

## MATHEMATICAL MODEL FOR EXPOSURE OF VEGETATION TO PERSISTENT ORGANIC POLLUTANTS

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### ABSTRACT

Risk assessment is a complex process of evaluating and reducing risk related to the application of the hazardous industrial chemicals, of which the most toxic are persistent organic pollutants (POPs), characterized by long half-lives, resistance to degradation, and acute and chronic toxicity. Most POPs are transported via atmosphere, water and biologically, causing bioaccumulation in living organisms, including human. Food web is a primary source of human exposure to a large number of environmental pollutants, and atmospheric exposure of plants is very significant for human exposure. This paper presents the mathematical model for the human dietary exposure to persistent atmospheric pollutants via food of plant origin. Model is based on the calculation of the human exposure factor which is derived from the dynamic equilibrium of the pollutant concentrations and processes of gain and loss of pollutants in plants (dry and wet deposition, adsorption, weathering and decay).

### INTRODUCTION

Food web is a primary source of human exposure to the large number of environmental pollutants. It is considered that over 90% of persistent pollutants enters the human body through the food. Content of pollutants in foodstuffs depends on their concentration in atmosphere ( $C_a$ ), water ( $C_w$ ) and soil ( $C_t$ ), from which they bioconcentrate and biomagnify in higher members of the trophic chain. Intake of atmospheric pollutants by plants greatly contributes to human exposure; however, this aspect is often neglected in experimental investigations, modeling and risk assessment (1,2,3).

Intake of atmospheric pollutants by plants occurs by absorption of gaseous contaminants through transpiratory system and leaf cuticle, and by deposition of

solid contaminants adsorbed on aerosol particles onto exposed leaf surface (sedimentation in gravitation field or dissolved in raindrops). The main pathway of contaminant intake into plants is the leaf surface, while the intake via root or other plant organs can often be neglected. Reasons for the highest exposure of leaves are:

1. Leaf is the site of the closest contact between plants and the atmosphere,
2. Total leaf surface is up to 20 times larger than the soil surface on which the plants grow (leaf area index),
3. Intake of lipophilic chemicals from soil is limited due to the poor water solubility and strong sorption to the lipophilic phase in soil,
4. Permeability of plant surfaces is higher for non-polar substances (4).

Non-volatile atmospheric substances are transported through cuticle into inner tissues, and gases and volatile substances enter both through cuticle and open stomata

#### POSTULATION OF THE MATHEMATICAL MODEL

Average daily exposure of humans via food of plant origin  $e_{v(a)}$  (mg/kg·day) depends on the total atmospheric concentration of contaminants  $c_a$  (gaseous and adsorbed to aerosol particles) and exposure factor  $F_{a/v}$ :

$$e_{v(a)} = F_{a/v} \cdot c_a \quad [1]$$

Exposure factor of humans can be expressed by the relationship between average daily intake of a contaminant and its atmospheric concentration:

$$F_{a/v} = U_v \cdot c_v / c_a \quad [2]$$

where:  $U_v$  – average daily intake of plant food per the unit of body mass (kg fresh mass/ kg BW·day);  $c_v$  – concentration of a contaminant in plants (mg/kg);  $c_a$  – atmospheric concentration of a contaminant (mg/m<sup>3</sup>).

In postulation of the exposure factors it is required that  $c_v = \Delta c_{v(a)}(+)=\Delta c_{v(a)}(-)=\text{const}$ , i.e. dynamic model-system in which the gain of a contaminant (by absorption and deposition) is at equilibrium with the contaminant loss (by evaporation, desorption and runoff). Daily gain  $\Delta c_{v(a)}(+)$  represents the sum of absorbed and deposited quantities (by dry and wet deposition) [Eq. 3], while the daily loss  $\Delta c_{v(a)}(-)$  equals the sum of amounts which run off and which evaporate from the exposed leaves [Eq. 4]:

$$\Delta c_{v(a)}(+) = c_v(\text{dep}) + c_v(\text{abs}) \quad [3]$$

$$\Delta C_{v(a)}(-) = c_v(r) + c_v(ev) \quad [4]$$

Persistent organic pollutants (POP) have relatively high vapour pressure: thus they are mostly found in air in a solid phase, adsorbed to the particles of smoke and dust with radius  $\leq 5\mu\text{m}$ . Under gravity the particles are deposited on the soil or vegetation. Deposition rate depends on the size and shape of the particles, their density, density of the fluid (air) and viscosity of air. In the equilibrium state, the flux of particles that accumulate on the unit surface is constant. If horizontal advective transport can be neglected and if time of falling is long enough, the stationary regime is reached:

$$\int_{t_1}^{t_2} \frac{dv}{dt} = 0 \Rightarrow v = \text{const} = v_o \quad [5]$$

Total gain of a pollutant by both dry and wet deposition equals:

$$C_{v(a)} = c_a(0,259(\rho-1,29) + \frac{P \cdot b}{K_{w/c}}) \cdot L \quad [6]$$

where:  $g$  – gravity acceleration of the Earth,  $\rho$  – density of spheroid particle,  $\rho_v$  – air density,  $r$  – radius of the spheroid particle,  $\eta$  – air viscosity,  $\phi$  – interceptive plant surface,  $M$  – average annual plant inventory,  $P$  – average daily precipitation rate (m/dan),  $b$  – runoff constant,  $K_{w/c}$  – partition coefficient of a contaminant between water and leaf cuticle,  $L$  – exposed leaf area index

The equilibrium concentration of a pollutant in leaf, as a result of its absorption and desorption equals:

$$C_{v(\text{abs})} = c_a \cdot \frac{K_1}{K_2} = c_a \frac{K_{c/w} \cdot RT}{H} \quad [7]$$

Total amount of a pollutant daily removed from the plant in processes of weathering, runoff and decay etc. depends on the pollutant concentration in/on vegetation and the removal constant  $G$ :

$$\Delta C_{v(a)}(-) = c_v \cdot G \cdot M \quad [8]$$

If all consumed plant food originates from the locality with atmospheric concentration of a pollutant  $c_a$ , it is possible to define the human exposure factor using expressions [6], [7] and [8]:

$$F_{a/v} = U_v \cdot \frac{(0.259(\rho - 1.29) + P \cdot b \cdot K_{C/W}) \cdot L + \frac{K_{C/W} \cdot RT}{H}}{G \cdot M} \quad [9]$$

## CONCLUSION

On the basis of the postulated model and the experimental values for the atmospheric concentration of persistent organic pollutants it is possible to calculate the average daily exposure of a human organism to these ubiquitous environmental toxicants, which represent a constant threat to human health due to various chronic, developmental and genetic effects. Proposed model is a contribution to the development of exposure analysis, which is one of the four basic phases in the complex process of risk assessment, a scientific discipline which gains its importance in the current situation of rapid development of industry and technology and the existence of innumerable anthropogenic hazardous chemicals.

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