Human health characterization factors of TiO_2 nanoparticles in indoor and outdoor environments

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Nano-TiO_2 properties

Self-cleaning coatings

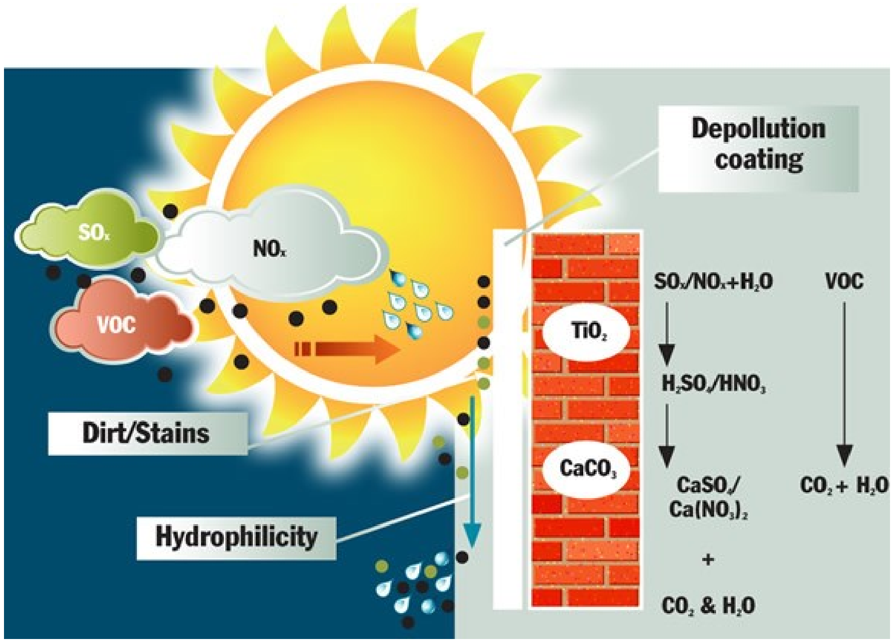


Photo-induced hydrophylic TiO_2 surface

Source: J. Chen, C.-sun Poon / Building and Environment 44 (2009) 1899–1906

Air depollution

Pollution removal mechanism of TiO_2 photocatalysis

Source: J. Chen, C.-sun Poon / Building and Environment 44 (2009) 1899–1906

Nanotoxicity assessment

- Uncertainties and knowledge gaps on behavior and toxicity of nanoparticles.

We cannot remain silent!!

- The LCA methodology can help to determine the potential impacts of nanoproducts and nanomaterials on human health and environment.

Pini M., Neri P., Ferrari A.M., **1° SEMINARIO TECNICO**, *Il contributo del dipartimento di scienze e metodi dell'ingegneria nello sviluppo del Life Cycle Assessment (LCA) per la gestione della sostenibilità ambientale* , Reggio Emilia, September 18, 2013

Pini M., Neri P., Montecchi R., Ferrari A.M., *"Life Cycle Assessment of nanoTiO_2 functionalized porcelainized stoneware tiles"*, **247th ACS National Meeting & Exposition**, Dallas, Texas, March 16-20, 2014

Collaboration

EMPA - Swiss Federal Laboratories for Materials Science and Technology, Technology and Society Laboratory, ERAM Group St. Gallen, Switzerland

EMPA
Materials Science & Technology

Conference

Pini M., Salieri B., Ferrari A.M., Nowack B. and Hischier R. (2014) Nanosafe 2014, November 18-20, 2014, Grenoble, France, "*Framework For Human Health Characterization Factor Calculation Of* TiO_2 *Nanoparticles*".

Pini M., Salieri B., Ferrari A.M., Nowack B. and Hischier R. (2014) XXV Congresso della Societa' Chimica Italiana, Rende (CS), September 11, 2014, *“Life Cycle Assessment of building nanomaterials: indoor and outdoor issues”*.

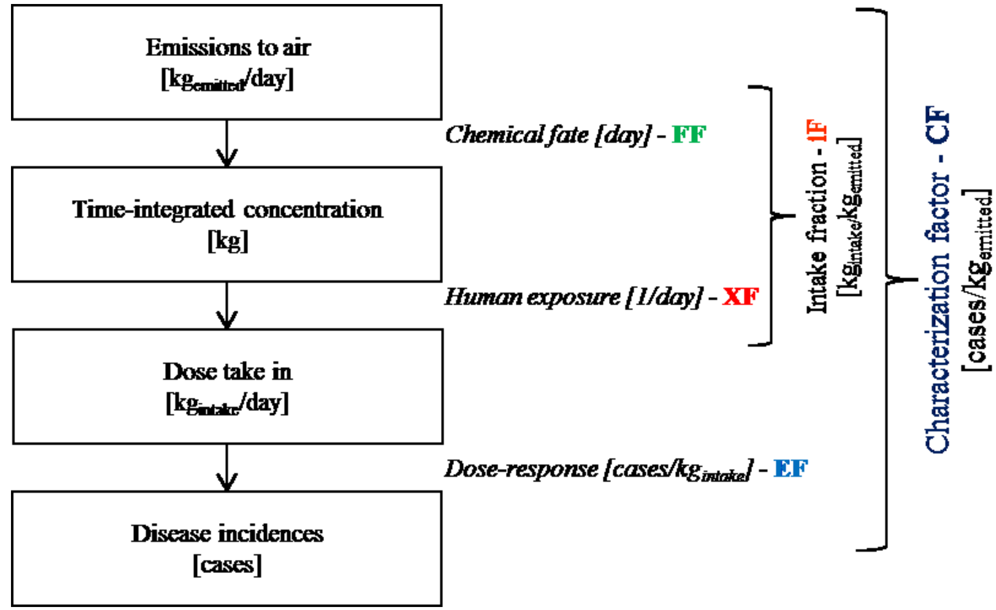
Publication

Pini M., Salieri B., Ferrari A.M., Nowack B. and Hischier R., " Human health characterization factors of TiO_2 nanoparticles in indoor and outdoor environments", International Journal of Life Cycle Assessment, Submitted.

USEtox^{TM} model (1)

CF is a quantitative representation of the *hazardousness* or *impact potential* related to the emission of pollutant.

CF can be estimated through three steps: *exposure*, *fate* and *effect*.

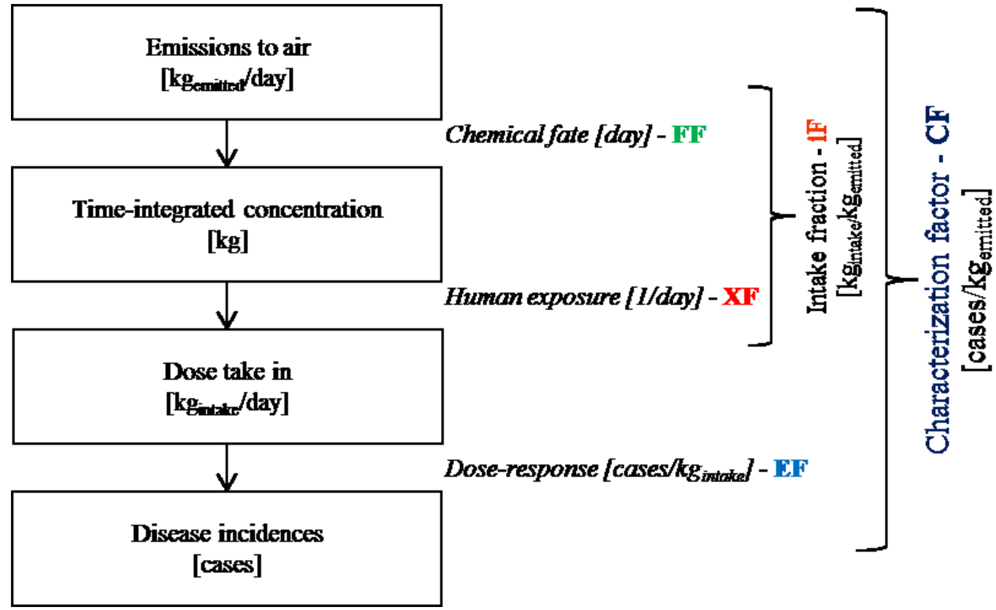


- CF = XF * FF * EF [cases/$kg_{emitted}$]
  - **XF** (Exposure Factor) *is the fraction of mass taken in by the population every day* [$Kg_{\_intake}$*day^{-1}*$Kg_{\_in\ compartment}^{-1}$]
  - **FF** (Fate Factor) *links the pollutant mass in a given compartment to the quantity released into any considered compartment. It accounts the multimedia transport between the environmental media (air, soil, water, run-off system, etc.)* [$Kg_{\_in\ compartment}$*$kg_{\_emitted}^{-1}$*day]
  - **EF** (Effect Factor) *relates the quantity taken in by the population (via inhalation) to the probability of adverse effects of the pollutant in human* [cases/$kg_{\_intake}$]

USEtox^{TM} model (2)

CF is a quantitative representation of the *hazardousness* or *impact potential* related to the emission of pollutant.

CF can be estimated through three steps: *exposure*, *fate* and *effect*.



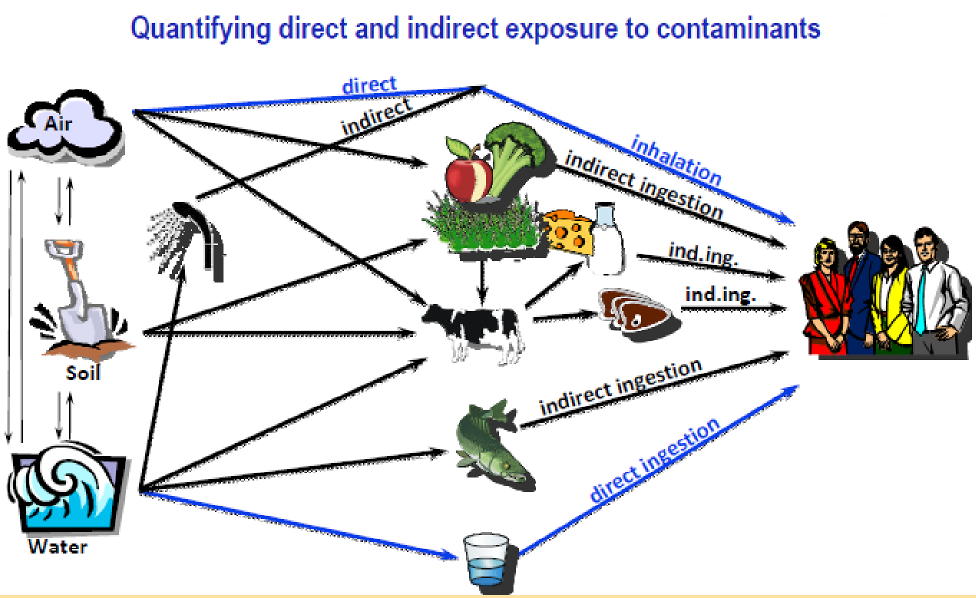
- CF = XF * FF * EF [cases/kg$_{emitted}$]

- iF = XF * FF [kg_$_{intake}$/kg_$_{emitted}$]

The fraction of an emission emitted into a compartment that is taken in by the exposed population through a given intake pathway.

Assumptions

- One-box model
- Steady state conditions
- Direct human exposure (e.g. inhalation of air, ingestion of water)
- Compartment: air



Indoor intake Fraction

$$iF = \frac{INH * POP}{V * m * k_{ex}}$$

Independent of the studied substance

- **INH** is the average human inhalation rate = **13 m^3*day^{-1}** *USEtox™*
- **POP** is the indoor exposed population (*occupational exposure*)
- **V** is the indoor volume
- **m** is the mixing factor (unitless) = **1** *Humbert et al., 2011*
- **k_{ex}** is the air exchange rate (h^{-1}) = **3 h^{-1}** *Humbert et al., 2011*

Outdoor intake Fraction

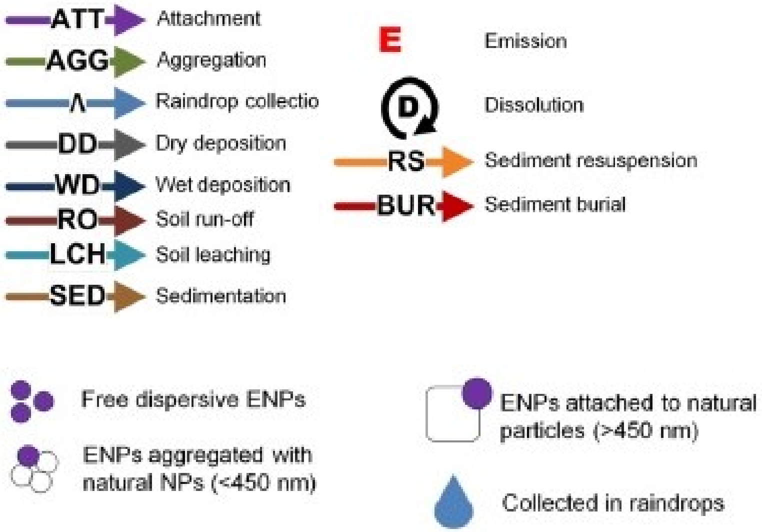
$$iF = \frac{INH * POP}{V} * \overline{FF}$$

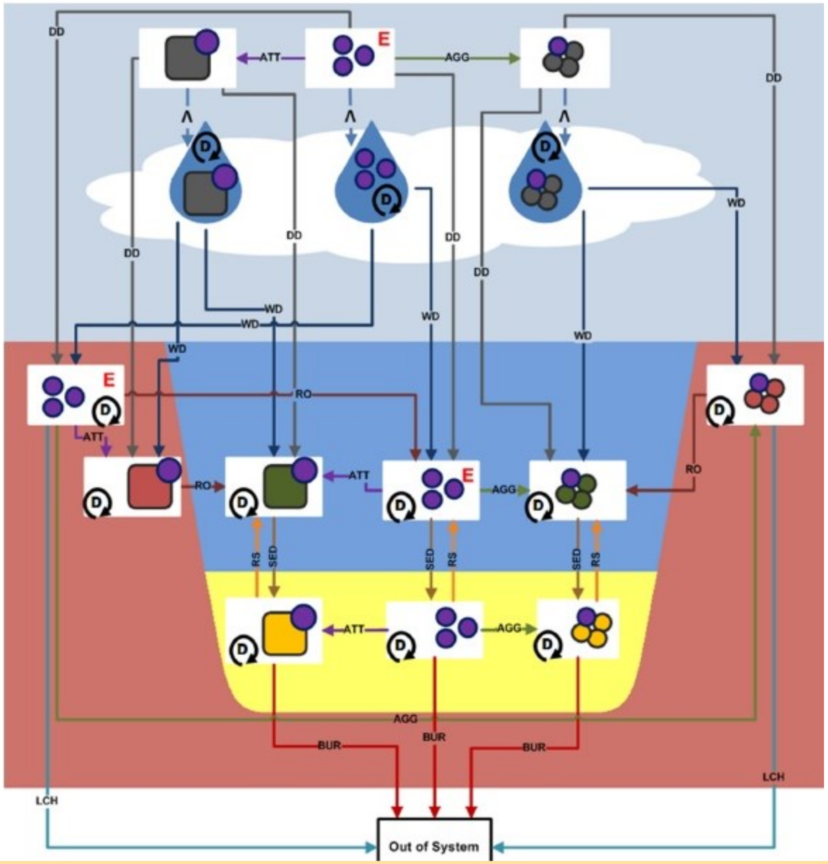
- **INH** is the average human inhalation rate = **13 m^3*day^{-1}**
- **POP** is the exposed population → Switzerland: 8112200 inhabitants
- **V** is the outdoor volume:
  - atmospheric height: 1 km. *ECB Technical Guidance Document on Risk Assessment, 2003*
  - area of Switzerland: 41285 km^2.
- $\overline{\boldsymbol{FF}} = -\overline{K}^{-1}$, where $\overline{K}$ is the rate coefficient matrix, which accounts transport and removal processes between the environmental media.

SimpleBoxModel4Nano (SB4N) assesses the ENPs transport and removal rates in and across air, rain, surface waters, soil, and sediment compartments.

Outdoor FF

One box model and Steady state conditions





Rate constant values for nano-TiO_2 calculated by SB4N

Meesters and co-author estimated the transport and removal processes for nano-TiO_2 considering the input parameters and systemic dimensions of *Mueller and Nowack, 2008* study.

Area, Height, Volume of Atmosphere, Soil and Water

TiO_2-NPs radius, TiO_2-NPs mass density, Aggregation and Attachement efficiency

Outdoor intake Fraction

System Matrix of the rate constants *for each compartment and physical-chemical form* $\bar{K}$ [day^{-1}]

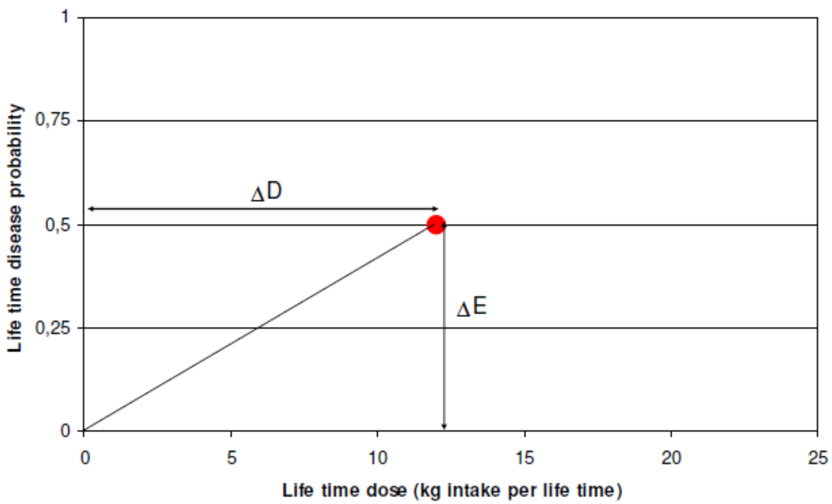
k [day^{-1}]	Free in atmosphere	Agg in atmosphere	Att in atmosphere	Free in rain	Agg in rain	Att in rain	Free in soil	Agg in soil	Att to soil	Free in water	Agg in water	Att in water	Free in sediment	Agg in sediment	Att in sediment
Free in atmosphere	-(ΣkrAfree)	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Agg in atmosphere	kaggA	-(ΣkrAagg)	0	0	0	0	0	0	0	0	0	0	0	0	0
Att in atmosphere	kattA	0	-(ΣkrAatt)	0	0	0	0	0	0	0	0	0	0	0	0
Free in rain	kΛARfree	0	0	-(ΣkrRfree)	0	0	0	0	0	0	0	0	0	0	0
Agg in rain	0	kΛARagg	0	0	-(ΣkrRagg)	0	0	0	0	0	0	0	0	0	0
Att in rain	0	0	kΛARatt	0	0	-(ΣkrRatt)	0	0	0	0	0	0	0	0	0
Free in soil	kdepASfree	0	0	kdepRSfree	0	0	-(ΣkrSfree)	0	0	0	0	0	0	0	0
Agg in soil	0	kdepASagg	0	0	kdepRSagg	0	kaggS	-(ΣkrSagg)	0	0	0	0	0	0	0
Att to soil	0	0	kdepASatt	0	0	kdepRSatt	kattS	0	-(ΣkrSatt)	0	0	0	0	0	0
Free in water	kdepAWfree	0	0	kdepRWfree	0	0	krunSWfree	0	0	-(ΣkrWfree)	0	0	krsSEWfree	0	0
Agg in water	0	kdepAWagg	0	0	kdepRWagg	0	0	krunSWagg	0	kaggW	-(ΣkrWagg)	0	0	krsSEWagg	0
Att in water	0	0	kdepAWatt	0	0	kdepRWatt	0	0	kerosionSWatt	kattW	0	-(ΣkrWatt)	0	0	krsSEWatt
Free in sediment	0	0	0	0	0	0	0	0	0	kdepWSEfree	0	0	-(ΣkrSEfree)	0	0
Agg in sediment	0	0	0	0	0	0	0	0	0	0	kdepWSEagg	0	kaggSE	-(ΣkrSEagg)	0
Att in sediment	0	0	0	0	0	0	0	0	0	0	0	kdepWSEatt	kattSE	0	-(ΣkrSEatt)

Matrices: $\overline{FF} = -\overline{K}^{-1}$

$\overline{iF} = \overline{XF} * \overline{FF}$

Effect Factor

1) The human-toxicological EF is calculated under the assumption of linearity in concentration–response up to the point in which the life time disease probability is 0.5.



2) $$EF = \frac{0.5}{ED_{50h}^{lifetime}} \ [\text{cases/kg}_{\text{intake}}]$$

3) $$ED_{50h}^{lifetime} = \frac{ED_{50}^{a,t,j} * BW * LT * N}{AF_a * AF_t}$$

Carcinogenic effects

$ED_{50}^{a,t,j}$ is the daily effect dose for animal *a*, time duration *t* and exposure route *j* that causes a disease probability of 50% [$mg*kg^{-1}*day^{-1}$].

AF_a = extrapolation factor for interspecies differences
AF_t = extrapolation factor for differences in time of exposure (2 for subchronic to chronic exposure and 5 for subacute to chronic exposure)
BW = body weight of humans
LT = average lifetime of humans; N = number of days per year

Non-carcinogenic effects

$ED_{50}^{a,t,j}$ can also be extrapolated from NOAEL (*no-observed adverse effect level*) and NOAEL from LOAEL (*low-observed adverse effect level*).

$ED_{50}^{a,t,j} = NOAEL^{a,t,j} * AF_N$ AF_N= 9 (Huijbregts et al., 2005)

$NOAEL^{a,t,j} = LOAEL^{a,t,j} / AF_L$ AF_L= 4 (Huijbregts et al., 2005)

Carcinogenic and Non-carcinogens effects (1)

Human Effects	References	Type of study and toxicity indicator	Toxicity value
Carcinogens	**NIOSH** National Institute for Occupational Safety and Health, 2011	• Sub-chronic oral study on rat. • Benchmark dose associated with a 4% inflammatory response= 0.0144 $m^2_{TiO_2}/g_{\text{rat-lung}}$.	$ED4^{rat,s\text{-}c,inh}$ 0.3 mg/kg-bw/day
Non-carcinogens	**SCCS** Scientific Committee on Consumer Safety, 2013	• Sub-chronic oral study on mice. • NOAEL.	$ED_{50}^{mice,s\text{-}c,inh}$ 62.5 mg/kg-bw/day

Carcinogenic and Non-carcinogens effects (2)

Indoor

- N = number of working days per year = 240 days/year (*European labour law, 99/70/EC*)
- LT = 45-years working lifetime (*NIOSH, 2011*)

Outdoor

- N = number of day per year = 365 days/year
- LT = average lifetime of humans = 70 years

Human health effect	INDOOR EF_i	OUTDOOR EF_o
Carcinogenic	1.45	6.11E-1
Non-carcinogenic	1.72E-2	7.26E-3

Characterization Factors nano-TiO_2

$$CF = iF * EF \ [cases/kg_{emitted}]$$

Indoor

Human Health effect	iF_i	EF_i	CF_i [cases/$kg_{emitted}$]
Carcinogenic ED_4	4.10E-04	1.45	**5.93E-04**
Non-carcinogenic NOAEL	4.10E-04	1.72E-2	**7.04E-06**

Outdoor

Human Health effect	iF_o	EF_o	CF_o [cases/$kg_{emitted}$]
Carcinogenic ED_4	2.53E-05	6.11E-1	**1.55E-05**
Non-carcinogenic NOAEL	2.53E-05	7.26E-3	**1.84E-07**

Humbert et al., 2009

Particular Matter

North America scenario

Indoor iF

Industry= 3.3E-5

Outdoor iF

Urban box= 6E-6

Humbert et al., 2011

PM 2.5 μm

Generic continent

Outdoor iF= 1.5E-5

Europe

Outdoor iF= 1E-5

Benzene	USEtox - CF - Outdoor
Cancinogenic	1.47E-02
Non-cancinogenic	3.72E-03

Characterization Factors nano-TiO_2

$$CF = iF * EF \ [DALY/kg_{emitted}]$$

Severity assessment → Endpoint Characterization Factors

Default damage severity factors of *11.5 DALY/cases(cancer)* and of *2.7 DALY/cases(non-cancer)* have been adopted (Huijbregts et al., 2005).

DALY = *Disability-adjusted life year is a measure of overall disease burden, expressed as the number of years lost due to ill-health, disability or early death.*

Indoor

Human Health effect	$CF_{S,i}$ [$DALY/kg_{emitted}$]
Carcinogenic ED_4	**6.82E-03**
Non-carcinogenic NOAEL	**1.90E-05**
Non-carcinogenic LOAEL	**9.51E-04**

Outdoor

Human Health effect	$CF_{S,o}$ [$DALY/kg_{emitted}$]
Carcinogenic ED_4	**1.78E-04**
Non-carcinogenic NOAEL	**4.96E-07**
Non-carcinogenic LOAEL	**2.48E-05**

Conclusions

- Human Health CFs of TiO_2 nanoparticles have been performed for both *indoor* and *outdoor* enviroments and *carcinogens* and *non-carcinogens* effects following USEtox^{TM} model.

- Challenge: ~~ED4~~ → ED50 ED4 ←→ ED50

- Indoor iF_i the FF_i could be improved including aggregation, attachment rates in indoor environment.

- Outdoor FF_o could be re-modeling for a wide geographic area using SB4N model.

Thank for your attention!

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