# The task of finding the chemical composition
## of an unknown medium by multi-energy radiography method

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# Scheme of experiment

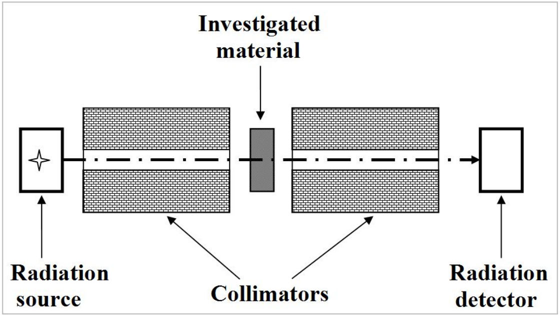


Figure: Scheme of experiment

Radiation flux is collimated by direction and energy
We use the following notation:
$0.1\ Mev = E_1 < E_2 < \ldots < E_{\overline{N}} = 20\ Mev$ – energies set, $N \leq \overline{N} = 20$
$X_0$ - unknown substance, $\rho_0$ - its density, $l$ - thickness
$h_k = h(E_k)$ , $H_k = H(E_k)$ – incoming and outgoing radiation flux densities

# Statement of the problem of chemistry

$X_1, \dots, X_N$ – chemical elements composing $X_0$
$\rho_{x1}, \dots, \rho_{xN}$ – densities of $X_1, \dots, X_N$
$w_1, \dots, w_N$ – weight fractions of $X_1, \dots, X_N$ – **UNKNOWN**
$\mu_{xik} = \mu_{xi}(E_k)$ – coefficients of radiation attenuation of $X_1, \dots, X_N$

$\rho_0, \quad \mu_{0k} = \mu_0(E_k)$ – density and coefficient of attenuation of $X_0$ – **UNKNOWN**

For each energy value $E_k$ radiation transfer equation gives

$$H_k = h_k \exp(-l\mu_{0k}) \ \ or \ \ -l\mu_{0k} = \ln(\frac{H_k}{h_k}); \quad k = 1, \dots, N. \tag{1}$$

For each energy value $E_k$ the equality holds:

$$\mu_{0k} = \rho_0 \sum_{i=1}^{N} w_i \frac{\mu_{xik}}{\rho_{xi}}. \tag{2}$$

Substituting the equality (2) into the formula (1) we have the system:

# Statement of the problem of chemistry

$$\sum_{i=1}^{N} \frac{\mu_{xik}}{\rho_{xi}} \cdot (l\rho_0 w_i) = \ln \frac{h_k}{H_k}; \quad k = 1, \ldots, N. \tag{3}$$

$$\sum_{i=1}^{N} w_i = 1 \tag{4}$$

$$w_i \geq 0; \quad i = 1, \ldots, N. \tag{5}$$

**The problen of chemistry:**
*Find the quantities* $\rho_0, w_i, i = 1, \ldots, N$ *satisfying equations* (3), (4) *and inequalities* (5) *provided that all other quantities included in* (3) *are know.*

Rewrite the system (3) in the form $Ax = b$ or

$$\sum_{i=1}^{N} A_{ki} x_i = b_k; \quad k = 1, \ldots, N, \tag{6}$$

where $A_{ki} = \mu_{xik}/\rho_{xi} = \mu_{xi}(E_k)/\rho_{xi}; \; x_i = l\rho_0 w_i; \; b_k = \ln(h_k/H_k)$.

# Perturbation of the solution

Rewrite the system (6) in the form

$$Ax = b$$

and represent $x$ and $b$ as
$x = x_T + \delta x$, where $x_T$ – true solution to a system (6), $\delta x$ – perturbation of solution
$b = b_T + \delta b$, where $b_T$ – true value of the vector $b$, $\delta b$ – perturbation of $b$, then

$$A(x_T + \delta x) = b_T + \delta b, \quad Ax_T = b_T, \quad A(\delta x) = \delta b \tag{7}$$

The singular decomposition of the matrix A is valid

$$A = USV^T, \tag{8}$$

where $S = \mathrm{diag}\{\sigma_1, \dots, \sigma_\mathrm{N}\}$ – diagonal matrix, $V$ and $U$ – orthogonal matrices.
Matrix $A$ is almost always non-degenerate; in this case

$$A^{-1} = VS^{-1}U^T \tag{9}$$

$\Omega = \{\delta b |\ \delta b \in \mathbb{R}^N, ||\delta b|| = 1\}$ – the unit sphere $A^{-1}(\Omega) = VS^{-1}(\Omega)$ is an ellipse with semiaxes $\{\sigma_1^{-1}, \dots, \sigma_N^{-1}\}$

We use the following notation:

$E^{(p)} = (E_1^{(p)}, E_2^{(p)}, \ldots, E_N^{(p)})$ – a vector formed from energies satisfying condition $E_1^{(p)} < E_2^{(p)} < \ldots < E_N^{(p)}$.

$C_{20}^N = \frac{20!}{N! \cdot (20-N)!}$ – number of different vectors $E^{(p)}$

$A^{(p)}$ – non-degenerate matrix of system (6) corresponding to the vector $E^{(p)}$

We will conduct a series of experiments on the irradiation of the sample. Each series consists of $N$ experiments in which the sample is irradiated to light at each energy $E_1^{(p)}, E_2^{(p)}, \ldots, E_N^{(p)}$

$b^{(p;n)} = b_T^{(p)} + \delta b^{(p;n)}$ – the result of such an experiment in the n-th series of measurements

$\widehat{\Pi}^{(p)} = \{z|\ z = (z_1, \ldots, z_N) \in \mathbb{R}^N,\ |z_k| \le r_k,\ k = 1, \ldots, N\}$ – parallelepiped in the space of the right-hand parts of the system (6)

$\widehat{T}^{(p)} = [A^{(p)}]^{-1}(\widehat{\Pi}^{(p)})$ – the inverse image of $\widehat{\Pi}^{(p)}$

$\Omega \quad = \{\delta b|\ \delta b \in \mathbb{R}^N, ||\delta b|| = 1\}$ – the unit sphere in the space of the right-hand parts of the system (6)

# Finding a set containing a solution to a problem

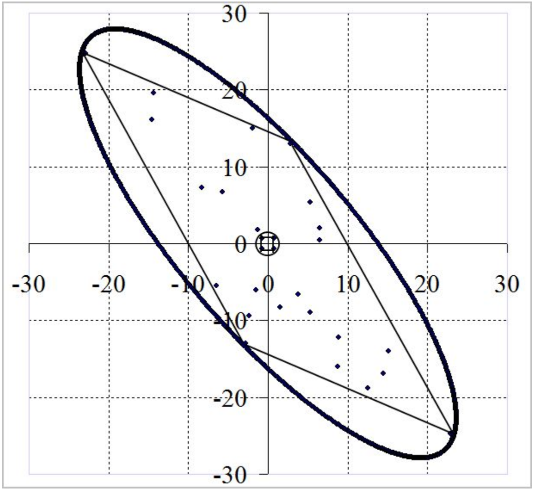


Figure: Small square $\widehat{\Pi}^{(p)}$ with a side $\sqrt{2}$ and a unit ball $\Omega$ belong to the space of the right-hand parts of the system (6) and limit possible perturbations of the system. Parallelogram $[A^{(p)}]^{-1}(\widehat{\Pi}^{(p)})$ and ellipse $[A^{(p)}]^{-1}(\Omega)$ are inverse images of these two figures.

For any $n$-th series of irradiation of the sample we have:

$$x_T \in x_T + \delta x^{(p;n)} + [A^{(p)}]^{-1}(\widehat{\Pi}^{(p)}) \tag{10}$$

$x_T + \delta x^{(p;n)} = [A^{(p)}]^{-1}(b_T + \delta b^{(p;n)}) = [A^{(p)}]^{-1}(b^{(p;n)})$ and $[A^{(p)}]^{-1}(\widehat{\Pi}^{(p)})$ are known

From inclusion (10) we hawe:

$$x_T \in Q_n = \bigcap_{i=1}^{n}(x_T + \delta x^{(p;i)} + [A^{(p)}]^{-1}(\widehat{\Pi}^{(p)})) \tag{11}$$

Under some assumptions we have: $\mathrm{diam}(Q_n) \to 0$ when $n \to \infty$

**We assume that the following is valid:**

1) for any energy vector $E^{(p)} = (E_1^{(p)}, E_2^{(p)}, \ldots, E_N^{(p)})$ and any $k = 1, \ldots, N$ we know a number $r_k > 0$ such as for any $n$

$$|\delta b_k^{(p;n)}| = |b_{T,k}^{(p)} - b_k^{(p;n)}| \leq r_k; \tag{12}$$

2) for any energy vector $E^{(p)}$ any $\varepsilon > 0$ and any facet of polyhedron $\widehat{\Pi}^{(p)}$ there exists $n$-th series of measurements such as the distance between $\delta b_k^{(p;n)}$ and the facet is less than $\varepsilon$

3) radiation detector has no systematic errors

## Theorem

*If assumptions 1), 2), 3) are fulfilled the diameter of the set*

$$Q_n = \bigcap_{i=1}^{n} (x_T + \delta x^{(p;i)} + [A^{(p)}]^{-1}(\widehat{\Pi}^{(p)})) \tag{13}$$

*tends to zero when n tends to infinity*

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