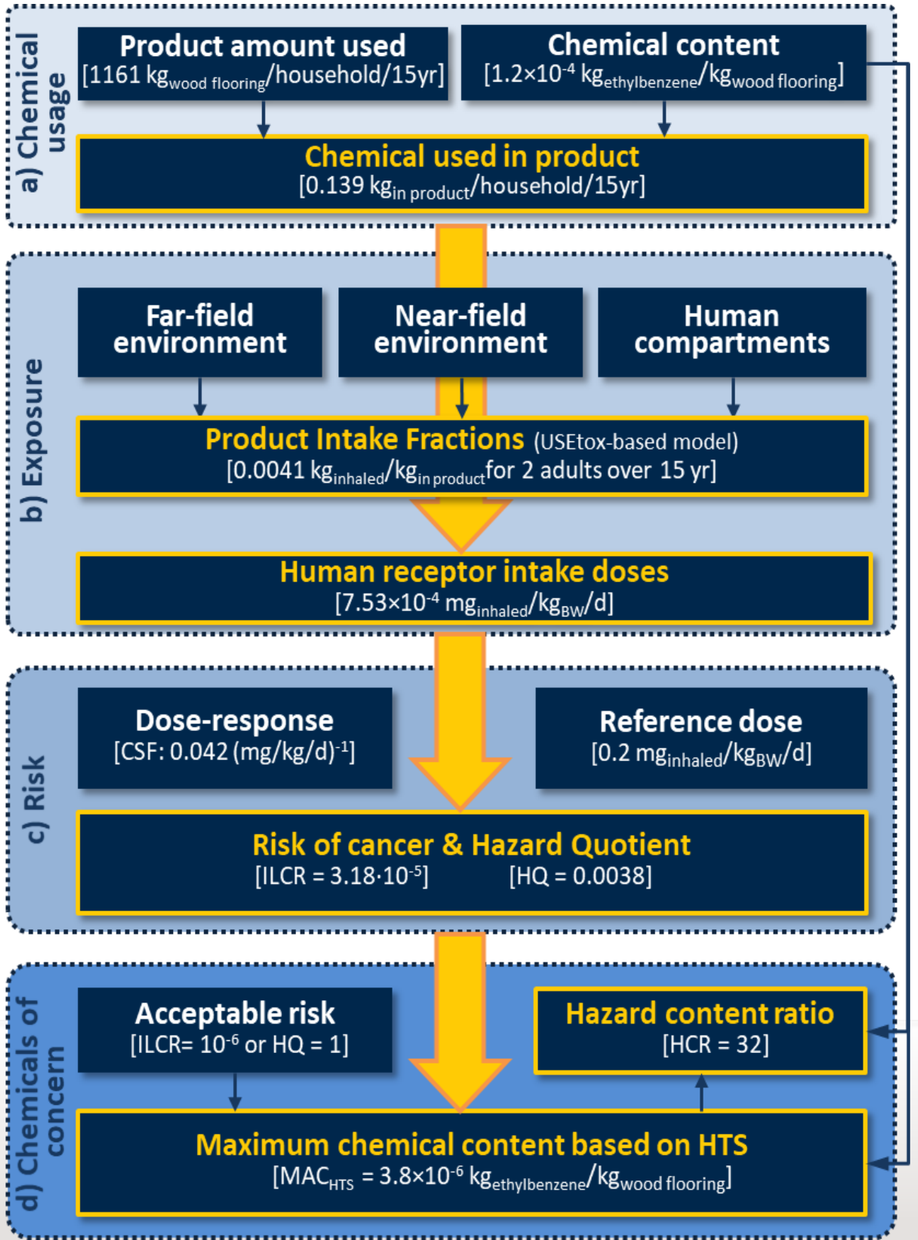
Formaldehyde is a probable human carcinogen and breathing in formaldehyde can also cause eye, nose and throat irritation.

→ Launch USEtox and activate the Building material interface

Activate Building material interface

Assessment framework

USEtox 3.0beta



For building occupants:

- Inhalation
- Dust ingestion
- Direct dermal contact
- Gaseous dermal uptake

Prioritization criteria:

- $HCR = \frac{Actual\ content}{MAC_{HTS}} > 10$

HQ: hazard quotient. ILCR: incremental lifetime cancer risk. CSF: cancer slope factor. HCR: hazard content ratio. MAC_{HTS}: maximum chemical content based on high-throughput screening.

Start from compartment of entry → direct transfers

Formaldehyde in wood flooring

0.29 kg

Chemical mass in product

96 m2 x 12 kg/m2 = 1160 kg

$2.5 \cdot 10^{-4}$

Product usage

Chemical content

Product life cycle

Far-field points of entry

Ambient Air

Water

Soil

Landfill

(WWTP) Waste Water Treatment Plant

0%

Near-field points of entry

Object interior

Food & beverage

Inside enclosed devices

Object surface

Dust

Skin surface

99.5%

Indoor air

0.5%

0.04 ppm

Direct human points of entry

Epidermis

Gastrointestinal tract

Respiratory tract

Fantke et al. 2018. Environ Health Perspect 126: 125001

Start from compartment of entry → direct transfers

Formaldehyde in wood flooring

Far-field points of entry

Ambient Air

Water

Soil

Landfill

(WWTP) Waste Water Treatment Plant

0.002%

Chemical mass in product

0.29 kg

Near-field points of entry

Object interior

Food & beverage

1.3%

Direct human points of entry

Epidermis

Inside enclosed devices

Object surface

Gastrointestinal tract

Dust

Skin surface

0.04 ppm

2.2%

0.6%

Indoor air

Respiratory tract

Product usage

Chemical content

Product life cycle

Fantke et al. 2018. Environ Health Perspect 126: 125001

Building material interface: Formaldehyde in wood flooring

If you want to modify other cells than the unlocked green cells or navigate freely, please use the "review, unprotect sheet" excel command

ASSESSMENT OF CHEMICAL IN BUILDING MATERIALS

Fill in the green highlighted cells as input data - other data are automatically calculated

Save user-input indoor settings

CHEMICAL SELECTION and CONTENT	Unit	Data	Comment
CAS RN		50-00-0	Give the chemical CAS number to
Row Number in Substance data		54	Row number in the substance da
Chemical name		Formaldehyde	Chemical name
Chemical mass fraction in product	$kg_{chemical}/kg_{product}$	2.50E-04	This is the mass fraction of the ch

INDOOR SETTING	Unit	Default data	User-input data
HomeRowNr		10	
HomeName		OECD countries average 2+1 children household	
Volume of house	m^3	236	
Ventilation rate of house	h^{-1}	0.79	
Total number of adults	-	2	
Total number of children	-	1	

Save current chemical-product for batch run

Save user-input product

PRODUCT INPUTS				
Product characteristics	Unit	Default data	User-input data	Comment
Product row number	-	81		
Product name	-	Flooring - Wood - 15y		
Product area	m^2	96.76		Area of the building material that is in contact with indoor air
Product thickness	m	0.015		Thickness of the building material
Product density	kg/m^3	800		Density of the building material
Product mass	kg	1161.12	-	Mass of the building material, calculated from the area, thickness and density.
Use duration of the building material	d	5475		Exposure, risks and impacts are calculated as average over use duration, which refers to the total time that the building material stays in the house.
Show more product inputs				

REGION	Unit	Data	Comment
RegionRowNr		7	
RegionName		Default USEtox	

Supporting intermediary data

Exposure and risk results Summary

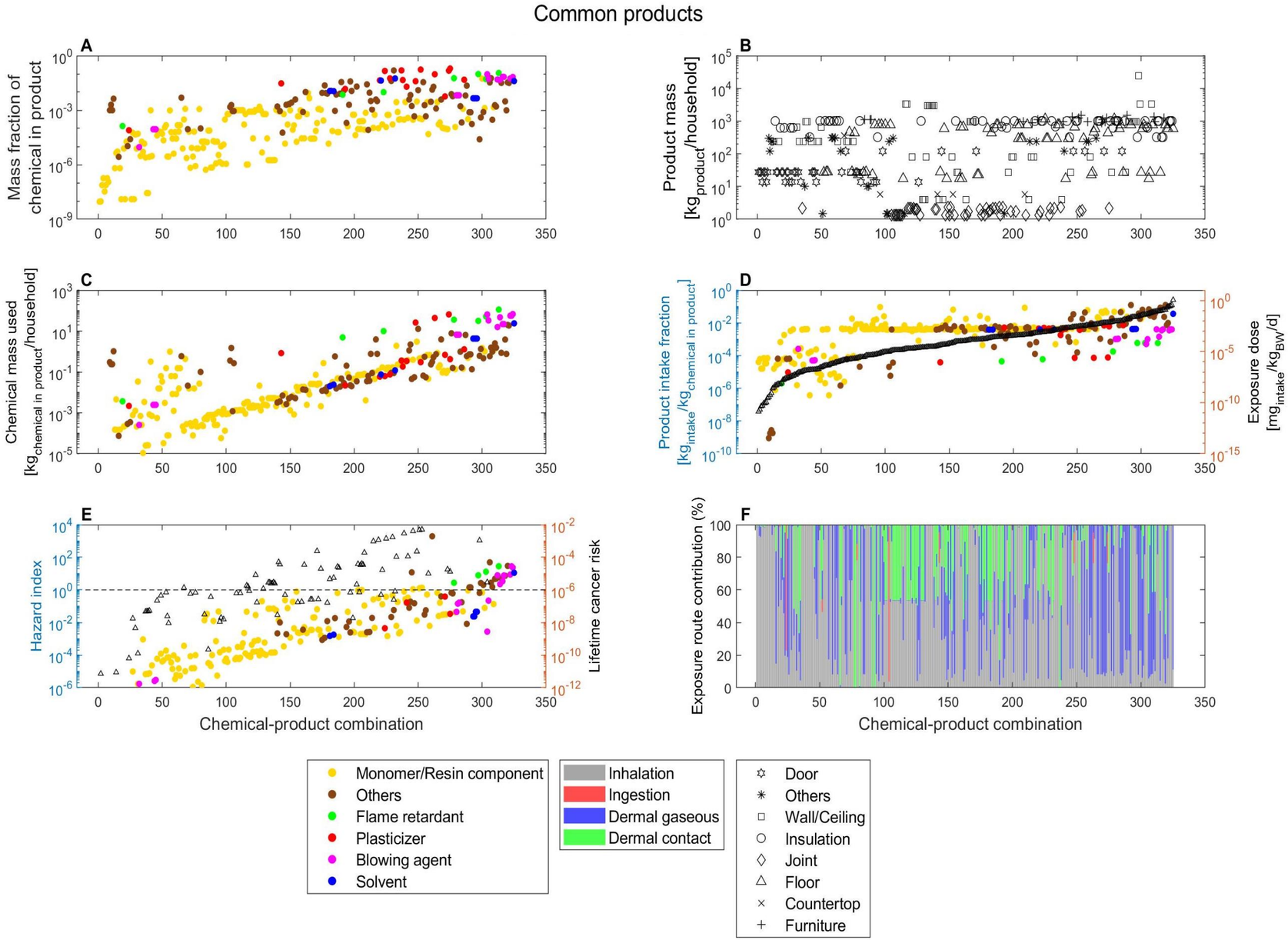
User characteristics	
Household Adult	2
Body weight BW [kg_{body}/person]	80
Household Child	1
Body weight BW [kg_{body}/person]	13.8
Use duration [d]	5475

Product characteristics	
Product mass [kg]	1.16E+03
Weight fraction wf [$kg_{chemical}/kg_{product}$]	2.50E-04
Chemical inventory mass [$kg_{chemical}$/house]	2.90E-01

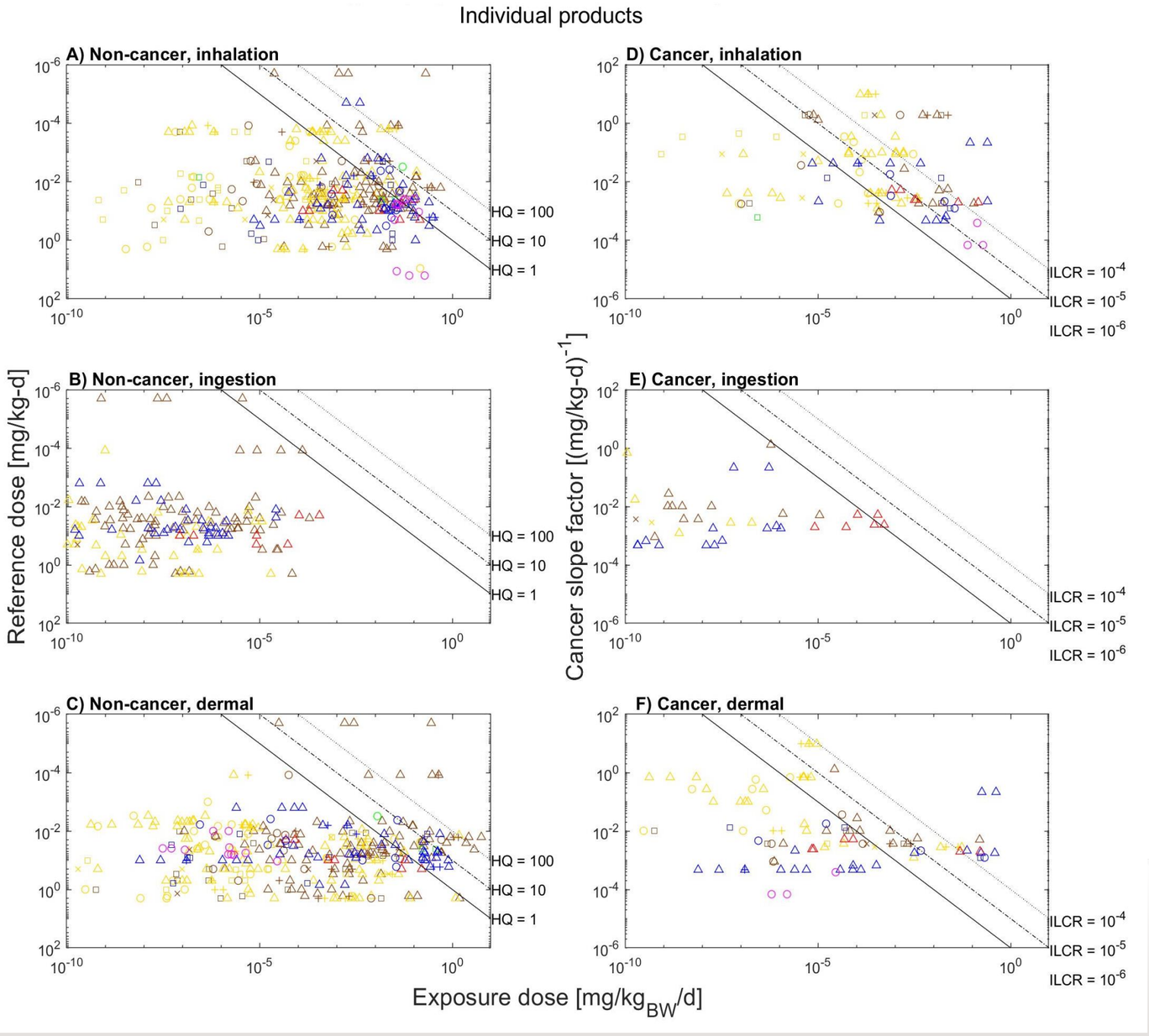
to:	Exposure Average daily dose $D_{exposure}$ [$mg/kg_{body}/d$]	Cancer risk Incremental lifetime risk ILCR [-]	Noncancer-general Hazard quotient HQ [-]	Noncancer-rep/dev Hazard quotient HQ [-]	Hazard Content Ratio How many time is wf too hi HCR=wf/MAC [-]	Maximum Chemical Content Max content not to exceed Cancer Risk and HQ targ MAC [$mg_{chemical}/mg_{product}$]
total.inhal.householdA	1.53E-03	3.31E-03	7.79E-01	1.75E-01		
total.ing.householdA	2.84E-09	1.19E-11	1.42E-08	1.58E-07		
total.derm.householdA	3.69E-03	1.55E-05	1.85E-02	2.06E-01		
total.intake.householdA	5.22E-03	3.33E-03	7.97E-01	3.81E-01		
total.inhal.householdC	5.08E-03	6.62E-03	8.04E-01	1.81E-01		
total.ing.householdC	1.19E-07	3.00E-10	5.95E-07	6.63E-06		
total.derm.householdC	1.10E-02	2.77E-05	5.49E-02	6.11E-01		
total.intake.householdC	1.61E-02	6.65E-03	8.59E-01	7.93E-01		
Hazard Content Ratio_adult	-	3.33E+03	7.97E-01	3.81E-01	3.33E+03	7.51E-08
Hazard Content Ratio_child	-	6.65E+03	8.59E-01	7.93E-01	6.65E+03	3.76E-08
Target for MAC	-	1E-06	1	1		

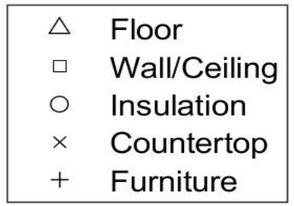
Cumulative impact results

Data and Results

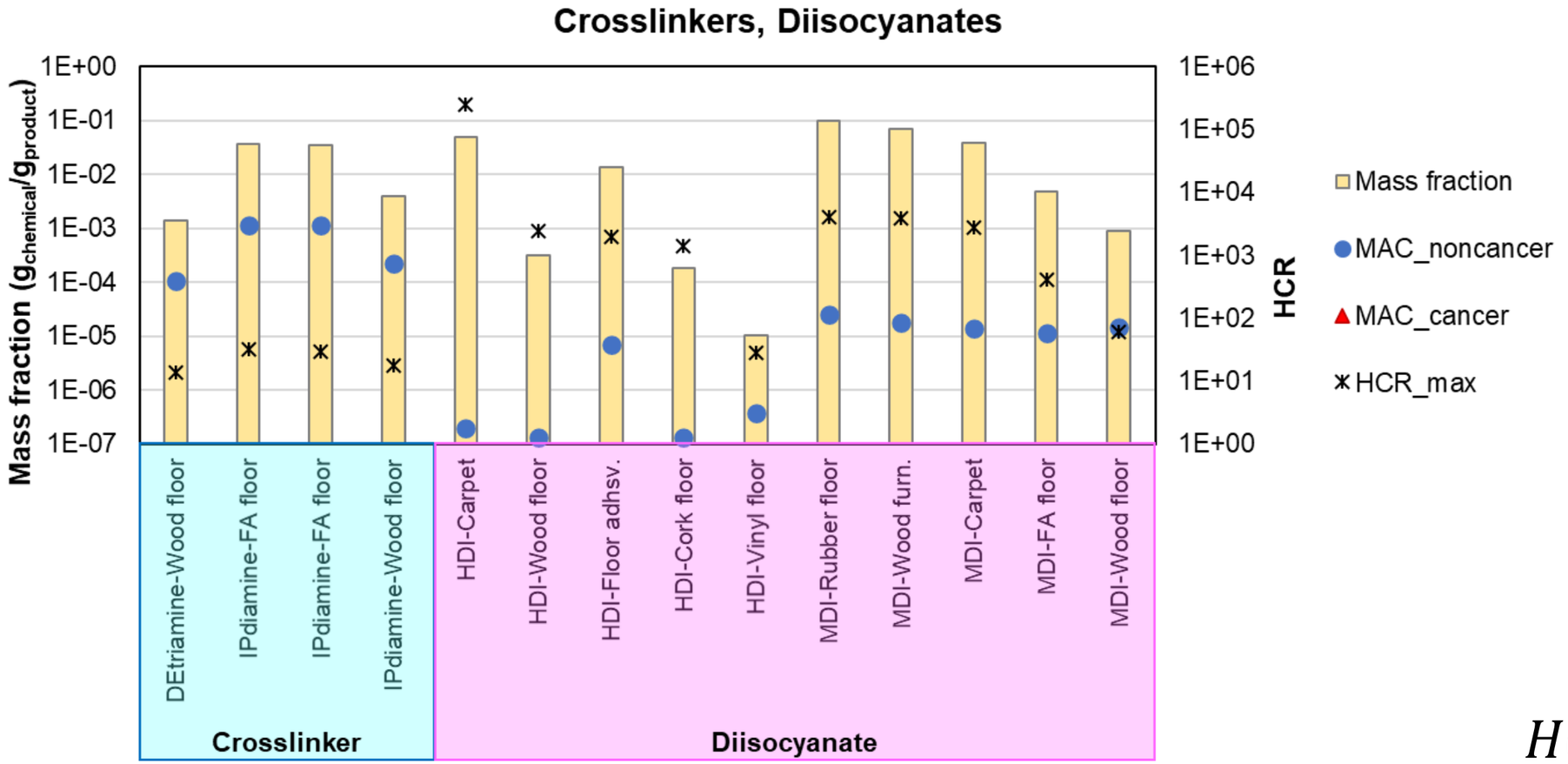


Consumer Exposure and Risk by Pathway





Identified Chemicals & Building Products of Concern



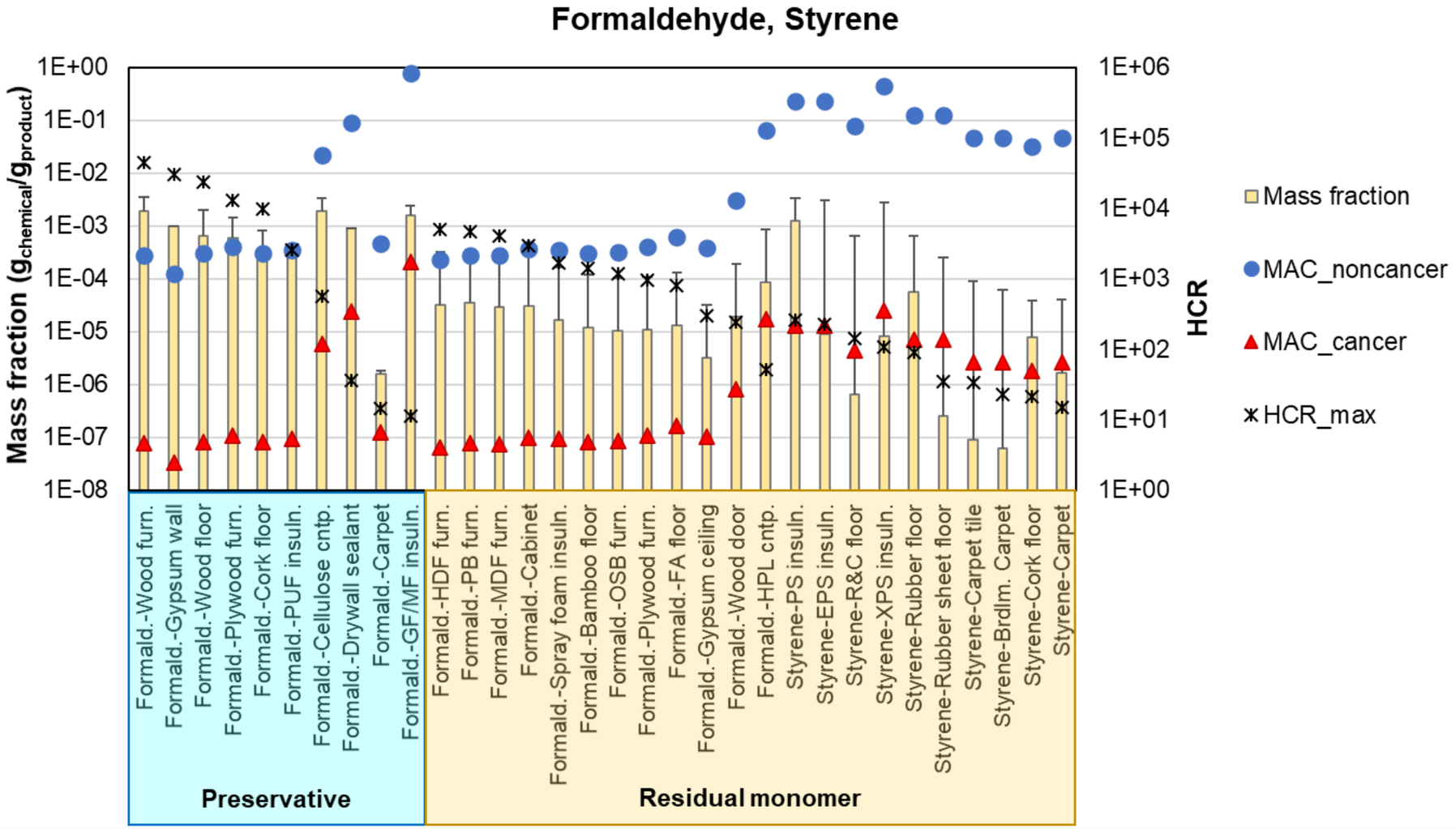
DEtriamine: diethylenetriamine. IPdiamine: isophorone diamine.

FA floor: fluid-applid flooring.

- HDI and MDI indicate great concern due to noncancer effects.
- HDI: 1,6-hexamethylene diisocyanate.
- MDI: 4,4’-methylene bisphenyl diisocyanate

$$HCR = \frac{Actual\ content}{MAC_{HTS}}$$

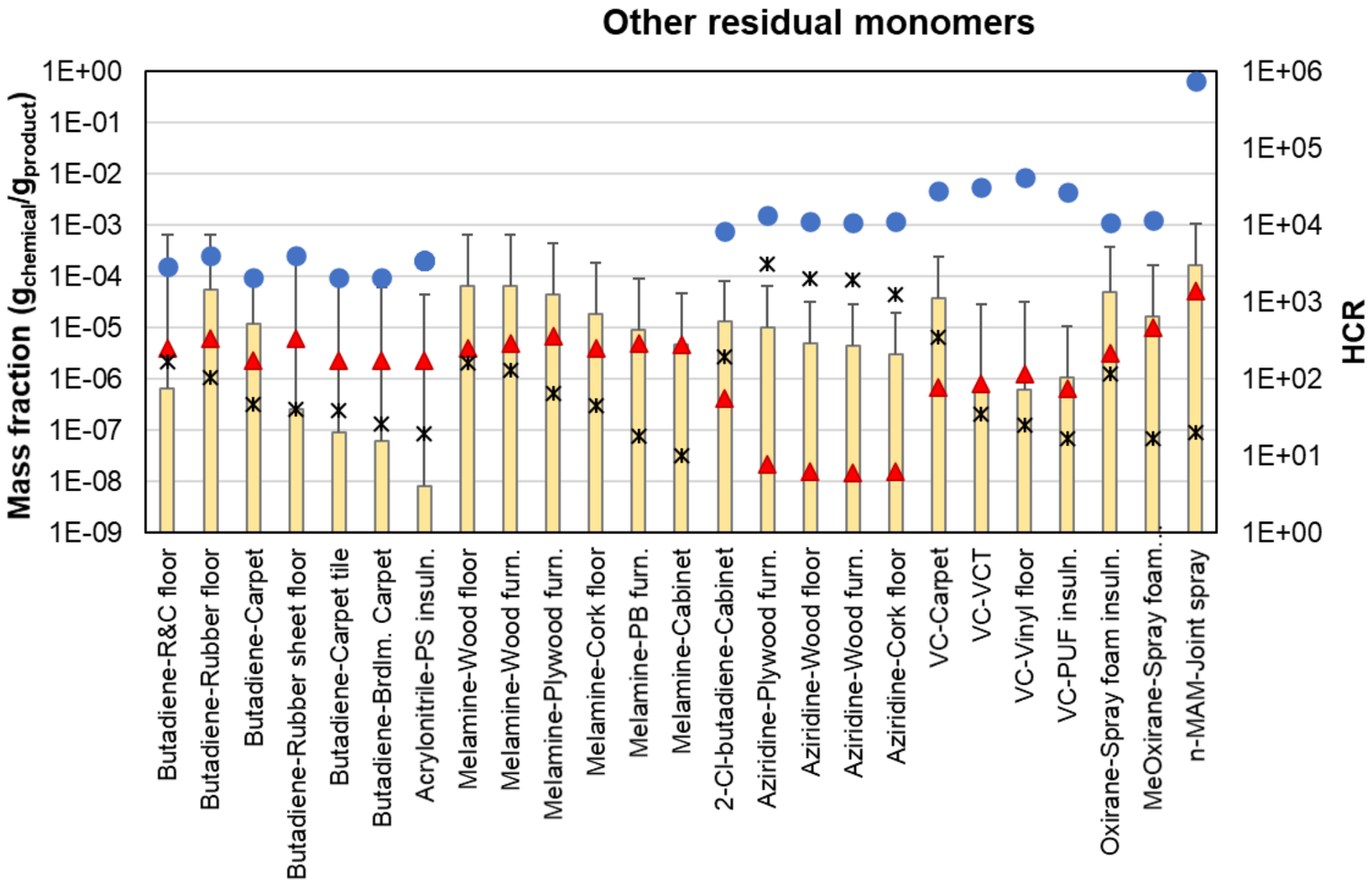
Identified Chemicals & Building Products of Concern



- Formaldehyde with HCRs up to 52,000, all based on cancer effects.
- Usage of formaldehyde-containing resins may need to be completely avoided.
- Formaldehyde as biocide may be replaced by thiabendazole, CIT, etc.

Insuln: insulation. Cntp: countertop.

Identified Chemicals & Building Products of Concern

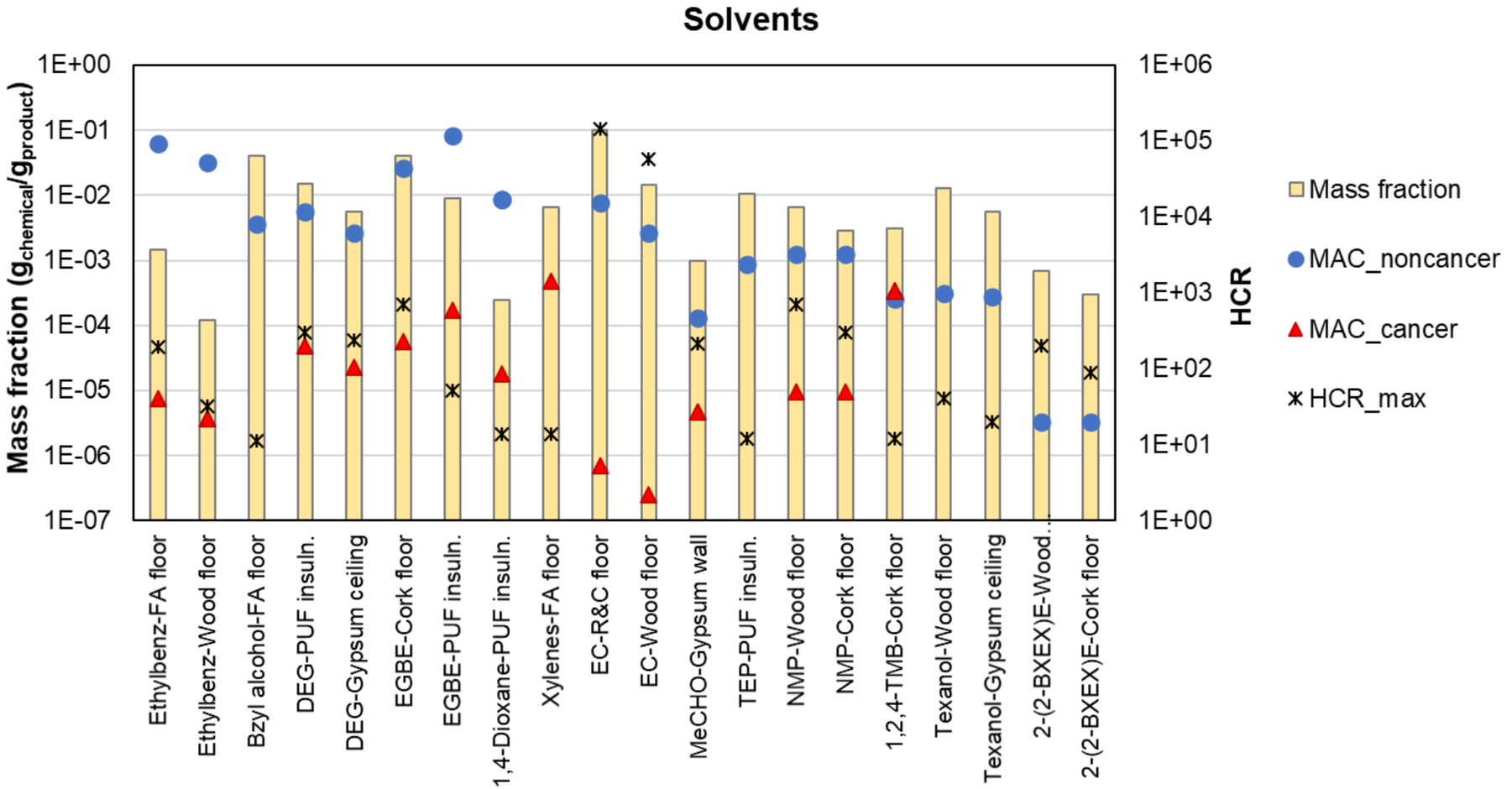


- Aziridine
- Vinyl chloride
- 2-Chloro-1,3-butadiene
- 7 others

Butadiene: 1,3-butadiene. 2-Cl-butadiene: 2-chloro-1,3-butadiene. VC: vinyl chloride.

MeOxirane: 2-methyloxirane. n-MAM: n-methylol acrylamide.

Identified Chemicals & Building Products of Concern



- Ethyl carbamate (EC) with extremely high HCR of 58,000 to 140,000 based on cancer effects.

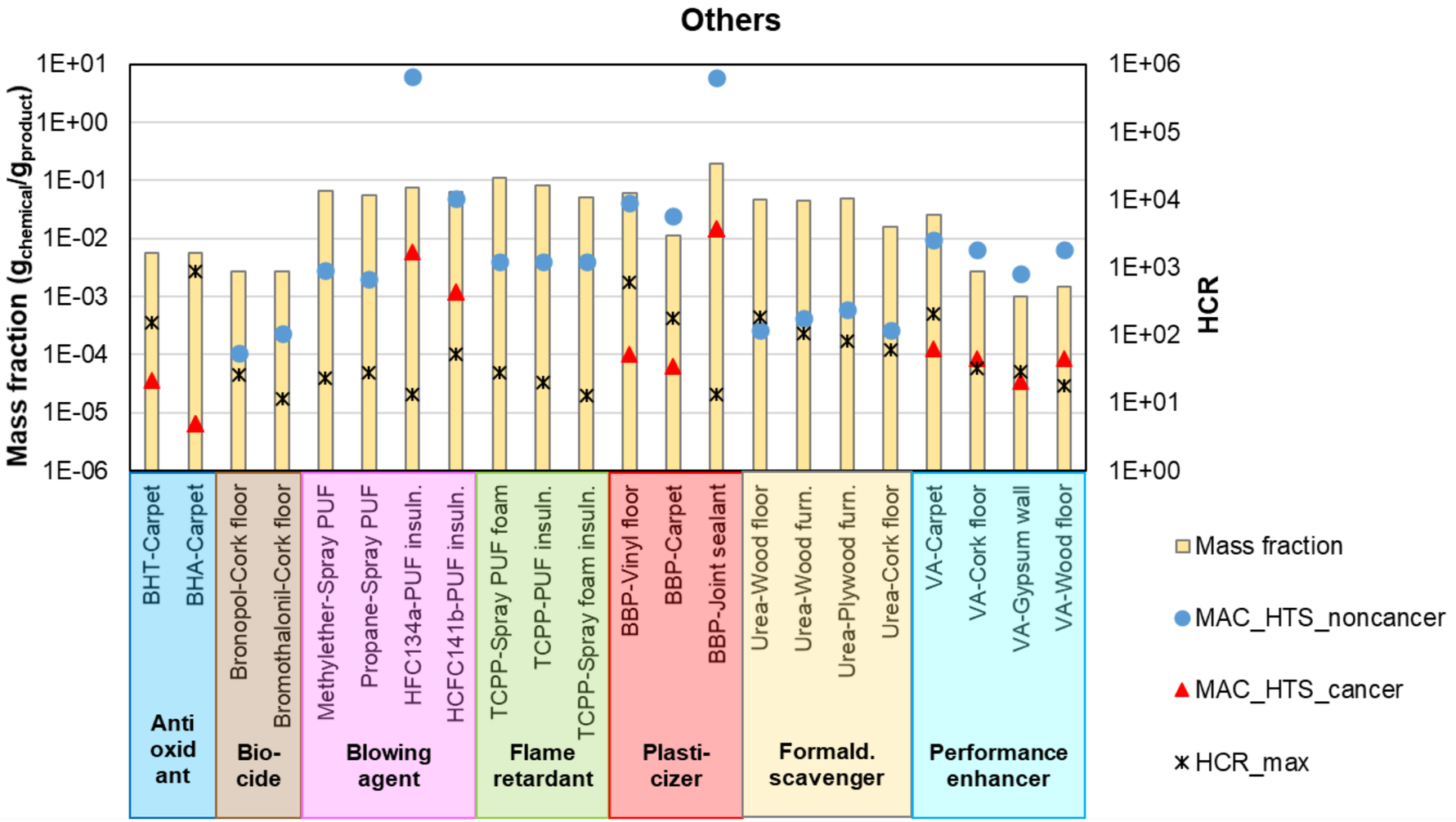
Ethylbenz: ethylbenzene. Bzyl alcohol: benzyl alcohol. DEG: diethylene glycol.

EGBE: Ethylene glycol monobutyl ether. EC: ethyl carbamate. MeCHO: acetaldehyde.

TEP: triethyl phosphate. NMP: N-Methylpyrrolidone. 1,2,4-TMB: 1,2,4-trimethylbenzene.

2-(2-BXEX)E: 2-(2-butoxyethoxy)ethanol.

Identified Chemicals & Building Products of Concern



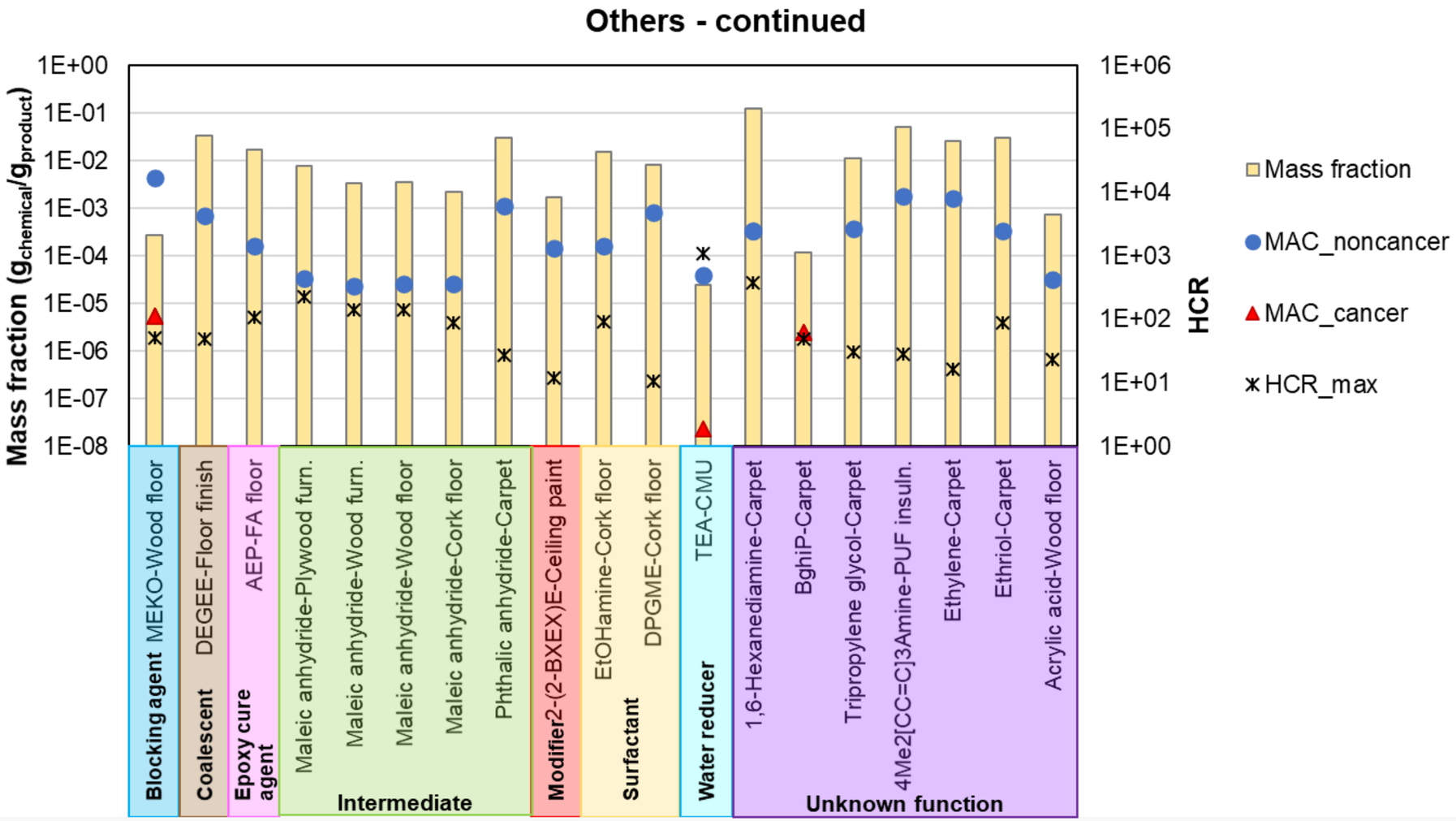
- Only one phthalate plasticizer BBP is identified as CoC.
- Only one flame retardant, tris(1-chloro-2-propyl)phosphate (TCPP) is identified as CoC.

BHT: Butylated hydroxytoluene. BHA: butylated hydroxyanisole.

TCPP: Tris(1-chloro-2-propyl)phosphate. BBP: Butyl benzyl phthalate.

VA: vinyl acetate.

Identified Chemicals & Building Products of Concern



MEKO: methyl ethyl ketoxime. DEGEE: diethylene glycol monoethyl ether. AEP: Aminoethylpiperazine. Ethriol: 1,1,1-tri(hydroxymethyl)propane.

2-(2-BXEX)E: 2-(2-butoxyethoxy)ethanol. EtOHamine: ethanolamine. DPGME: dipropylene glycol monomethyl ether.

TEA: triethanolamine. BghiP: benzo[g,h,i]perylene.4Me2[CC=C]3Amine: tetramethyldipropylenetriamine.

Summary – Building materials interface

- USEtox enables us to assess thousands of chemicals in 100+ different types building materials
- It combines far-field and near-field exposures, accounting for multiple exposure pathways
- Exposure in the near-field environment are usually dominant, but environmental exposures can remain high for persistent and bio-accumulating chemicals
- Enables both a risk and a damage-oriented approach
- The building material interface enables us to easily inputs new products and perform batch mode calculations

USEtox applied to assess chemicals in indoor paints

USEtox paint interface – chemical selection

	A	B	C	D	E	F
1	If you want to modify other cells than the unlocked green cells or navigate freely, please use the "review, unprotect sheet" excel command					
2		***ASSESSMENT OF CHEMICAL IN INTERIOR PAINTS***				
3		*Fill in the green highlighted cells as input data - other data are automatically calculated*				
4		***CHEMICAL SELECTION and CONTENT***		Unit	Data	Comment
5		**CAS RN**			50-00-0	Give the chemical CAS number to sel
6		**Row Number in Substance data**			34	Row number in the substance data lis
7		**Chemical name**			Formaldehyde	Chemical name
8		**Chemical mass fraction in product**		[$kg_{chemical}/kg_{product}$]	7.50E-05	This is the mass fraction of the chemi

	A	B	C
182			
183		Available chemicals	
184			
185		1002-53-5	DIBUTYLTIN
186		100-37-8	N,N-Diethylethanolamine
187		100-40-3	4-Vinylcyclohexene
188		100-41-4	Ethylbenzene
189		100-42-5	Styrene
190		100-45-8	3-Cyclohexene-1-carbonitrile
191		100-51-6	Benzyl alcohol
192		100-52-7	Benzaldehyde
193		1008-80-6	NAPHTHALENE, DECAHYDRO-2,3-DIMETHYL-
194		100-97-0	Methenamine
195		101-39-3	2-Propenal, 2-methyl-3-phenyl-
196		1014-60-4	BENZENE, 1,3-BIS(1,1-DIMETHYLETHYL)-
197		101-67-7	Benzenamine, 4-octyl-N-(4-octylphenyl)-
198		101-68-8	4,4'-Diphenylmethane diisocyanate

Give the chemical CAS number to select the chemical in the list below (row 184 onwards)

Give the mass fraction of the chemical in the toy

USEtox paint interface – Product characteristics and usage

PRODUCT CHARACTERISTICS	Unit	Data	Comment
Product Mass	kg	4.77E+00	Mass of paint applied
Density	kg/m^3	1.25E+03	Density of the paint
Product area	m^2	42	Area that is painted, typically 42 m2 pe
Initial liquid thickness	m	9.09E-05	Liquid thickness when the paint is fres
Material type for Dm	-	Synthetic rubber	Select the paint main matrix, or closes
Material type for Kma	-	Latex and solvent-based paint	Select the paint main matrix, or "gener
Material type for Kmw	-	Generic	Select the paint main matrix, or "gener
Solid fraction of paint	-	0.80	Fraction of mass remaining when pair
Average liquid thickness	m	8.18E-05	Calculated as average between intial t
Solvent system of the paint	-	water	Main solvent of the paint. "dry" means p
Solvent chemical CAS RN	-	7732-18-5	CAS number of the main solvent
Viscosity of paint	centipoise	4	Viscosity of the paint, not the pure sol

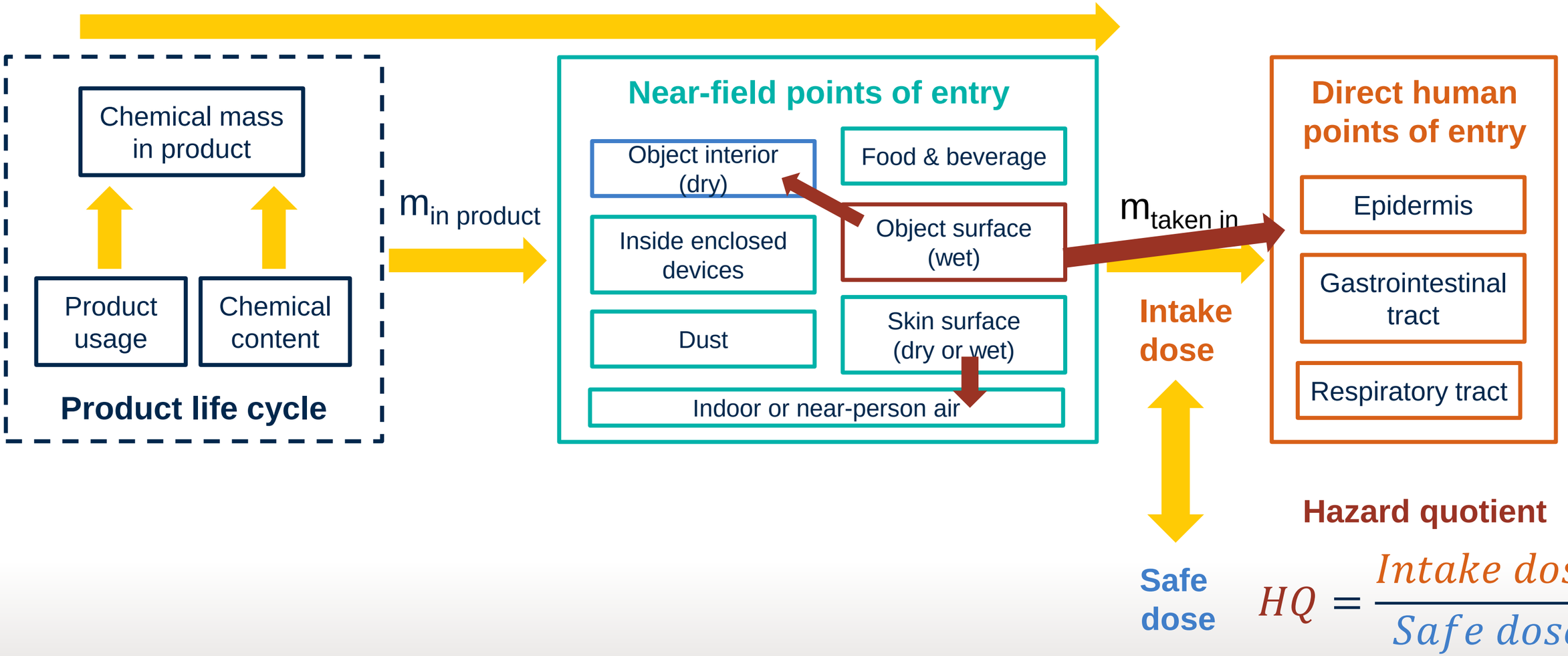
USAGE DATA	Unit	Data	Comment
Use duration of the finished paint	d	1	Exposure, risks and impacts are calculated as average over use duration
Dermal contact area	-	hands one-sided	Select the part of the body in direct contact with the painted area
Dermal contact area_adult	m^2	4.90E-02	
Dermal contact frequency_adult	min/min	0	Fraction of the day an adult might touch the painted area
Fraction of ingested dust for adults	-	0.00E+00	
Dermal contact area_child	m^2	1.40E-02	
Dermal contact frequency_child	min/min	0.00E+00	Fraction of the entire day a child might touch the painted area
Fraction of ingested dust for children	-	0.00E+00	
Total time touching different objects, both hands	min/hr	9.91E+01	
Fraction of time at home_adult	-	0.644	Will be used to adjust exposures
Fraction of time at home_child	-	0.772	Will be used to adjust exposures
Relative humidity indoors	%	70	

USEtox paint interface – Indoor exposure

INDOOR EXPOSURE			
HomeName		Non-OECD countries average (airtight building) 2+1 household	
OccupationName		Industry, non-OECD	
User scenario		adult	
Temperature for product use	°C	25	Indoor temperature

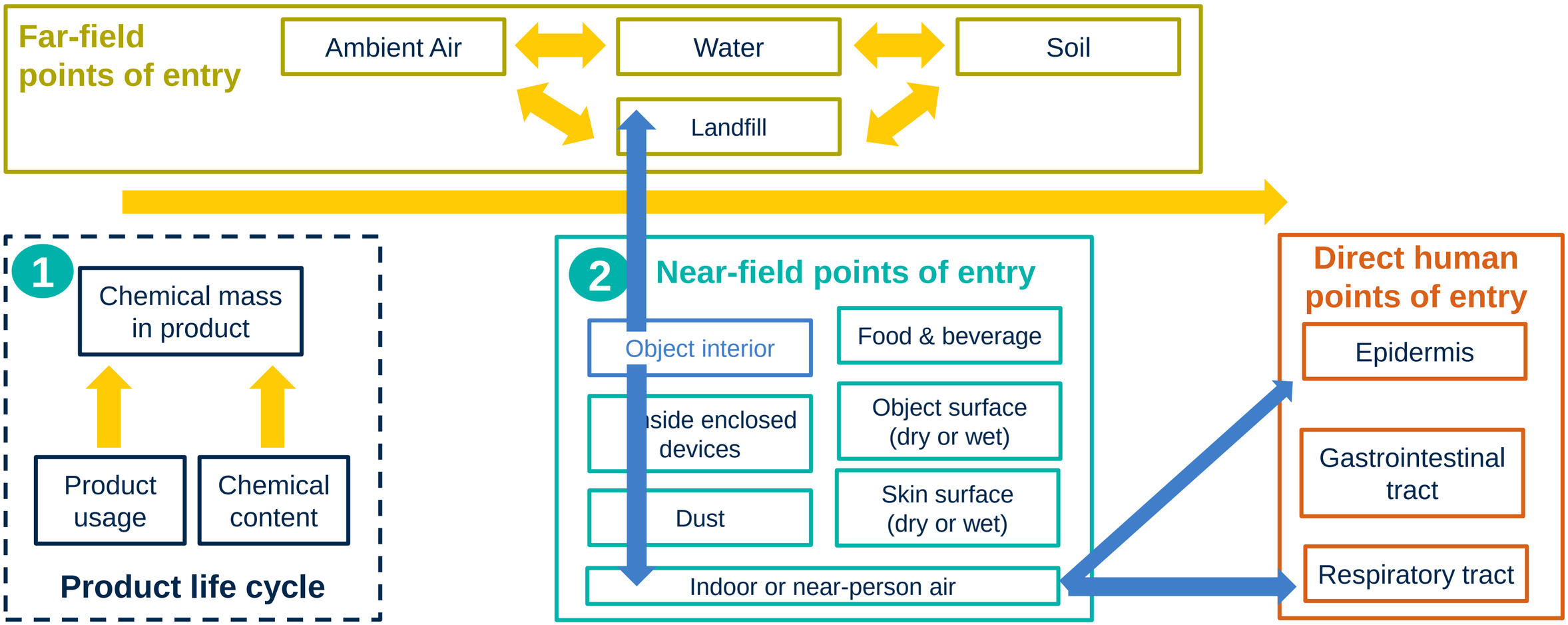
Near field consumer exposure to chemicals in wet paint

Product intake fraction: $PiF = \frac{m_{taken\ in}}{m_{in\ product}}$



Fantke et al. 2018. Environ Health Perspect 126: 125001

Near field bystander exposure to chemicals in dry paint



Fantke et al. 2018. Environ Health Perspect 126: 125001

0.20 kg DEHP/kg toy

0.2 kg toy

Volatilization 0.19%

→ Inhalation child 0.8 ppm

→ Gaseous dermal 0.08 ppm

$$I_{dust\ ingestion} = PiF_{i,p}^{tot} \cdot m_{i,p}$$

$$= 1.8\% \cdot 0.04\ kg = 0.00072\ \text{kg}$$

Results – Product and user characteristics , transfer fractions & exposures

Supporting intermediary data

Mass balance
Direct transfer fractions
[$kg_{to\ compartment}/kg_{inventory\ mass}$]

to:	From paint
indoor air	1.00E+00
dust.userA	0
dir.derm.userA	1.16E-08
dust.householdC	0
dir.derm.householdC	0
Left in dried paint	0
Total	1.00E+00

Exposure
Product intake fractions
[$kg_{intake}/kg_{inventory\ mass}$]

to:	From paint
total.inhal.userA	3.39E-03
total.ing.userA	0
total.derm.userA	2.22E-05
total.intake.userA	3.41E-03
total.inhal.householdC	1.15E-03
total.ing.householdC	0
total.derm.householdC	4.13E-06
total.intake.householdC	1.16E-03
Acceptable range	

Exposure and risk results Summary

User characteristics

User Adult	1
Body weight BW [kg_{body}/person]	70
Household Child	1
Body weight BW [kg_{body}/person]	13.8
Use duration [d]	1

Product characteristics

Product mass [kg]	4.77E+00
Weight fraction wf [$kg_{chemical}/kg_{product}$]	7.50E-05
Chemical inventory mass [$kg_{chemical}$/toy]	3.58E-04

Exposure
Average daily dose
D_{child}
[$mg/kg_{body}/d$]

to:	
total.inhal.userA	1.73E-02
total.ing.userA	0
total.derm.userA	1.13E-04
total.intake.userA	1.74E-02
total.inhal.householdC	2.99E-02
total.ing.householdC	0
total.derm.householdC	1.07E-04
total.intake.householdC	3.00E-02
Hazard Content Ratio_adult	

Relative risks and maximum chemical content

to:	Cancer toxicity Cancer slope factor CSF [(mg/kg$_{bodyw}$/d)$^{-1}$]	Non cancer safe dose Reference Dose RfD [mg/kg$_{bodyw}$/d]
total.inhal.userA	1.90E+00	2.24E-03
total.ing.userA	3.68E-03	2.00E-01
total.derm.userA	3.68E-03	2.00E-01
total.intake.userA	-	-
total.inhal.householdC	7.60E+00	6.32E-03
total.ing.householdC	1.47E-02	2.00E-01
total.derm.householdC	1.47E-02	2.00E-01
total.intake.householdC	-	-
Acceptable range	<10^{-4} to 10^{-6}	<1

to:	Cancer risk Incremental lifetime risk ILCR [-]	Non cancer characterization Hazard quotient HQ [-]	Hazard Content Ratio How many time is wf too high to reach target HCR=wf/MAC [-]	Maximum Chemical Content Max content not to exceed Cancer Risk and HQ targets MAC [mg$_{chemical}$/mg$_{product}$]
total.inhal.userA	3.29E-02	7.74E+00		
total.ing.userA	0	0		
total.derm.userA	4.16E-07	5.66E-04		
total.intake.userA	3.29E-02	7.74E+00		
total.inhal.householdC	4.54E-02	4.73E+00		
total.ing.householdC	0	0		
total.derm.householdC	3.15E-07	5.35E-04		
total.intake.householdC	4.54E-02	4.73E+00		
Hazard Content Ratio_adult	3.29E+04	7.74E+00	3.29E+04	2.28E-09
Hazard Content Ratio_child	4.54E+04	4.73E+00	4.54E+04	1.65E-09
Target for MAC	1E-06	1		

Chemicals in paints: Cumulative intake and impacts

Cumulative impact results

	Cancer damage [DALY/paint application]	Non cancer damage [DALY/paint application]	Total damage [DALY/paint application]	Damage per person-d [µDALY/person-d]	Damage per person-d [min. lost/person-d]
User adult	1.48E-05	2.79E-08	1.48E-05	1.20E+01	6.32E+00
Household adult	9.05E-06	1.71E-08	9.06E-06	7.35E+00	3.87E+00
Household child	5.03E-06	9.46E-09	5.04E-06	4.09E+00	2.15E+00
Population	7.50E-08	1.42E-10	7.52E-08	6.11E-11	3.21E-11
Total	5.11E-06	9.61E-09	5.12E-06	-	-

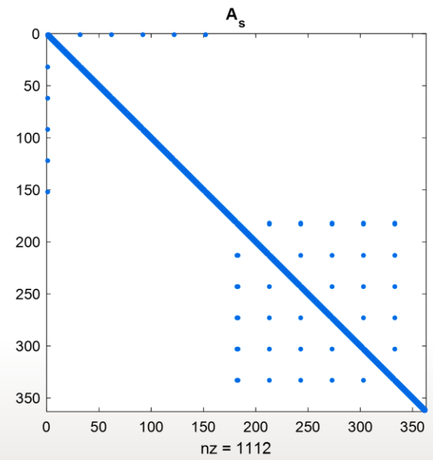
MATERIAL & METHOD: Modelling energy and mass conservation

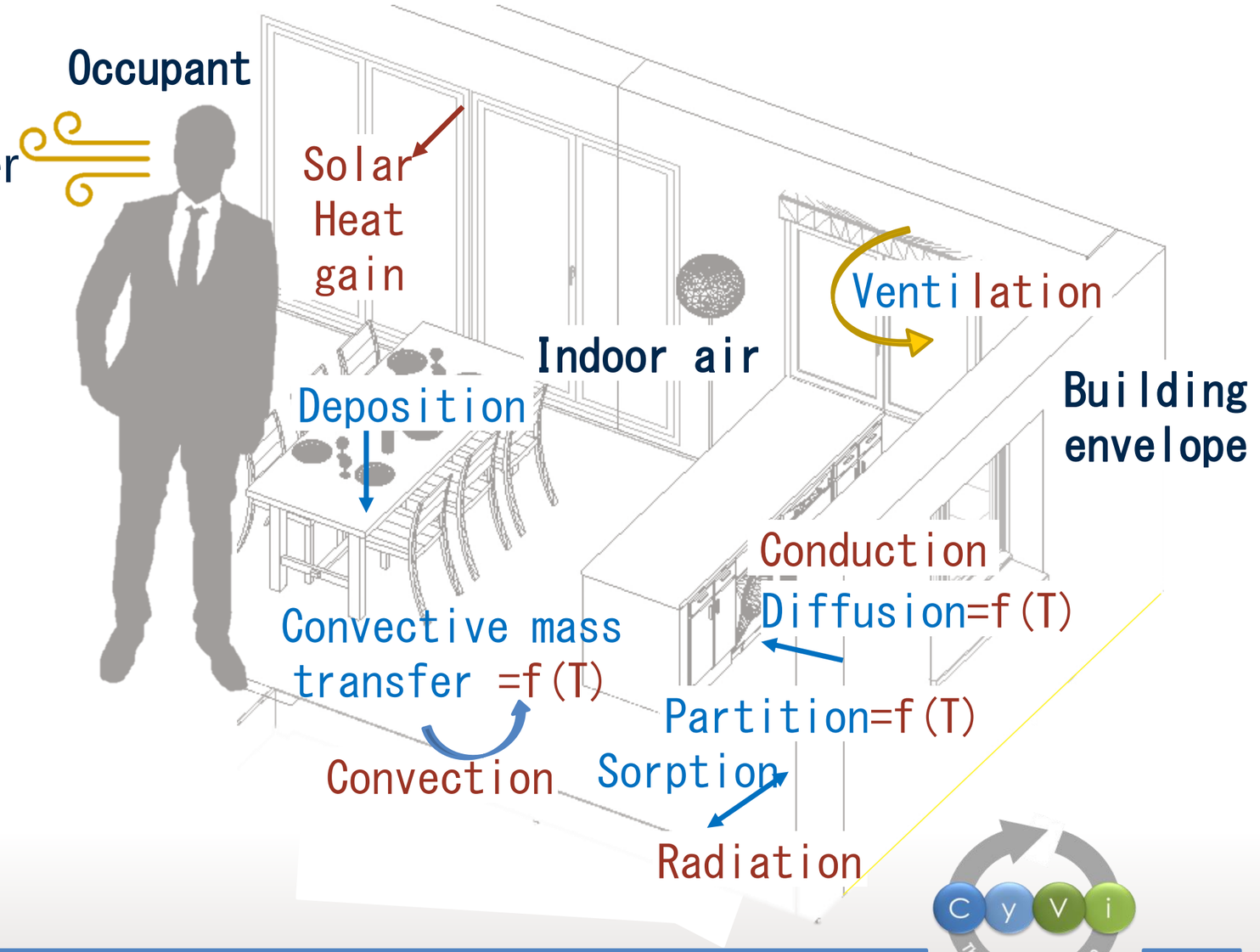
System of 2N coupled ordinary differential equations, with N the number of nodes in the building envelope

$$\begin{bmatrix} \frac{dC_i}{dt} \\ \cdots \\ \frac{dT_i}{dt} \end{bmatrix} = A_s \begin{bmatrix} C_i \\ \cdots \\ T_i \end{bmatrix} + B_s$$

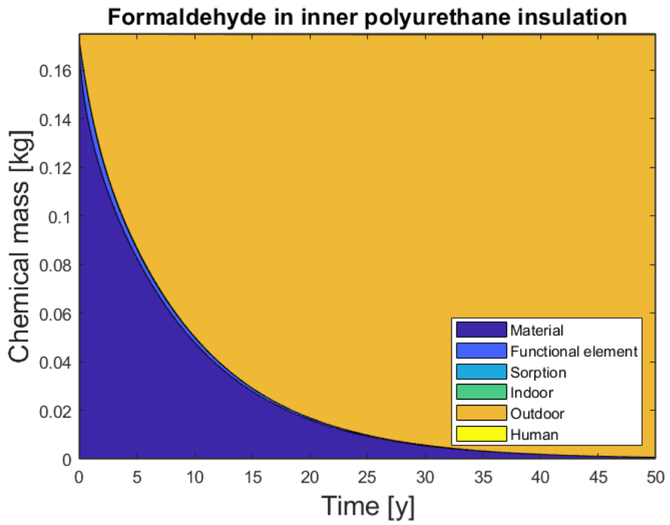
Mass transfer

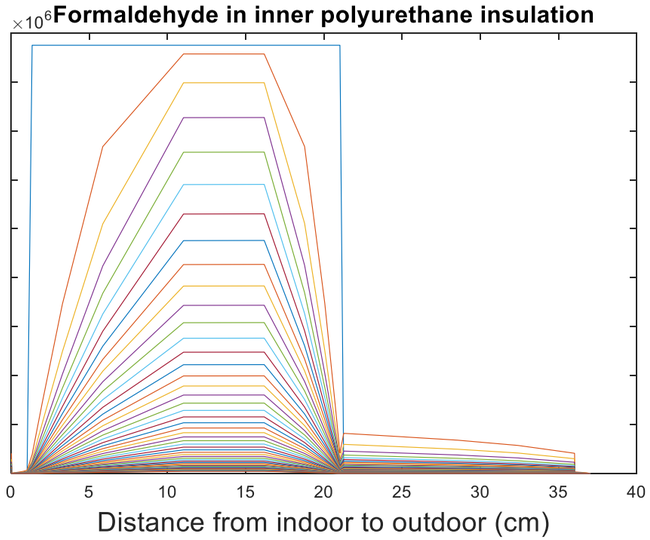
Heat transfer

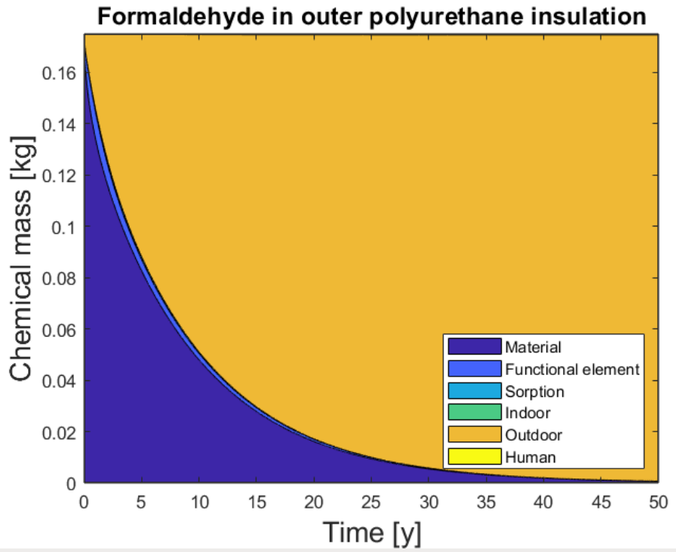


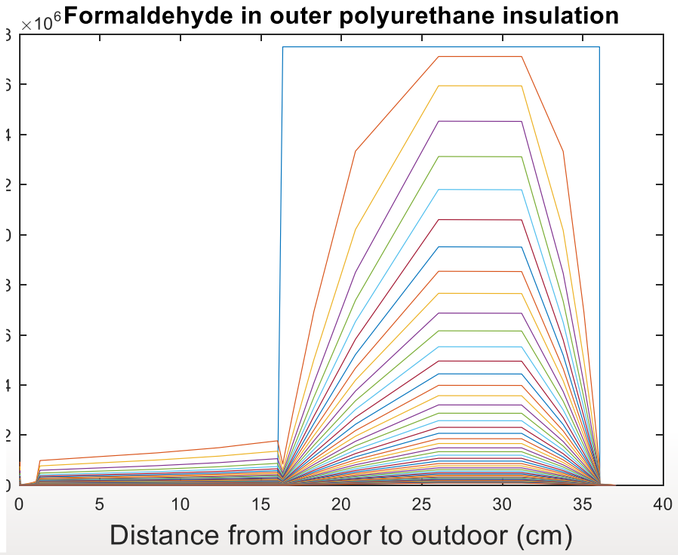


Results: What matters for indoor exposure?
Surprisingly, not the position of the insulation inner/outer for VOCs









100% emitted after 50years for every insulation system

Inner insulation:

PiF = 0.20%

Human health damage= 0.0041 DALY

Outer insulation:

PiF = 0.20%

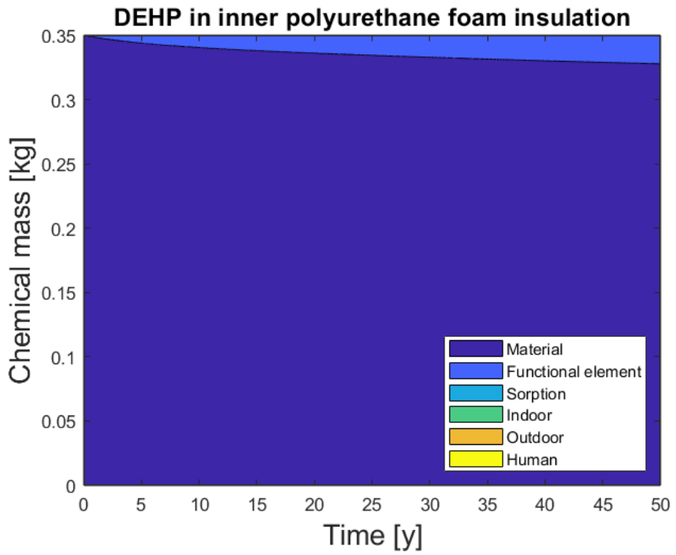
Human health damage= 0.0041 DALY

Outer insulation, 30cm-concrete:

PiF = 0.20%

Human health damage= 0.0041 DALY

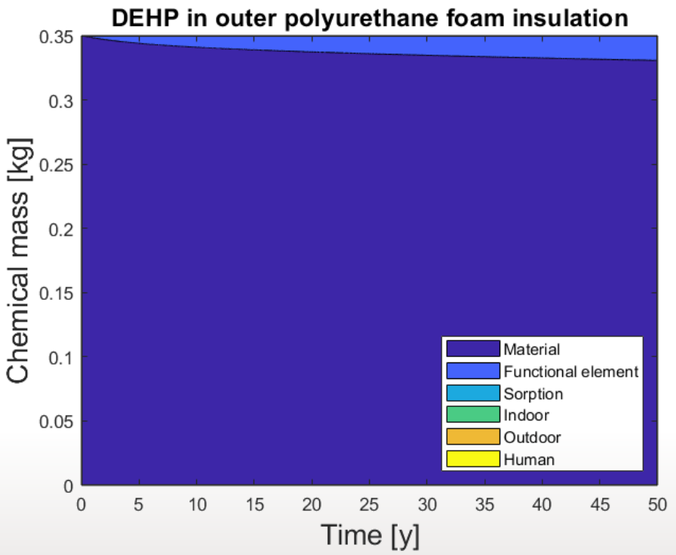
RESULTS: WHAT MATTERS FOR INDOOR EXPOSURE?
Large influence of insulation position for SVOCs such as DEHP!



Inner insulation:

PiF = $3.86e^{-7}$ $kg_{intake}/kg_{initial}$

Human health damage= $8.8e^{-7}$ DALY



Outer insulation:

PiF = $9.91e^{-10}$ $kg_{intake}/kg_{initial}$

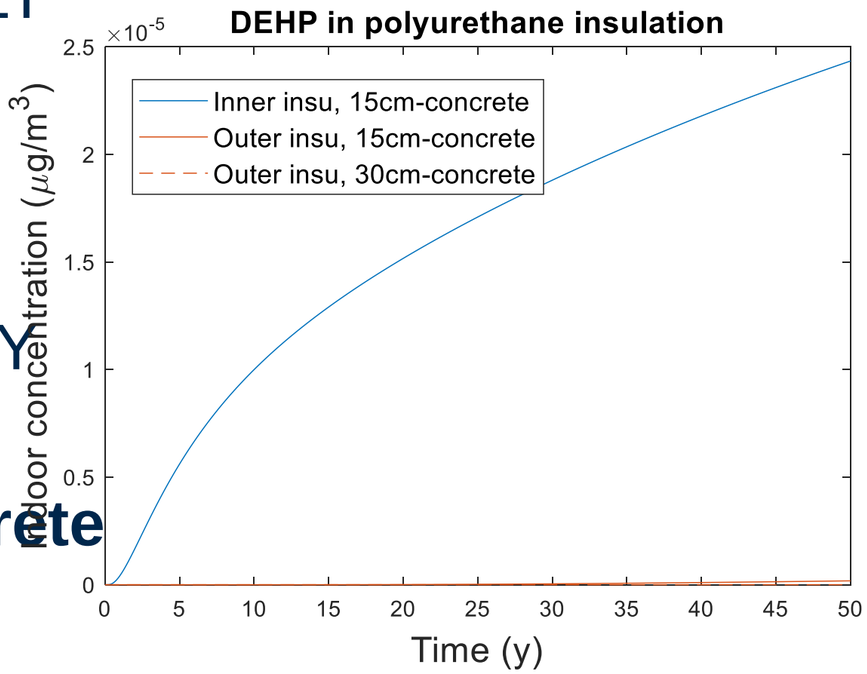
Human health damage= $1.3e^{-9}$ DALY

Outer insulation with 30cm-concrete

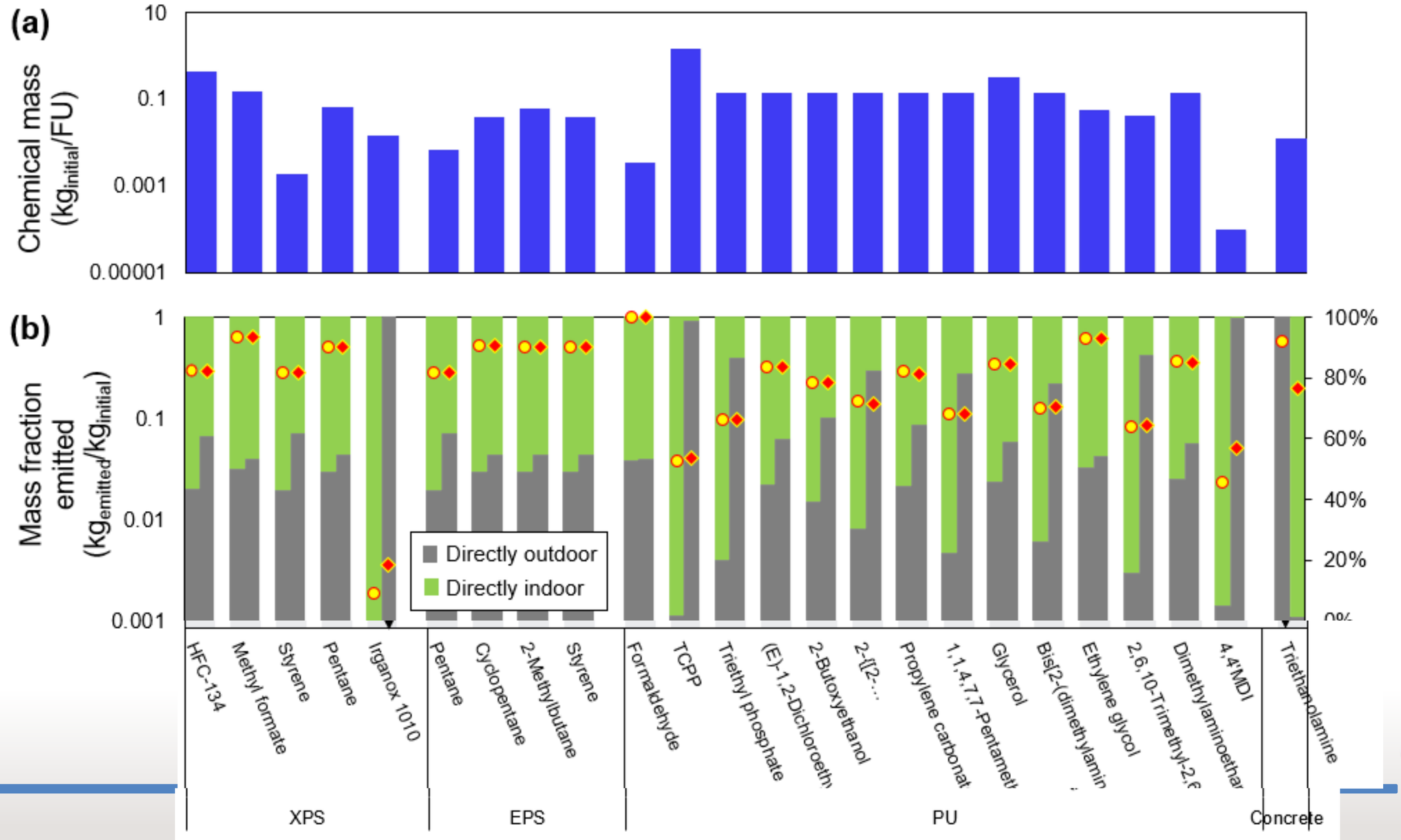
PiF = $9.40e^{-12}$ $kg_{intake}/kg_{initial}$

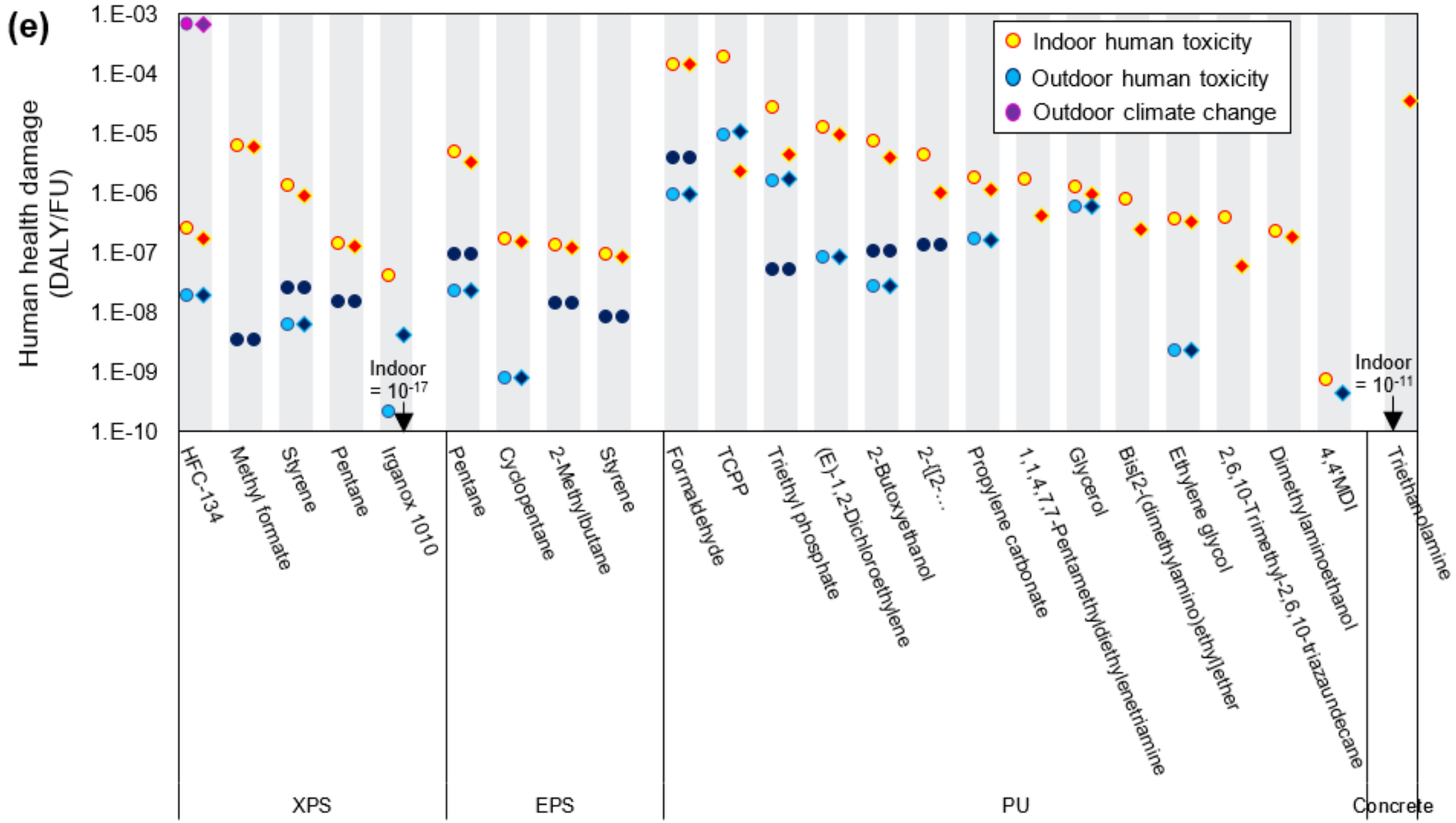
Human health damage= $7.0e^{-14}$ DALY

0.01%, 0.04% and 0.04% emitted after 50years for inner and outer insulation respectively



(a) Initial chemicals mass/m2 of three insulations and mass fraction emitted directly indoor (green) and directly outdoor (grey) for inner (circle) & outer (diamond) insulation




(e)
Human health damage (DALY/FU)
1.E-03
1.E-04
1.E-05
1.E-06
1.E-07
1.E-08
1.E-09
1.E-10
Indoor human toxicity
Outdoor human toxicity
Outdoor climate change
Indoor = 10-17
Indoor = 10-11
HFC-134
Methyl formate
Styrene
Pentane
Irganox 1010
Pentane
Cyclopentane
2-Methylbutane
Styrene
Formaldehyde
TCPP
Triethyl phosphate
(E)-1,2-Dichloroethylene
2-Butoxyethanol
2-[[2-...
Propylene carbonate
1,1,4,7,7-Pentamethyldiethylenetriamine
Glycerol
Bis[2-(dimethylamino)ethyl]ether
Ethylene glycol
2,6,10-Trimethyl-2,6,10-triazaundecane
Dimethylaminoethanol
4,4'MDI
Triethanolamine
XPS
EPS
PU
Concrete

Human health damage over the complete life cycle for 1 m2 of the inner (a) and outer (b) insulation thickness and of the air renewal rate without (c) and with (d) heat exchanger