IMPROVEMENT OF CALCULATIONS OF THE TOTAL CHARACTERIZATION FACTOR IN THE USETOX MODEL INCLUDING A REGIONAL APPROACH

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TOMSK POLYTECHNIC UNIVERSITY ТОМСКИЙ ПОЛИТЕХНИЧЕСКИЙ УНИВЕРСИТЕТ

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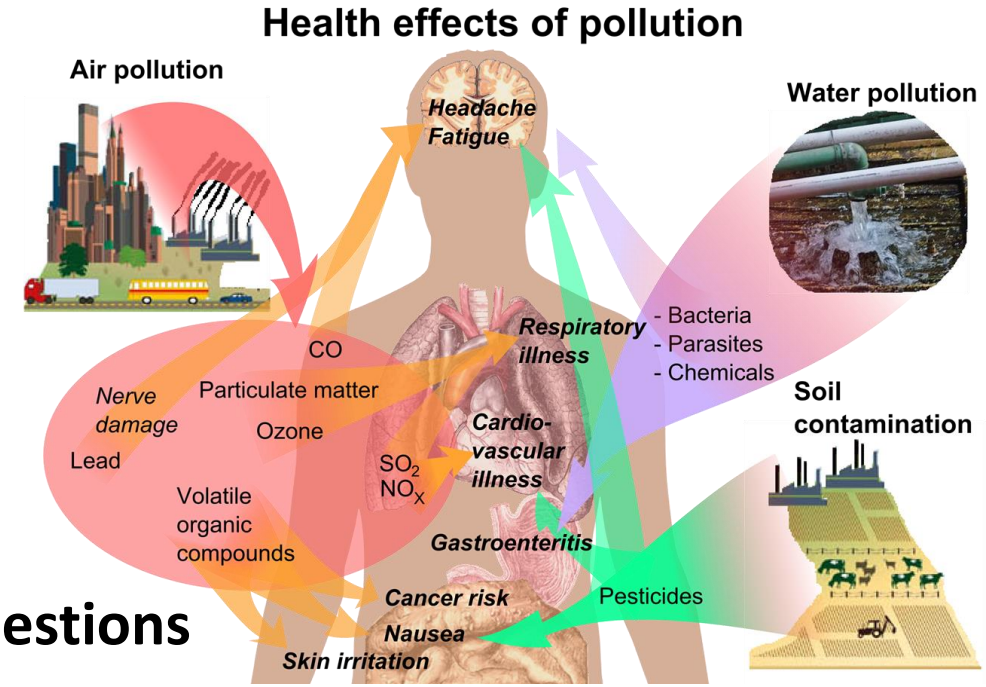
Arts et Métiers Sciences et Technologies

Contexte



Research questions

How can we analyze the chemical elements content in biological materials?

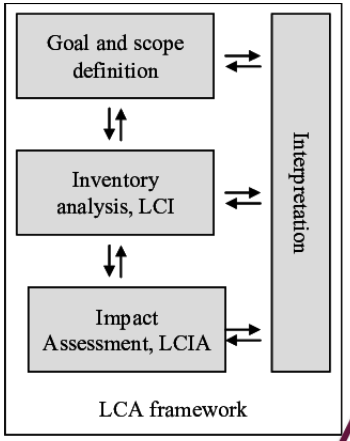
What are the main sources of negative influence on human health?

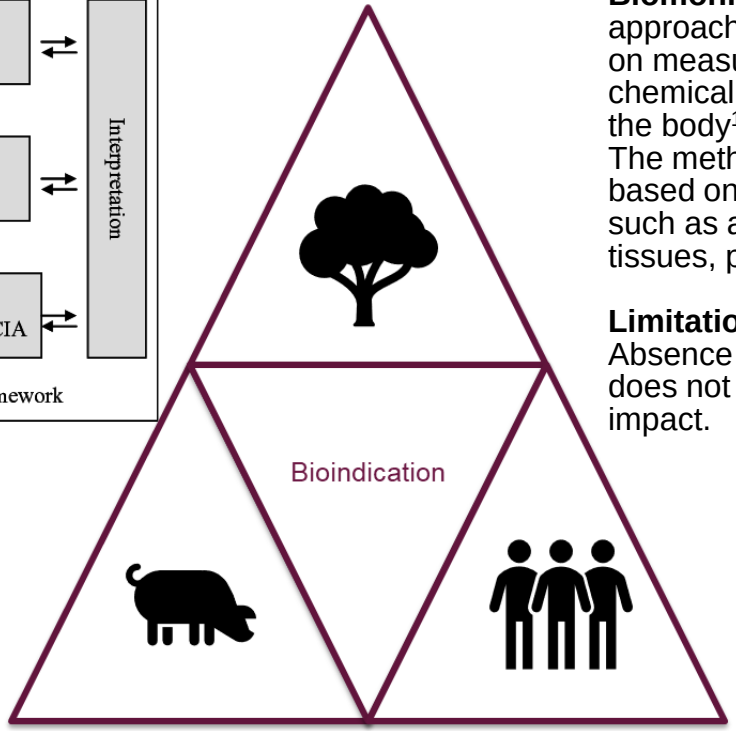
Which methods should we use to assess chemicals' impact on the population?

Which methods should we use to assess chemicals' impact on population?

Life Cycle Impact Assessment (LCIA) is vital phase of any LCA. Life cycle impact assessment (LCIA) aims at understanding and quantifying the magnitude and significance of the potential environmental impacts of a product or a service throughout its entire life cycle.
LCIA models (e.g. the **USEtox**) is a sufficient tool to model the human health and ecosystems impact.

Limitations of the method:
Lack of spatial differentiation





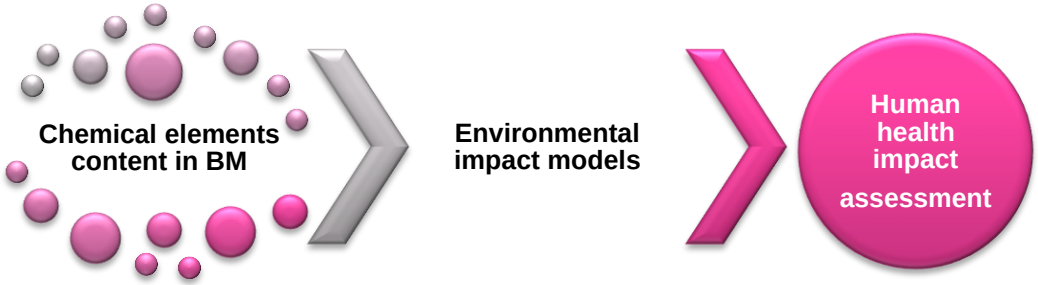
Biomonitoring is an analytical approach which focuses directly on measuring the volume of toxic chemical compounds present in the body[1].
The methods of **bioindication** is based on analysis of the biota such as animal and human tissues, plants or microorganisms.

Limitation of method:
Absence of scale of impact, that does not allow to normalize the impact.

1. Standards, T. I. International Standard ISO 14040 1991, *1991*.
2. The International Standards Organisation INTERNATIONAL STANDARD ISO 14044 assessment Requirements and guilelines. *Int. J. Life Cycle Assess.* **2006**, *2006*, 652–668, doi:10.1007/s11367-011-0297-3.
3. Fantke, P.; Bijster, M.; Guignard, C.; Hauschild, M.; Huijbregts, M.; Jolliet, O.; Kounina, A.; Magaud, V.; Margni, M.; McKone, T.; Posthuma, L.; Rosenbaum, R. K.; van de Meent, D.; van Zelm, 2, R. *USEtox® 2.0, Documentation version 1*; 2017; ISBN 978-87-998335-0-4.

1 - Kowalski, 1974; Glazovskaya, 1988; Saet et al., 1990; Alekseenko, 2006; Rikhvanov et al., 2006; Yazikov et al., 2010; Strakhovenko, 2011; Baranovskaya et al., 2015

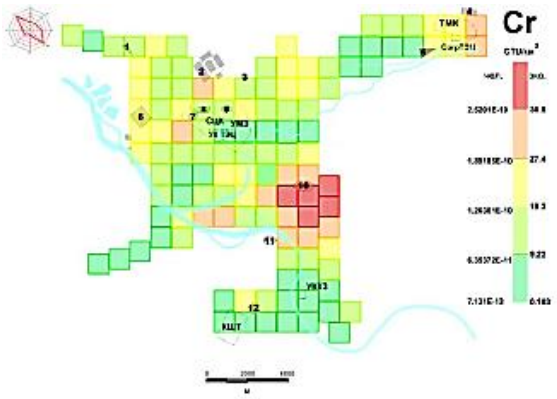
How can we assess the technological environmental impact and human health impact?
According to the previous investigations we have a wide massive of analytical data of chemical elements content in biomaterials in the studied areas.

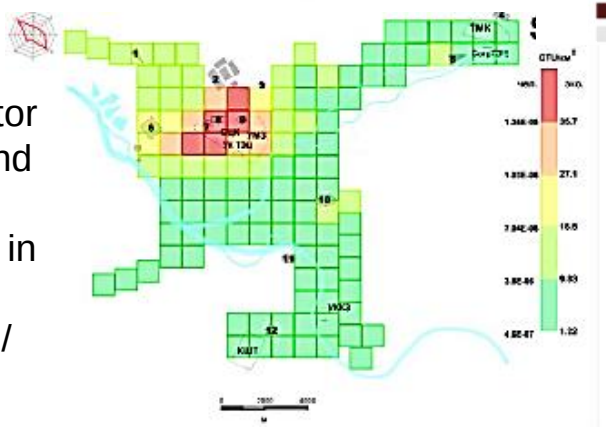


Research methods

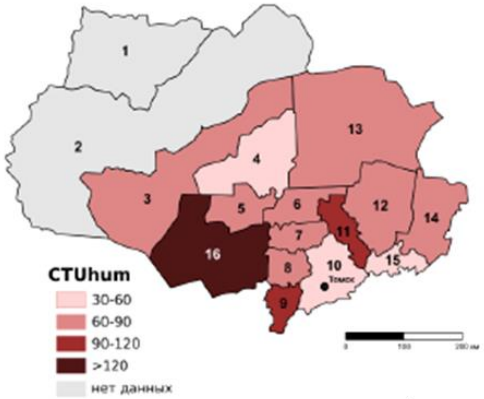
Modeling part:	Characterization factor modification and calculation
Experimental part:	Measurement of the concentration coefficient of microelements

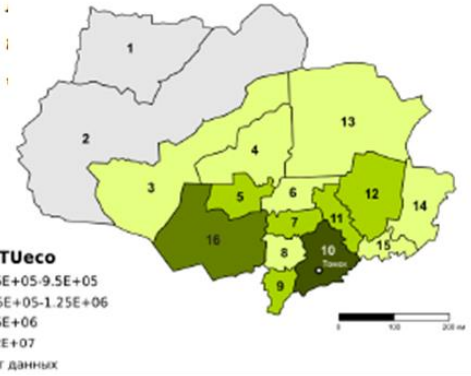
The examples of previous work made with utilization of LCA methods in human health and ecosystem impact assessment.





Mapping of the Characterization factor value (for humans and ecosystems), calculated for Cr, Sb in the city of Ust-Kamenogorsk (CTU / km2)
According to A.R. Yalaltdinova, 2015





The Characterization factor of Br [CTU], human health and ecosystem impact.
According to T. Perminova, 2017

Modeling part

$$IS = \sum_i \sum_x CF_{x,i} \times M_{x,i}$$

Modification

$$CF = EF \times XF \times FF$$

Default values given by the USEtox model

- **Fate factor** (FF) [$kg_{in\ compartment}$ per $kg_{emitted}$/day] represents the persistence of a chemical in the environment (e.g. in days) as well as the relative distribution, and the exposure factor expresses the availability for human or ecosystem contact represented by the fraction of the chemical transferred to the receptor population in a specific time period such as a day.
- **Exposure factor** (XF) [kg_{intake}/day per kg $_{in\ compartment}$] describes the effective human intake of a specific environmental medium – air, water, soil – through inhalation and ingestion.
- **Effect factor** (EF) [kg_{intake}/day] reflects the impact on human health and the state of ecosystems due to the arrival of a chemical element / substance in the living organism in various ways (through air, water, soil or food).

The framework of calculations inside the model

The clarke concentration
(Clarke$_{biosphere}$) expresses the average concentration of metal in biosphere. [1]

Macroelements ($n\cdot10^{-3}$%...$n\cdot10$ %) Microelements(<$n\cdot10^{-3}$%)				Microelements (<$n\cdot10^{-3}$)			
Elements	%, content	Elements	%, content	Elements	%, content	Elements	%, content
O	70	Mn	$9{,}6\cdot10^{-3}$	Pb	$1\cdot10^{-4}$	Be	$4\cdot10^{-6}$
C	18	Al	$5\cdot10^{-3}$	Ni	$8\cdot10^{-5}$	Ga	$2\cdot10^{-6}$
H	10,5	Zn	$2\cdot10^{-3}$	Cr	$7\cdot10^{-5}$	Se	$2\cdot10^{-6}$
N	$3\cdot10^{-1}$	Sr	$1{,}6\cdot10^{-3}$	V	$6\cdot10^{-5}$	Ag	$1{,}2\cdot10^{-6}$
Ca	$5\cdot10^{-1}$	Ti	$1{,}3\cdot10^{-3}$	Li	$6\cdot10^{-5}$	W	$1\cdot10^{-6}$
K	$3\cdot10^{-1}$	B	$1\cdot10^{-3}$	Co	$4\cdot10^{-5}$	U	$8\cdot10^{-7}$
Si	$2\cdot10^{-1}$	Ba	$9\cdot10^{-4}$	La	$3\cdot10^{-5}$	Hf	$5\cdot10^{-7}$
Na	$2\cdot10^{-1}$	Cu	$3{,}2\cdot10^{-4}$	Y	$3\cdot10^{-5}$	Sb	$2\cdot10^{-7}$
P	$7\cdot10^{-2}$	Zr	$3\cdot10^{-5}$	Mo	$2\cdot10^{-5}$	Cd	$2\cdot10^{-7}$
S	$5\cdot10^{-2}$	Rb	$2\cdot10^{-4}$	I	$1{,}2\cdot10^{-5}$	Hg	$<n\cdot10^{-7}$
Mg	$4\cdot10^{-2}$	Br	$1{,}6\cdot10^{-4}$	Sn	$1\cdot10^{-5}$	Au	$n\cdot10^{-8}$
Cl	$2\cdot10^{-2}$	Br	$1{,}6\cdot10^{-4}$	As	$6\cdot10^{-6}$	Ra	$n\cdot10^{-12}$
Fe	$1\cdot10^{-2}$	F	$1{,}4\cdot10^{-4}$	Cs	$6\cdot10^{-6}$		

Default values

$$CF = \overbrace{EF \times FF}^{\text{Default values}} \times XF \longrightarrow \text{Modifications}$$

$$\textbf{B)}\ XF_{xp,i}^{inderect} = \frac{BAF_{xp,i} \times IR_{xp} \times P}{\rho_i \times V_i}$$

$$BAF_{xp,i} = \frac{C_{xp}}{C_i} \rightarrow CC_{Cr} = \frac{C_{Cr_{[Concentration\ of\ Cr]}}}{C_{Clarke}}$$

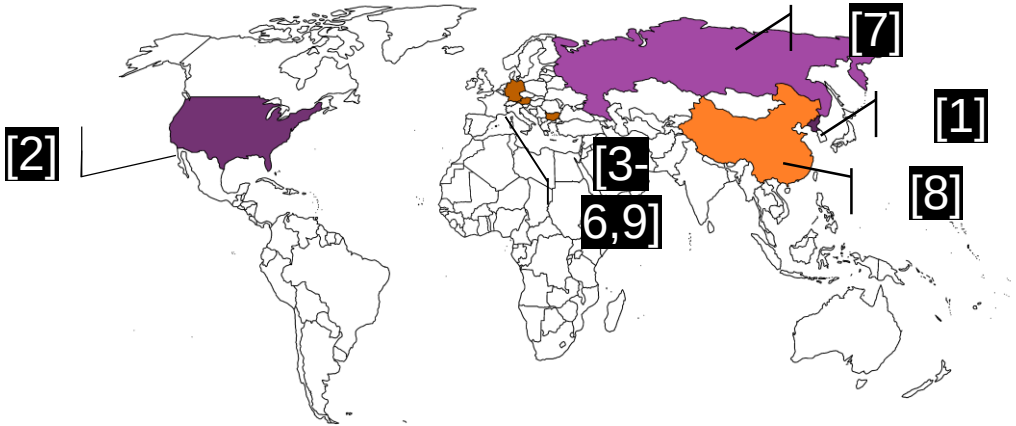
A) ICP-MS

Pork meat

[1] Glazovsky, N. . F. . Tekhnogennye potoki veschestva v biosfere Technogenic flows of matter in bioshepere. *Dobytcha water Resour. their Futur.* **1982**, 7–28.

Previous investigation results

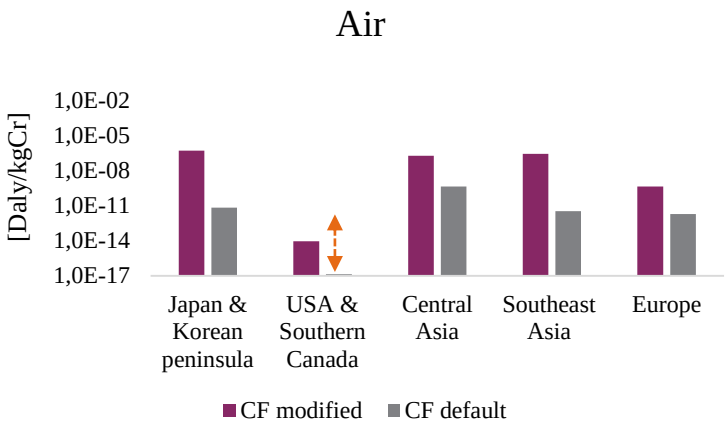
Sampling map of pork meat according to own investigation and literature references

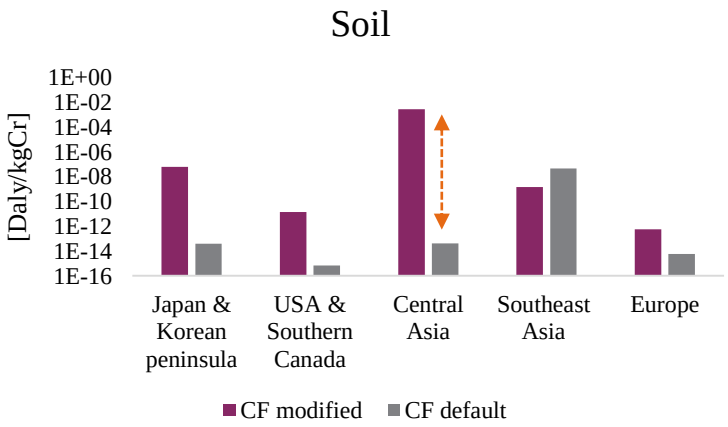


1. Korea; 2. USA; 3. Germany; 4. Austria; 5. Netherlands; 6. Belgium; 7. Russia; 8. China; 9. Serbia

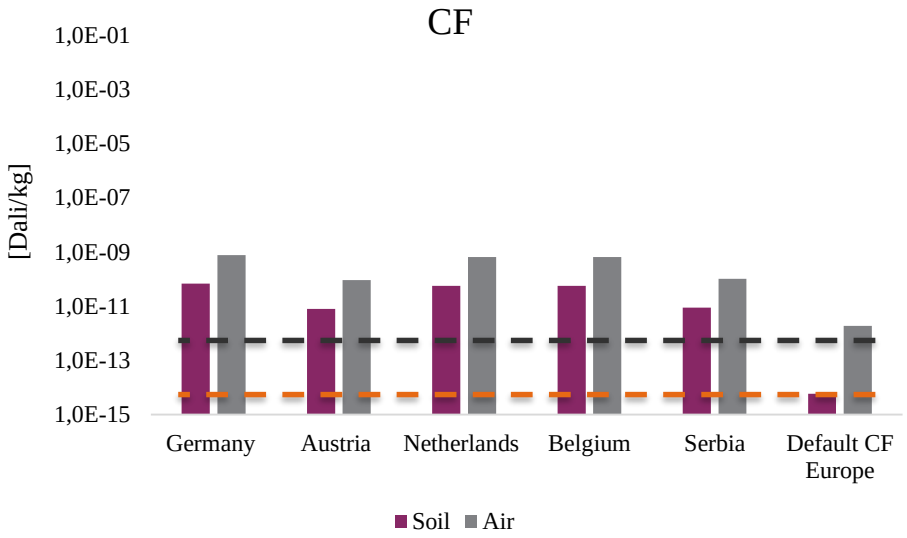
Country	Cr mean, [mg/kg]	St. deviation	Number of samples	Data of sampling [year]	Geo zone in USEtox model	Reference
Korea	0,003	0,0001	227	2016	Japan and Korean peninsula	Kim, J. S.; Hwang, I. M.; Lee, G. H.; Park, Y. M.; Choi, J. Y.; Jamila, N.; Khan, N.; Kim, K. S. Geographical origin authentication of pork using multi-element and multivariate data analyses
USA	0,0009	0,0001	36	2016	USA and southern Canada	
Germany	0,0006	0,0001	12	2016	Europe	
Austria	0,00007	0,00001	15			
Netherlands	0,0005	0,0001	14			
Belgium	0,0005	0,00001	19			
Serbia	0,08	0,01	192	2017		Nikolic, D.; Djinovic-Stojanovic, J.; Jankovic, S.; Stanisic, N.; Radovic, C.; Pezo, L.; Lausevic, M. Mineral composition and toxic element levels of muscle, liver and kidney of intensive (Swedish Landrace) and extensive (Mangulica) pigs from Serbia.
China	2,01	0,2	100	2016	Southern China	Zhao, Y.; Wang, D.; Yang, S. Effect of organic and conventional rearing system on the mineral content of pork

Previous investigation results



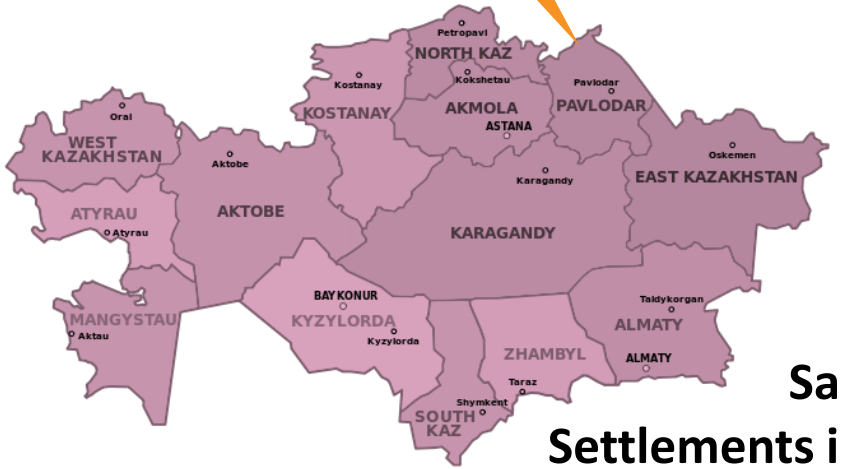


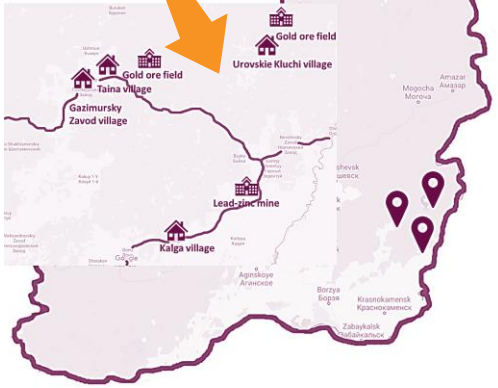
1. The significant difference between $CF_{modified}$ and $CF_{default}$ is found out. As in the level of s region, as in level of a country factor proposed be the USEtox model is lower than factor calculated with experimental results. Possibly the model underestimates results because it does not include the local data.
2. The importance of the local data is proved by the fact, the CF can vary greatly within <u>one administrative</u> unit.



The experimental part

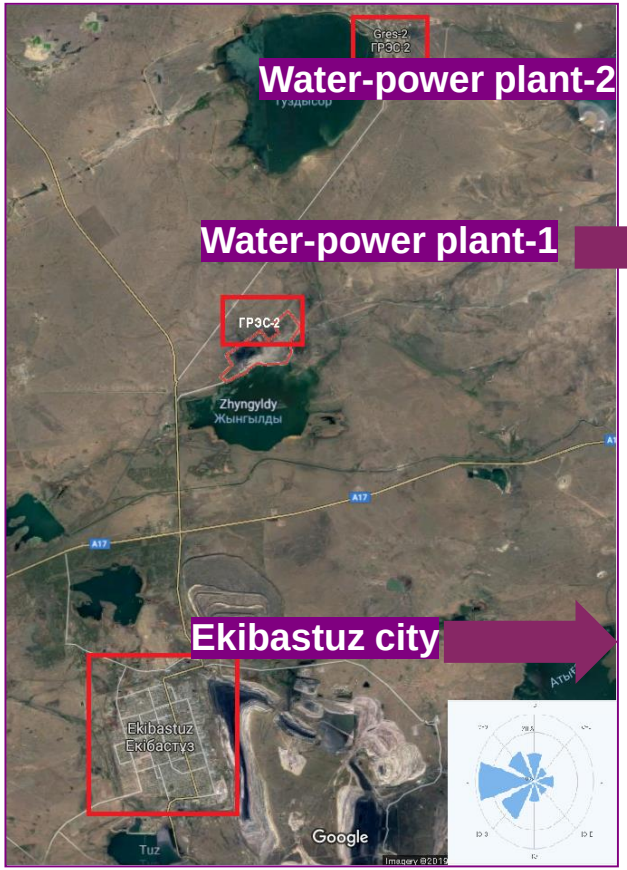
The areas are characterized by a complex ecological and geochemical situation caused by **natural anomalies, mining industry facilities, production facilities.**





Sampling areas:
Settlements in Kazakhstan and Russia

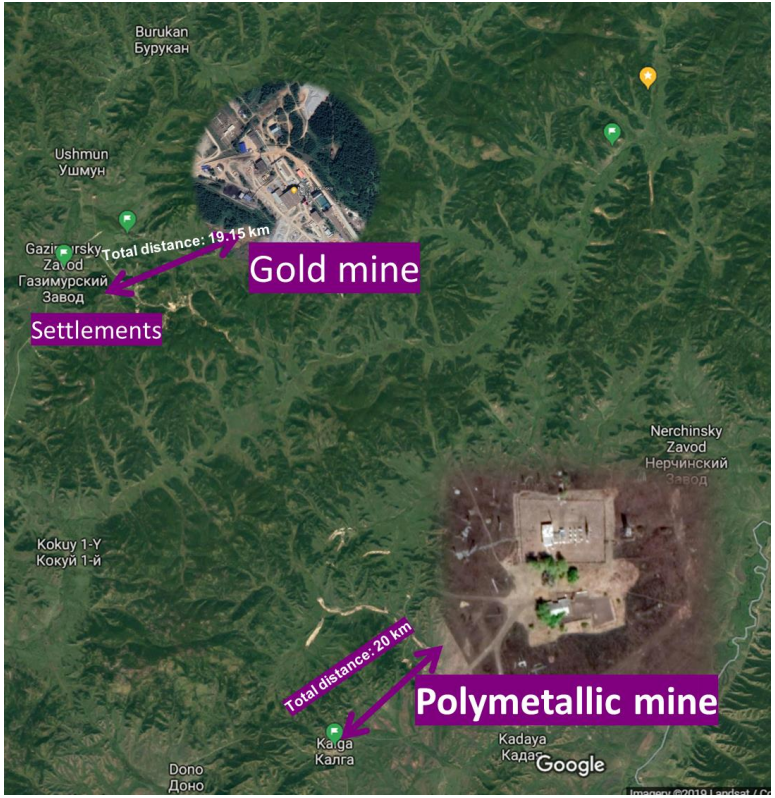
Sampling areas

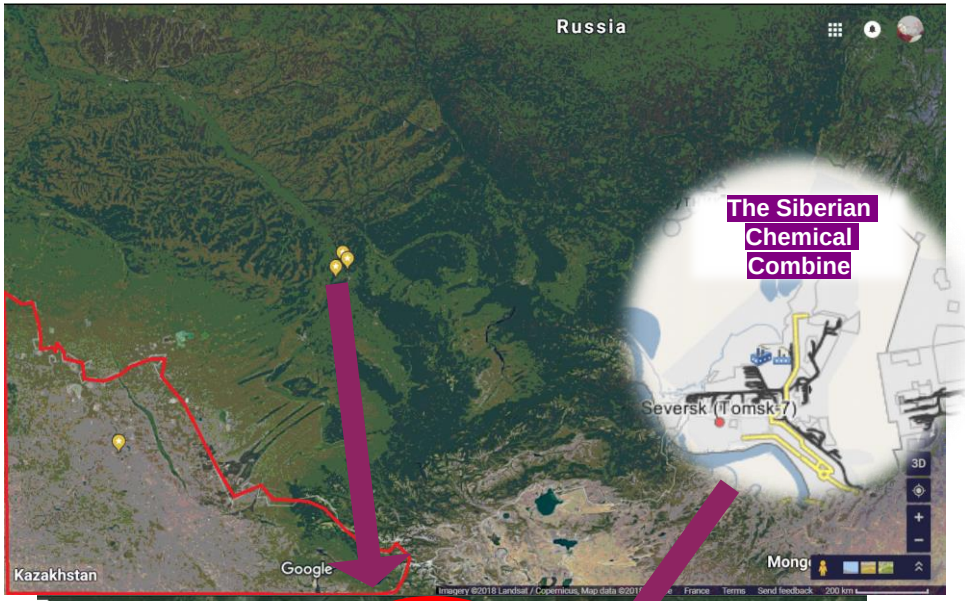


The population of this region is constantly under a high level of technogenic tension.
Coal mines and power facilities placed inside of the urban zone.

Sampling map Kazakhstan

Sampling map
Russia





The experimental part

Sampling areas

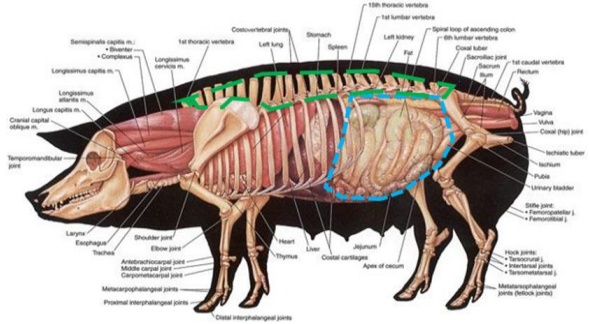
Why those areas?

- High level of risks of water and soil use;
- **A large number of fuel cycle facilities** (NFC “The Siberian Chemical Combine”, hydroelectric power station, fossil fuel burning power station);
- Natural anomalies.

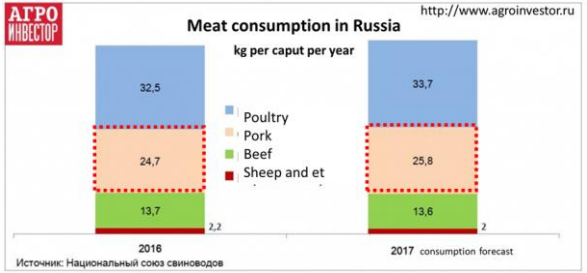
Methods of analysis of samples

- Samples were taken immediately after the death of the animal, packed in plastic bags and frozen.
- Neutron Activation Analysis is very sensitive and is therefore used to analyze for minor elements, which are present in very low concentrations.
- The analysis of the samples is carried out based on the IRT-T research nuclear reactor in the nuclear geochemical laboratory (YLL) of the Department of Geoecology of the National Research Tomsk Polytechnic University.

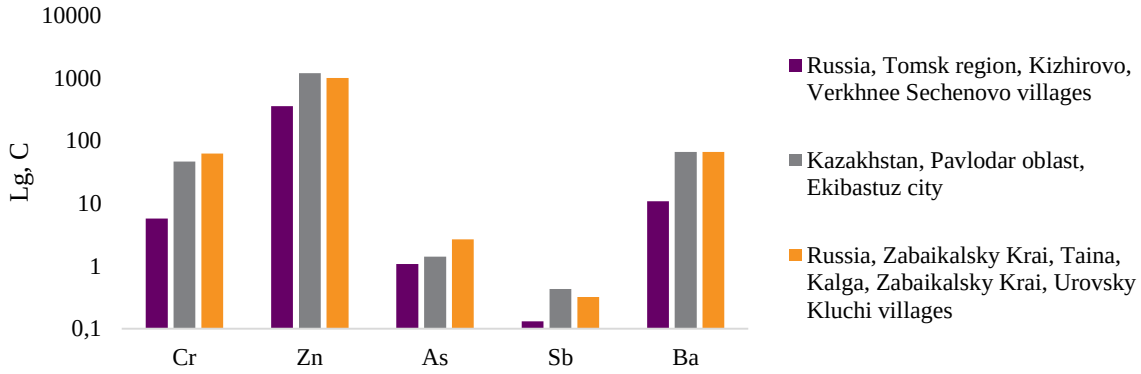
Samples are taken



Subject of study biological material (BM) (organs and tissues) of Sus scrofa domesticus



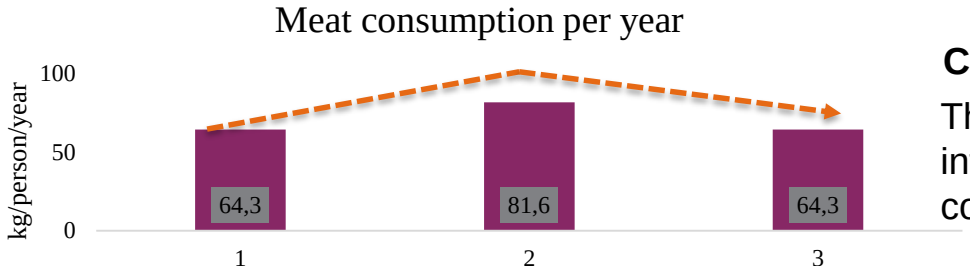
Pork occupies 37% of the world's meat production According to the Food and Agriculture Organization (FAO) classification, pork is one of the most indispensable foods.



The registration number of the element and the source data for calculating the exposure factor, the concentration coefficient relative to the noosphere clarke concentration [$kg_{intake\ /day}$ per $kg_{in\ compartment}$]

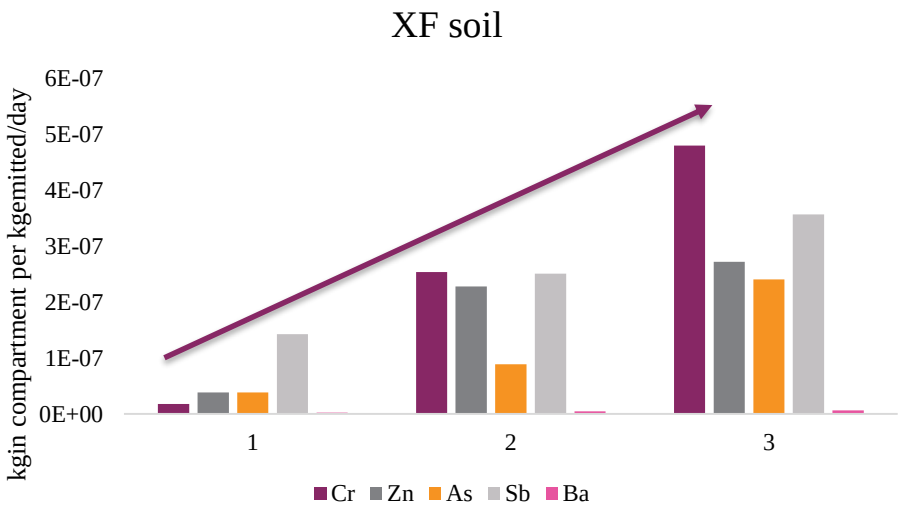
C/e	The concnetration clarke by Glazovsky	Russia, Tomsk region, Kizhirovo, Verkhnee Sechenovo villages	Kazakhstan, Pavlodar oblast, Ekibastuz city	Russia, Zabaikalsky Krai, Taina, Kalga, Zabaikalsky Krai, Urovsky Kluchi villages	CAS number of element in the USEtox model
Cr	0,00007	5,75	46,75	62,24	18540-29-9
Zn	0,002	359,20	1201,73	1008,18	23713-49-7
As	0,000006	1,08	1,41	2,67	22541-54-4
Sb	0,0000002	0,13	0,43	0,32	22537-51-5
Ba	0,0009	10,77	65,94	65,97	22541-12-4

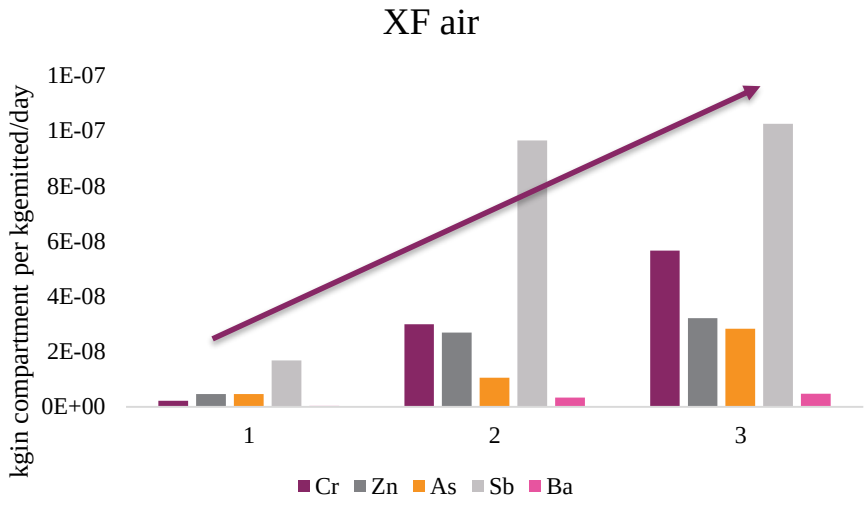
Results of data extrapolation



Conclusion

The main influence on the elements ingestion into the human body is not the amount of meat consumption, but its elemental composition.

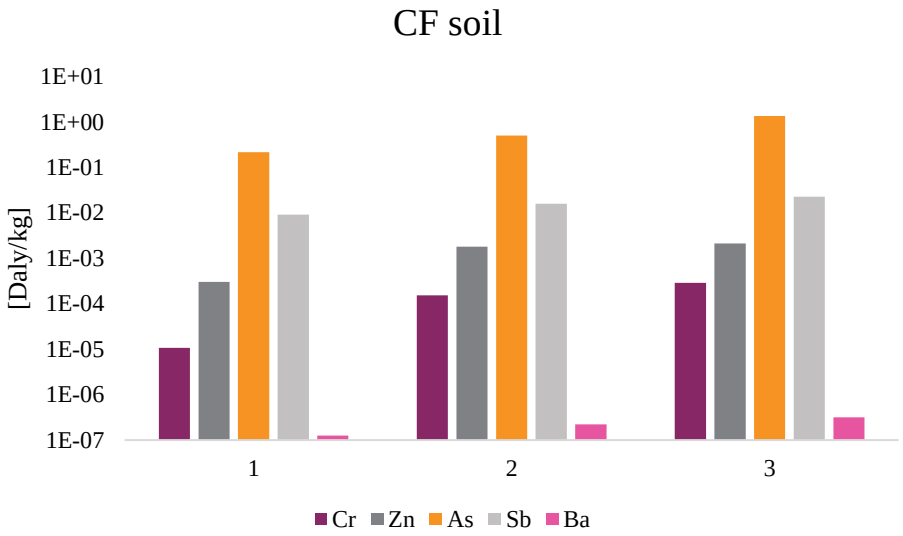


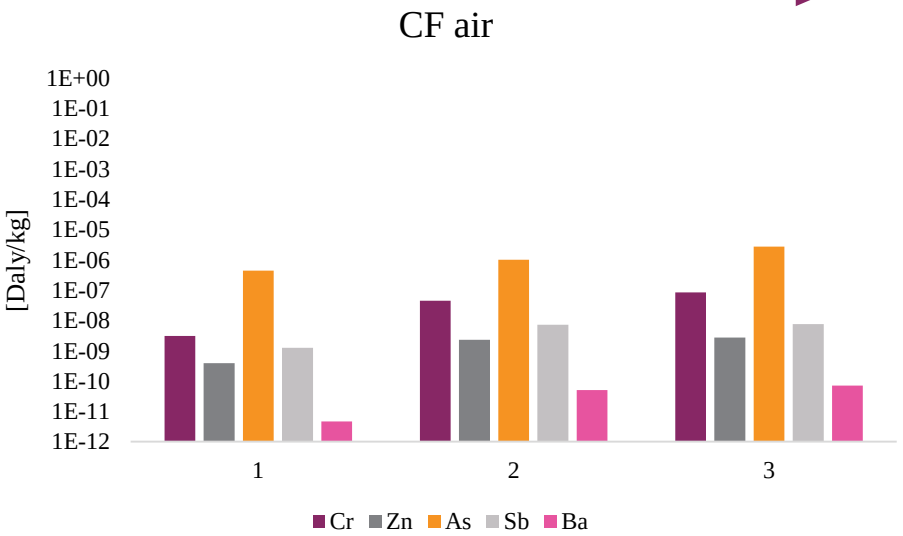


1 - Tomsk district (Russia); 2 - Pavlodar region (Kazakhstan); 3 - Zabaikalsky krai (Russia)

Results of data extrapolation

The Characterization factor in the studied geo zones of elements in pork meat via soils (right), CTU_H





The Characterization factor in the studied geo zones of elements in pork meat via air, CTU_H

1 - Tomsk district (Russia); 2 - Pavlodar region (Kazakhstan); 3 - Zabaikalsky krai (Russia)

Conclusions

General conclusions:

1. Integration of experimental data into the USEtox model is prepared;
2. The total Characterization factor is modified using own data.

Specific conclusions:

1. Generally, the introduction of elements into the body during normalization to the soil is much higher than during normalization to air. The highest exposure factor of all elements is determined for Zabaikalsky Krai region, the lowest one is for Tomsk region. No correlation between the consumption of meat products and the value of the exposure factor is found;
2. For most elements, the ranking of the CF_{hum} for entry from the soil is as follows: Zabailkasky Krai> Palodar Region> Tomsk Region. CF_{hum} calculated for ingestion with air follows the same tendency.

THANK YOU FOR ATTENTION!

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