Mathematical model for the assessment of limit concentrations of 2,3,7,8-tetrachlorodibenzo-para-dioxin in the environment.

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It is known that both the risk assessment of 2,3,7,8-tetrachlorodibenzo-para-dioxin and related compounds and the determination of their acceptable levels in the air, water, soil and food are difficult problems. Therefore investigations on methods that allow to assess safety concentrations of dioxins are highly actual.

In the beginning of the 80-s Rosenblatt a.o.[1,2] had suggested PPLV ("Preliminary Pollutant Limit Values")-approach. It was one of the first perspective methods that could be used in the regulatory policy.

Based on the principles of PPLV-approach we had developed a mathematical model LIMES (LIMits EStimation). The main purpose of this model is to let to regulatory managers and agencies estimate acceptable levels of toxicants in the environment.

LIMES allows to estimate limit concentrations of a toxicant when the complex exposure from the environment takes place (it means: from several sources by several pathways simultaneously). A toxicant may present in the air, water, bottom and suspended sediments of water basins, soil, dust. If a toxicant may migrate on food-chains it is necessary to take into account the exposure from foods produced at the polluted locations and to estimate limits in fish, vegetables, fruit, root crops, potatoes, different kinds of meat (beef, pork, chicken-meat), eggs, milk and milk products (cheese, butter, and so on). LIMES allows to do it both in the case of complex exposure and in the case of isolated exposure (one source by one pathway or several pathways).

LIMES may to weight roles of the ways on which a toxic compound may intake into human organism: oral (foods, water, soil, dust), inhalated (vapours, aerosols, dust), percutaneous (vapours, aerosols, soil, water, dust).

The model analyses limit concentrations when toxicant' exposure may be occured by different pathways. There are many that pathways. In our last version there are 14 pathways in the case of water and 29 pathways in the case of soil. There is the possibility to select necessary complex of pathways.

The main element of the model is the determination of the correspondence between the allowable daily intake (ADI) of the toxicant and concentrations in the environment. That determination takes into account partition coefficients between different environmental objects and rates of human's uptake.

The assessment of ADI for non-carcinogenic chemicals is based on safety factors (for different experimental doses: LD_{50}, $NOEL_{90}$, NOEL).

For carcinogens we used the method suggested by Moolgavkar[3]. He had developed biologically based "two-stage" model of carcinogenesis. Some later his approach had been improved by Thorslund a.o.[4]. They had suggested some more simple formulae. On the basis of Thorslund' formulae we had developed the program CARIES (CArcinogenic RIsk EStimation) that is used as LIMES' subroutine to estimate ADI of carcinogens. CARIES uses data of carcinogenic animal experiments and allows to define the dose connected with concrete risk level.

In our estimates, the dose of 2,3,7,8-tetrachlorodibenzo-para-dioxin for risk level $1:10^6$ during the life (70 years) is 0.52 pg/kg of human body weight/day. (Assessment was based on Kociba's experiment[5]).

Then we estimated limit concentrations for different numbers of pathways, different rations, different values of physico-chemical parameters of dioxin. Two variants: first, when isolated exposure is occured, and second, when complex exposure is occured, are presented in the table.

For comparison we suggest the limit concentrations for the dose 10 pg/kg/day. The risk level that corresponds to this dose is $18:10^6$.

There are many different values of ADI and limit concentrations of 2,3,7,8-tetrachlorodibenzo-para-dioxin. These values depend on the methodical approaches to the risk assessment. Di Domenico gives the most detailed and motivated list of dioxins' limit concentrations[6]. Our estimated limit concentrations had shown a good correspondence with those described by him.

So LIMES may to estimate allowable concentrations:

a) both for carcinogenic and for non-carcinogenic chemicals;

b) for selected kind of exposure - isolated (from one source on one pathway) or complex (different number of sources and different number of pathways);

c) for concrete location;

d) for selected risk level.

We suppose that such approaches as LIMES may be very important in the regulatory context. There are no enough objective methods to assess limit concentrations especially for complex exposure. In our opinion, the approach discussed is the most perspective since it allows to explain the behaviour of toxicant objectively on each step of the algorythm.

This approach may be used for deciding a very difficult problem: to estimate limit concentrations of several toxicants when complex and combinated exposure takes place. Practically, Table.

Environmental Limits for 2, 3, 7, 8-TCDD.

Matrix	ADI=0.52 pg/Kg/day		ADI=10 pg/Kg/day	
	risk level 1:10^6		risk level 18:10^6	
	complex	isolated	complex	isolated
Air, mg/cub. m	$6.5*10^{-10}$	$2.0*10^{-9}$	$1.3*10^{-8}$	$3.8*10^{-8}$
Surface water, mg/L	$4.5*10^{-11}$	$2.2*10^{-10}$	$8.7*10^{-10}$	$4.8*10^{-9}$
Drinking water, mg/L	$1.1*10^{-10}$	$1.4*10^{-8}$	$1.9*10^{-9}$	$2.6*10^{-7}$
Farming soil, mg/Kg	$8.5*10^{-9}$	$9.2*10^{-8}$	$1.6*10^{-7}$	$1.8*10^{-6}$
Soil in residential area, mg/Kg	$2.0*10^{-4}$	$5.8*10^{-4}$	$8.6*10^{-3}$	$1.1*10^{-2}$
Bottom sediments, mg/Kg	$1.6*10^{-7}$	$1.3*10^{-6}$	$3.0*10^{-6}$	$2.4*10^{-5}$
Meat, mg/Kg	$2.2*10^{-9}$	$2.0*10^{-7}$	$4.1*10^{-8}$	$3.7*10^{-6}$
Milk, mg/L	$5.5*10^{-11}$	$3.0*10^{-8}$	$1.0*10^{-9}$	$5.7*10^{-7}$
Butter, mg/Kg	$2.2*10^{-9}$	$7.0*10^{-8}$	$4.2*10^{-8}$	$1.0*10^{-6}$
Curds, mg/Kg	$1.6*10^{-9}$	$1.6*10^{-7}$	$2.9*10^{-8}$	$2.8*10^{-6}$
Cream, mg/Kg	$1.7*10^{-9}$	$1.9*10^{-7}$	$3.3*10^{-8}$	$3.6*10^{-6}$
Cheese, mg/Kg	$1.8*10^{-9}$	$2.3*10^{-7}$	$3.4*10^{-8}$	$3.8*10^{-6}$
Fish, mg/Kg	$4.6*10^{-8}$	$9.0*10^{-6}$	$6.0*10^{-7}$	$1.6*10^{-5}$
Vegetables/Fruit, mg/Kg	$3.7*10^{-9}$	$4.0*10^{-8}$	$1.4*10^{-8}$	$8.0*10^{-7}$
Potatoes, mg/Kg	$7.3*10^{-9}$	$1.1*10^{-7}$	$7.1*10^{-8}$	$2.7*10^{-6}$

that situation is more wide-spread situation, especially for dioxins and related compounds.

Limit concentrations of dioxins may be different in different locations that depends on the structure and quantities of foods in daily rations, rates of breathing and skin exposure connected with people's activities and so on. The important advantage of method discussed is to take into account this fact and to estimate specific limit concentrations. Now there is no any method in regulatory practice to do it.

We consider LIMES as the important element of an integrated system of complex risk assessment. That system may include models of behaviour of a toxicant in the environment (migration and fate in abiotic objects and in the biota, degradation and so on), analysis and prognosis of exposure and potential effects. The role of LIMES is to estimate safety limits of a toxic compound in the air, water, soil, suspended and bottom sediments of water basins, foods. It allows to compare safety concentrations and those predicted by other models that analyse dynamic levels of the environmental pollution.

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