DESIGN OF THE SABAT SYSTEM FOR UNDERWATER DETECTION OF DANGEREUS SUBSTANCES

M. Silarski
Jagiellonian University
on behalf of the SABAT collaboration

- Introduction
- Neutron Activation Techniques
- Application in the underwater environment
- Status of the project
- Summary

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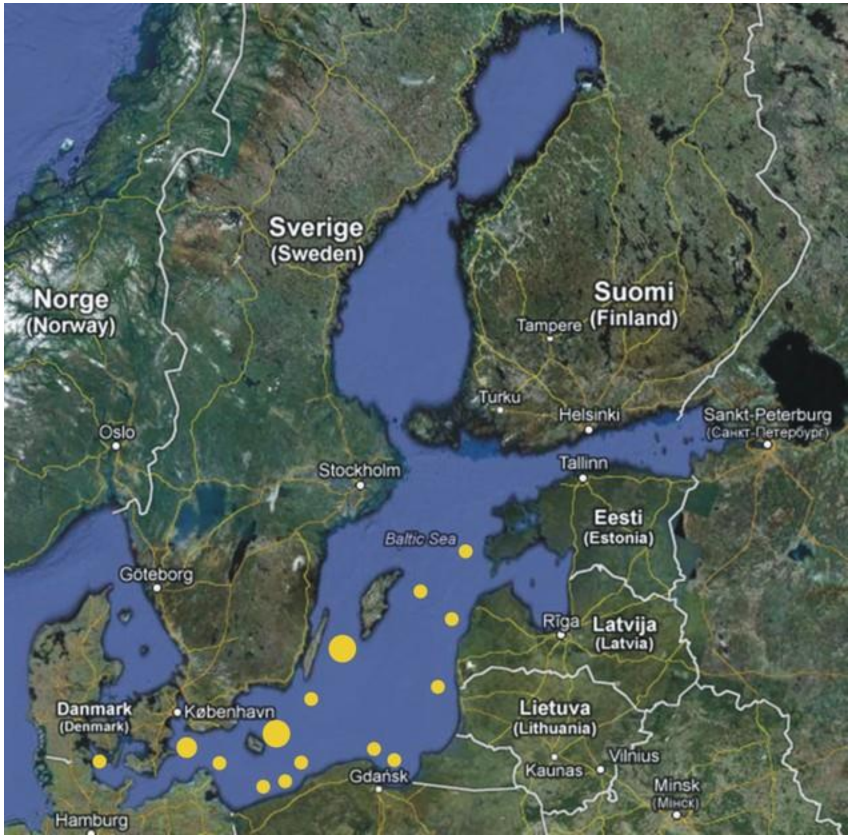
Introduction

- „Ghosts" of World Wars: ~250 kt of munition (including 65 kt of chemical agents) sunk in the Baltic Sea
- Main known contamined areas: Little Belt, Bornholm Deep (east of Bornholm) and the south-western part of the Gotland Deep
- **Unknown amount of chemical leftovers are spread around the Baltic Sea**
- Serious threat for people and environment
  - „Fake amber" on the coast
  - Mustard gas „fished" out the sea
  - Menace to navy
  - Genetic mutations of marine fauna



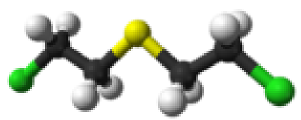
http://www.sfora.pl/polska/Napalm-w-Baltyku-Przed-katastrofa-nie-ma-ratunku-a52539

- **1/6 of the sunk munition released into Baltic = entire degradation of live in the sea and at its shores for 100 years!!**

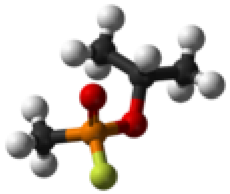
Introduction

❖ Main agents do deal with:

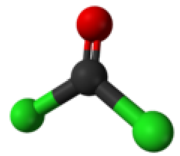
Mustard gas ($C_4H_8Cl_2S$)



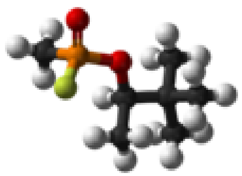
Sarin ($C_4H_{10}FO_2P$)



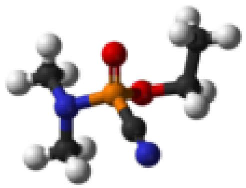
Fosgen ($COCl_2$)



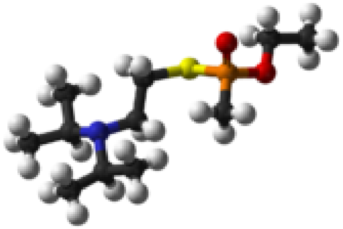
Soman ($C_7H_{16}FO_2P$)



Tabun ($C_5H_{11}N_2O_2P$)



VX ($C_{11}H_{26}NO_2PS$)



❖ Presently used detection methods:

- ❖ Sonars (shape and localization) + diver/robot inspection (evaluation of the ammunition shell and type)
- ❖ „By chance": during fishing, etc.

❖ **High economic and environmental costs has been preventing so far any activities aiming at extraction o these hazardous substances**

Neutron Activation Techniques

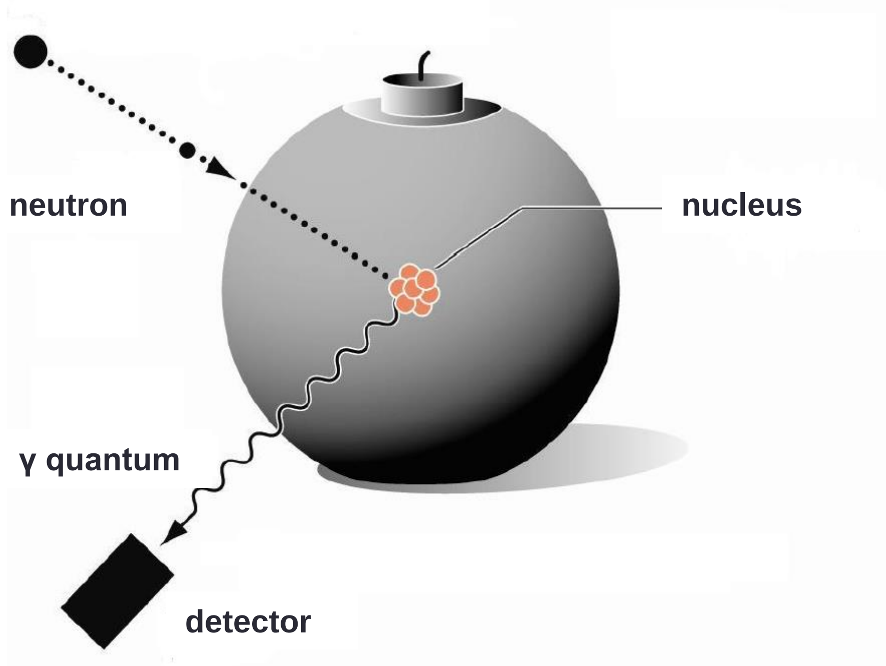
❖ Novel methods of **nondestructive** chemical threat detection based on neutron activation:

Thermal neutron capture (sources, D+Dgenerators)

Neutron inelastic scattering (D+D/**D+T** generator)

D+T → α + n

n + nucleus → nucleus + γ + n



Excited nuclei emit gamma quanta of energy characteristic of the element

Relative content of elements ⇔ Stoichiometry → **Identification**

Neutron Activation Techniques

❖ **Signature:**
gamma quanta of the following nuclei: ^{12}**C** (4.44 MeV), ^{16}**O** (6.13 MeV), ^{14}**N** (2.31 MeV, 5.11 MeV), ^{37}**Cl** (1.73 MeV, 3.1 MeV) ^{32}**S** (3.78 MeV) ^{31}**P** (1.27 MeV) ^{19}**F** (0.11 MeV, 0.197 MeV)

❖ High penetration allows detection of explosives/ which are hidden in vehicles, buried, etc.

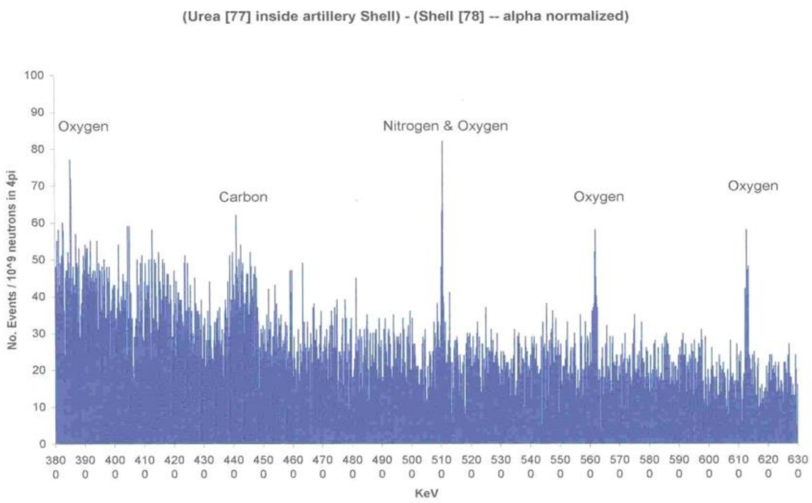
❖ The use of pulse generators and detection of correlated α particles allows to measure the neutron time of flight $\Leftrightarrow$ topographical picture of the chemical composition of the substance

http://www.calseco.com/

http://www.uncoss-project.org/

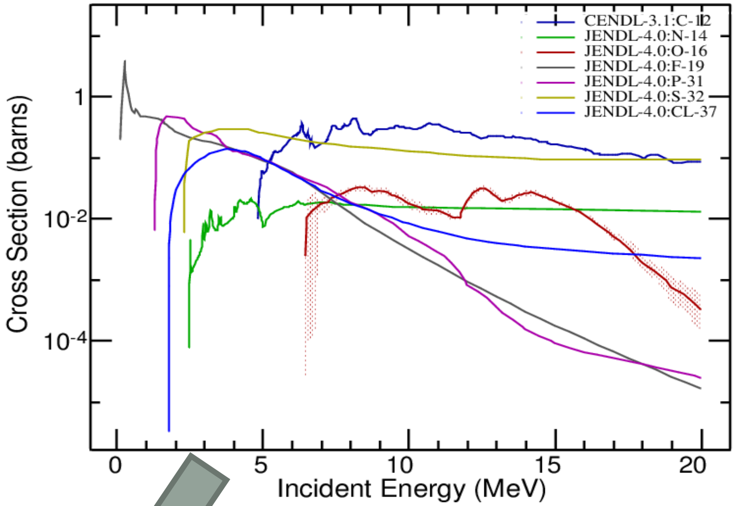
Neutron Activation Techniques

γ quanta detection

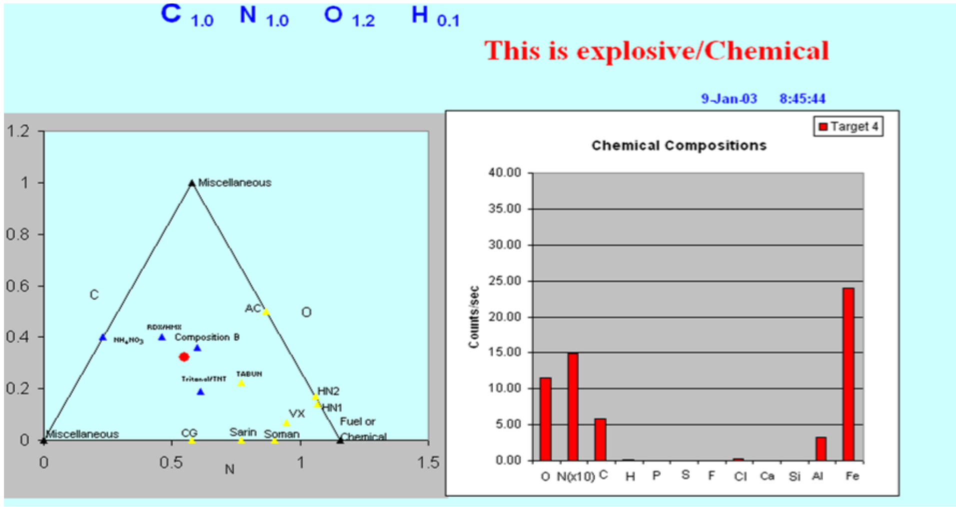


http://www.calseco.com/

Data analysis



Comparison with database of known substances & identification



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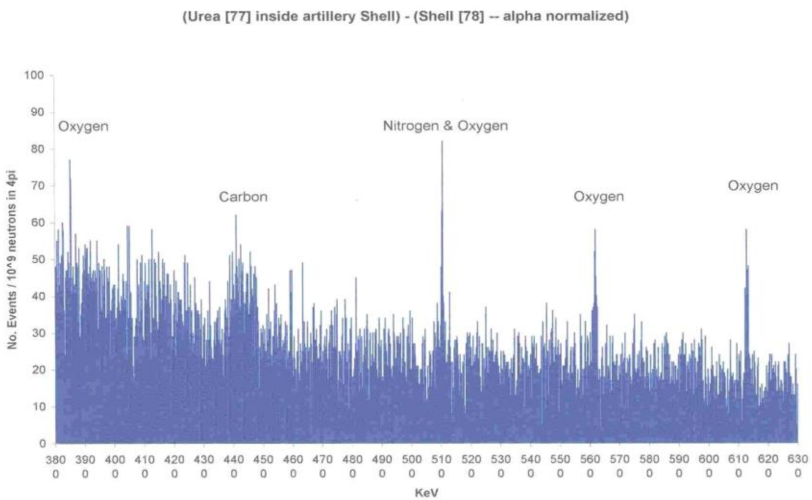
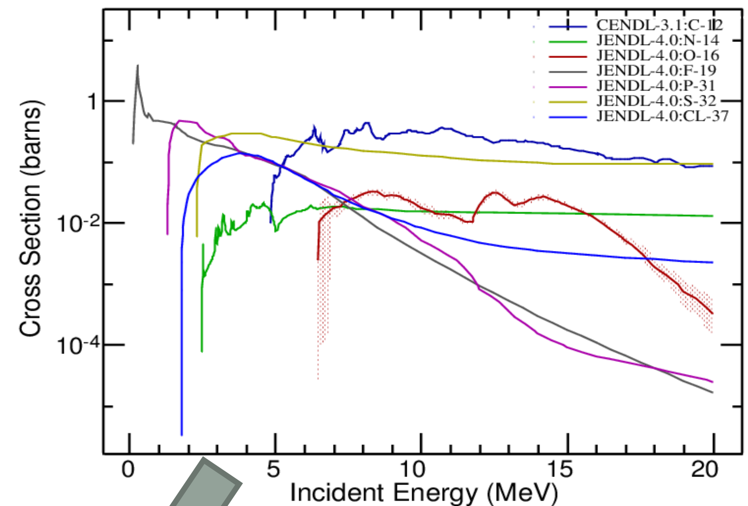
Neutron Activation Techniques

γ quanta detection

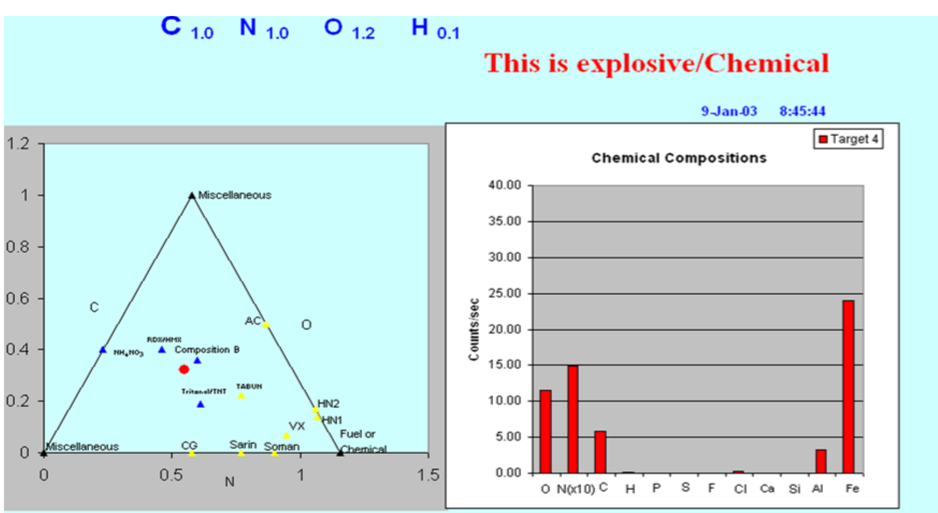


http://www.calseco.com/

Data analysis



Comparison with database of known substances & identification



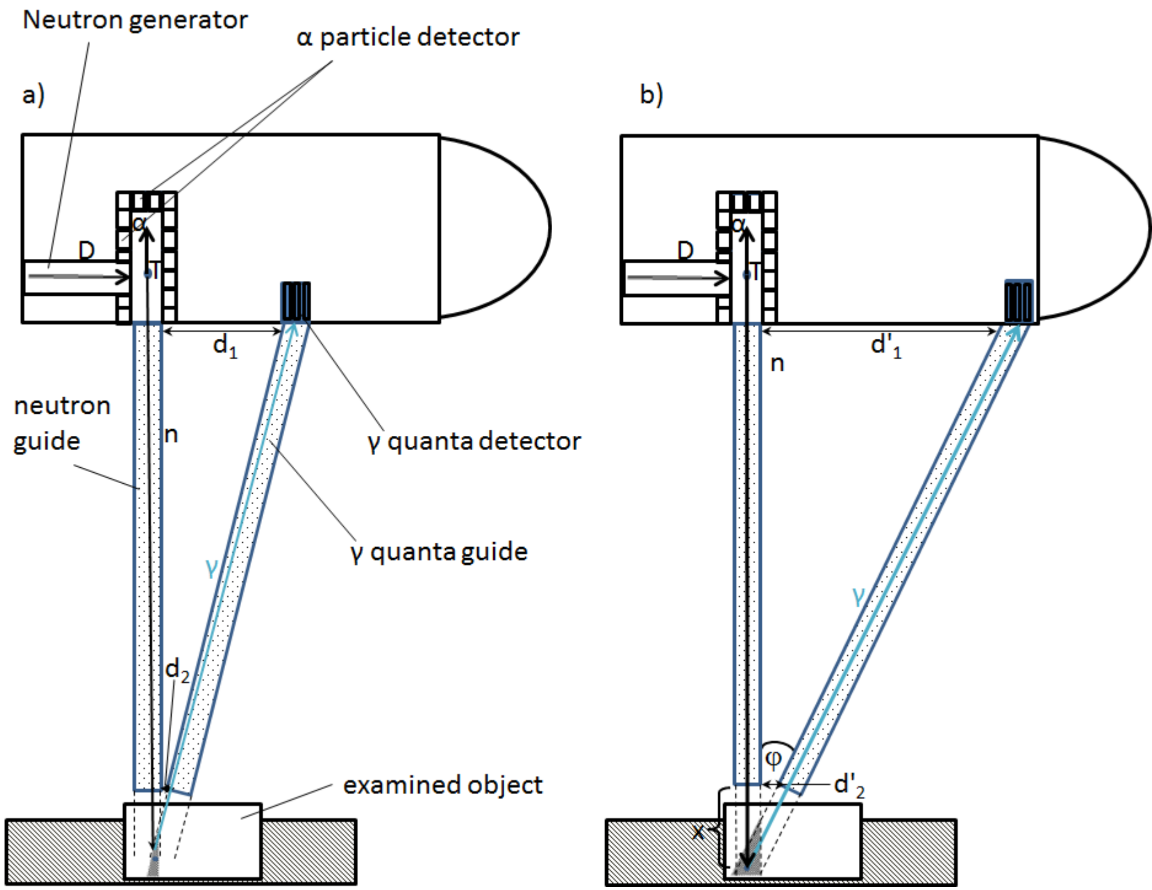
http://www.calseco.com/

Drawbacks:

- Small cross sections for some of the elements
- Decreased mobility due to detector cooling
- High neutron flux needed
- Insensitivity to the structure of molecul
- **High neutron attenuation in water**
- **High background from oxygen and nitrogen**

Underwater application

- The 14.1 MeV neutron generator with α particle detection
- Neutron and γ quanta attenuation in water minimized by guides filled with air or some other gas
- Changeable position and orientation of guides
- Position sensitive detector (**scintillator**)

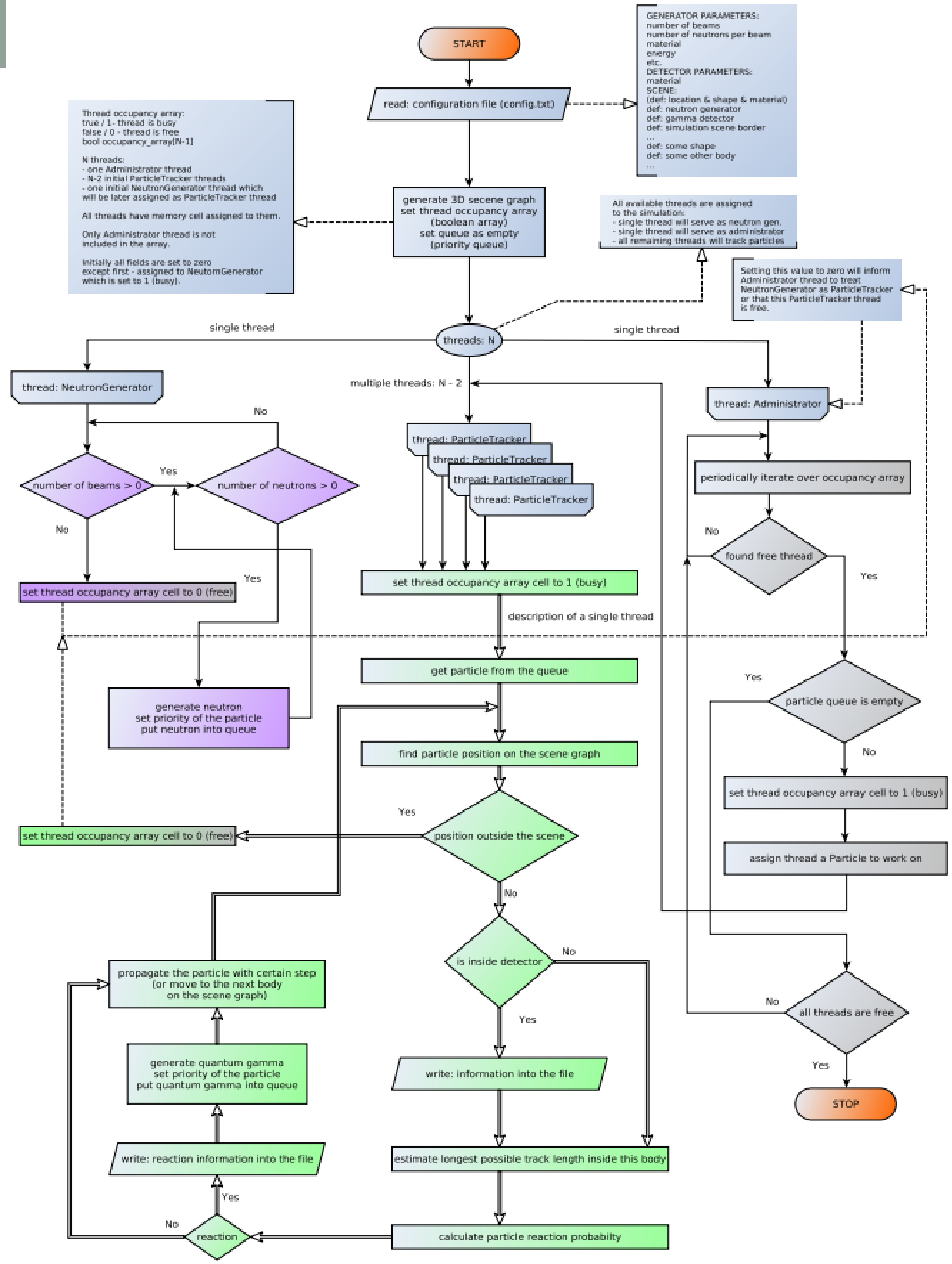


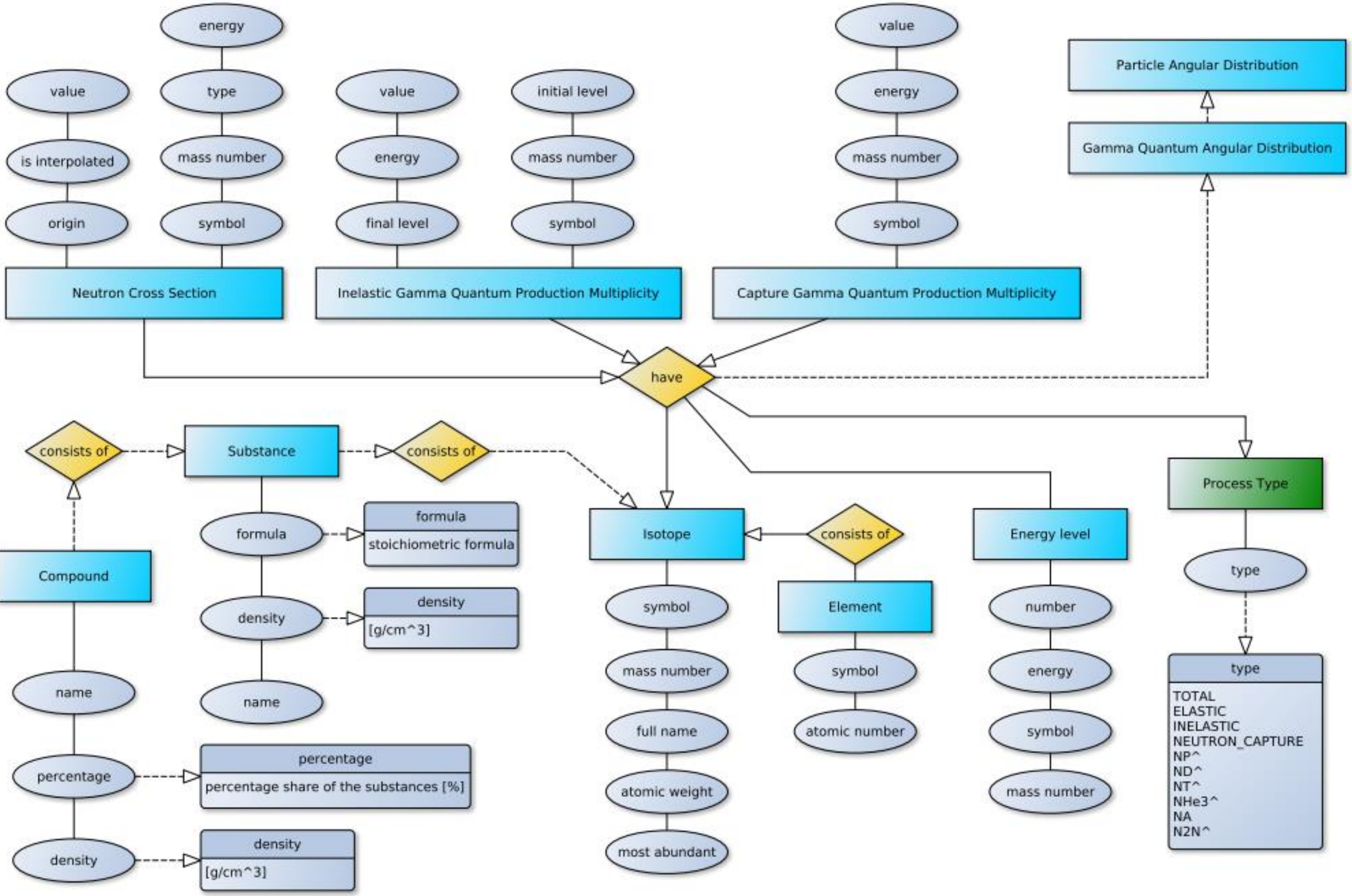
- Depth of neutron interaction determined from the time difference between neutron and γ quantum registration times:

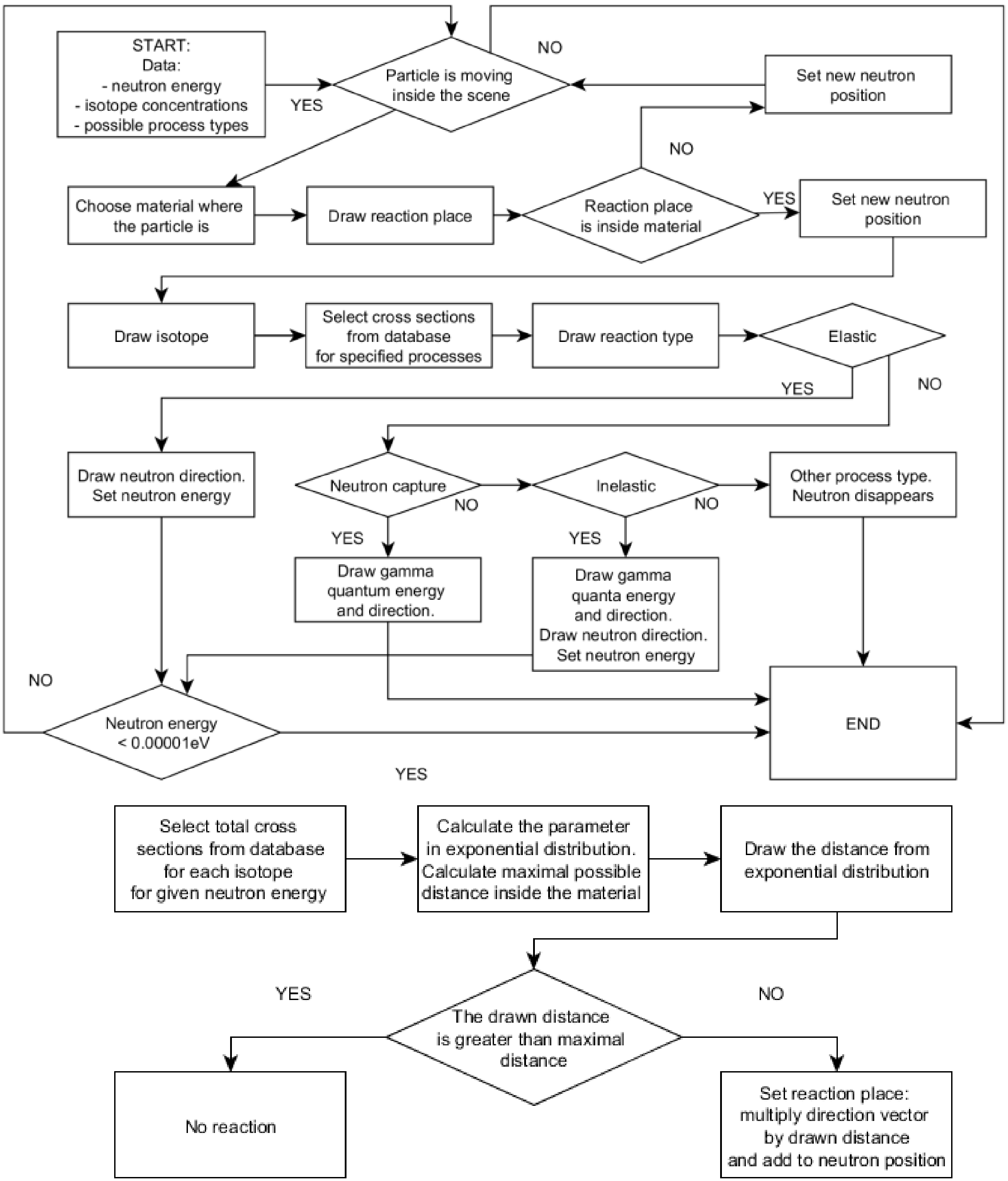
$$x = \left(\Delta t + \frac{l_\alpha}{v_\alpha} - \frac{l_n}{v_n} - \frac{l_\gamma}{c}\right)\frac{c v_n \cos\varphi}{c\cos\varphi + v_n}$$

Design of the first prototype: Monte Carlo simulations

- **Fast independent simulations devoted only to the NAA applications**
- Open source code (C++ as default programming language, standard version C++11)
- Target OS: Linux (Debian or Red Hat based)
- Multiple cores/threads (Open MPI standard & library)
- Parallel computing
- Physics: ENDF/ENSDF libraries used
- Database : SQLite3
- Relational DataBase Management System, most tables in the second normal or third normal form (2NF & 3NF)
- **Novel method of geometry definition and particle tracking based on hypergraphs**

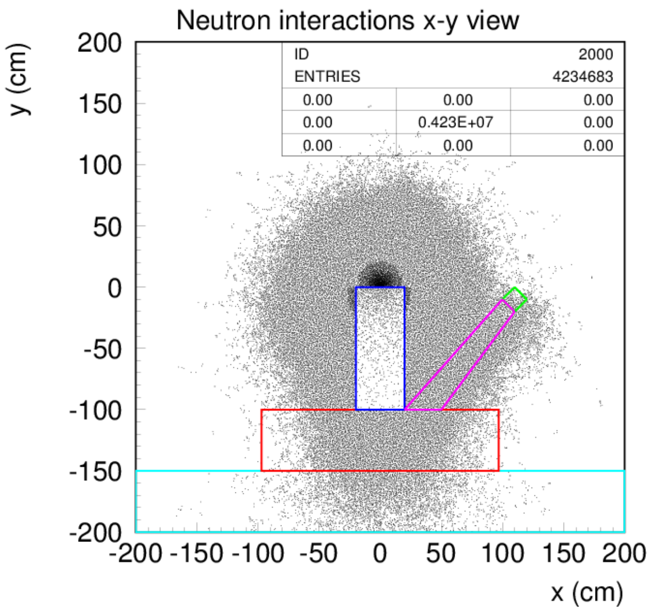


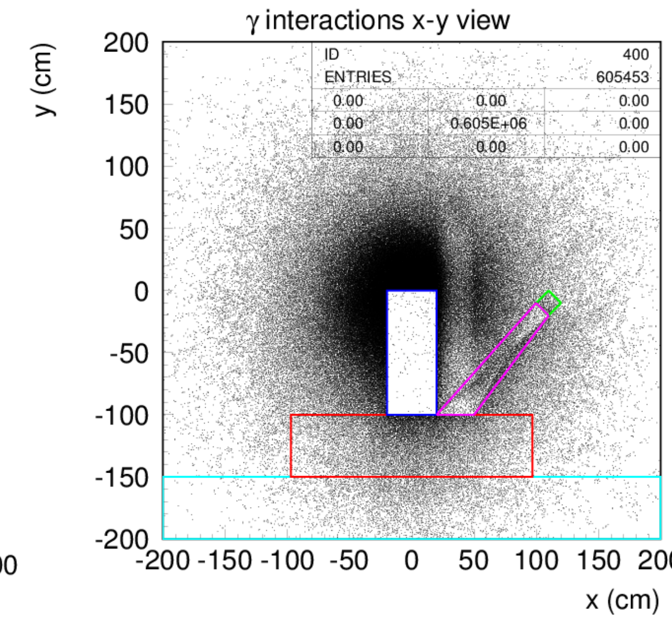

energy
value
type
value
initial level
value
energy
Particle Angular Distribution
is interpolated
mass number
energy
mass number
mass number
Gamma Quantum Angular Distribution
origin
symbol
final level
symbol
symbol
Neutron Cross Section
Inelastic Gamma Quantum Production Multiplicity
Capture Gamma Quantum Production Multiplicity
have
consists of
Substance
consists of
Process Type
formula
formula
stoichiometric formula
Isotope
consists of
Energy level
Compound
type
density
density
[g/cm^3]
symbol
Element
number
mass number
symbol
energy
type
name
name
full name
atomic number
symbol
TOTAL
ELASTIC
INELASTIC
NEUTRON_CAPTURE
NP^
ND^
NT^
NHe3^
NA
N2N^
percentage
percentage
percentage share of the substances [%]
atomic weight
mass number
density
density
[g/cm^3]
most abundant

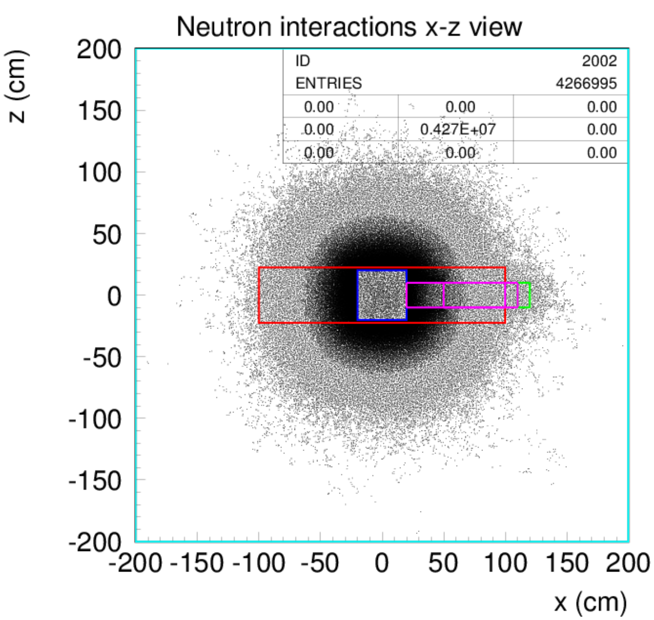

START:
Data:
- neutron energy
- isotope concentrations
- possible process types
Particle is moving inside the scene
YES
NO
Set new neutron position
Choose material where the particle is
Draw reaction place
Reaction place is inside material
NO
YES
Set new neutron position
Draw isotope
Select cross sections from database for specified processes
Draw reaction type
Elastic
YES
NO
Draw neutron direction. Set neutron energy
Neutron capture
NO
YES
Inelastic
NO
YES
Other process type. Neutron disappears
Draw gamma quantum energy and direction.
Draw gamma quanta energy and direction. Draw neutron direction. Set neutron energy
NO
Neutron energy < 0.00001eV
YES
END
Select total cross sections from database for each isotope for given neutron energy
Calculate the parameter in exponential distribution. Calculate maximal possible distance inside the material
Draw the distance from exponential distribution
YES
NO
The drawn distance is greater than maximal distance
No reaction
Set reaction place: multiply direction vector by drawn distance and add to neutron position

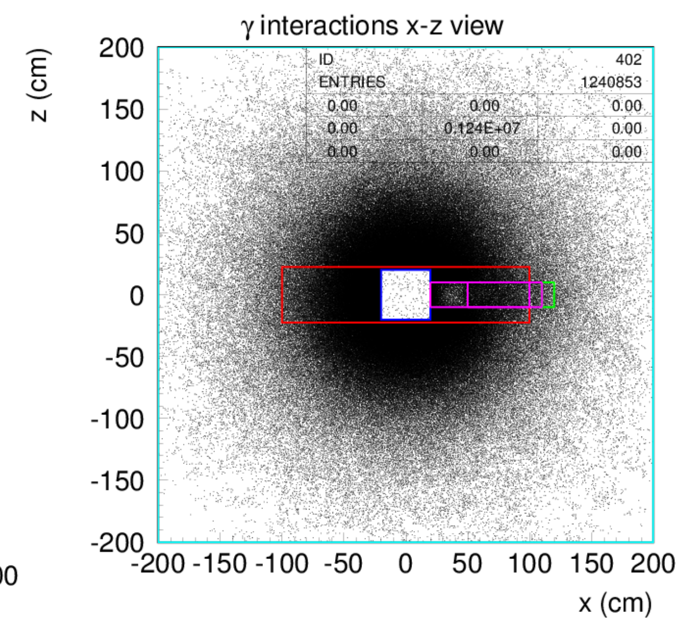
First results and validation of simulations

- The first test „scene”:
  - Container with mustard gass
  - Neutrons guide
  - Ge detector
  - γ quanta giude
  - Sea bottom (sand)
- Simulated (so far) interaction processes:
  - For neutron: capture, inelastic and elastic scattering
  - For γ quanta: Compton scattering, pair production and photoelectric effect
- Validation of the first version of the software almost finished







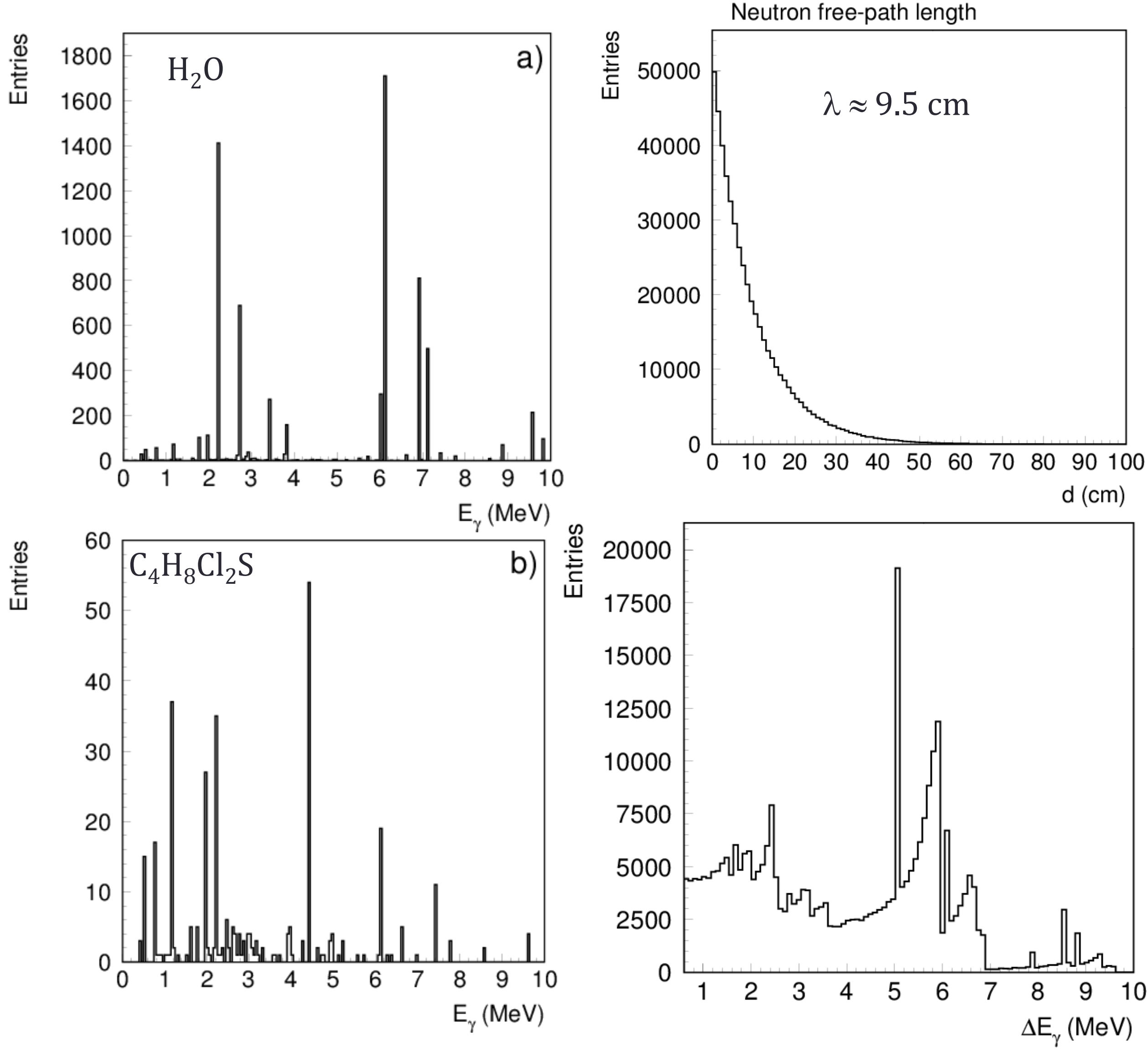


First results and validation of simulations

- Strong lines from the excitation of oxygen (~3 MeV, 6 MeV and 7 MeV), and characteristic line of neutron capture by hydrogen (about 2.2 MeV) visible

- For the container with mustard gas: big peak for gamma quanta emitted by carbon ^{12}C (E_γ = 4.43 MeV) and chlorine ^{37}Cl (~6 MeV)

- Hydrogen and sulfur compose one line at E_γ = 2.2 MeV ⇒ hard identification of ^{32}S.



Summary

- The chemical munitions sunk in seas constitute a very serious threat for environment and people
- Methods of detection used so far are not efficient enough to detect all contaminated sea areas
- Promising improvement: neutron activation techniques used on the submarine
- Design of the prototype of such device has started in the Institute of Physics of the Jagiellonian University
- We are developing a new fast simulation tool devoted to the Neutron Activation Analysis applications
- First simulations of complete identification system expected for the end of December 2015

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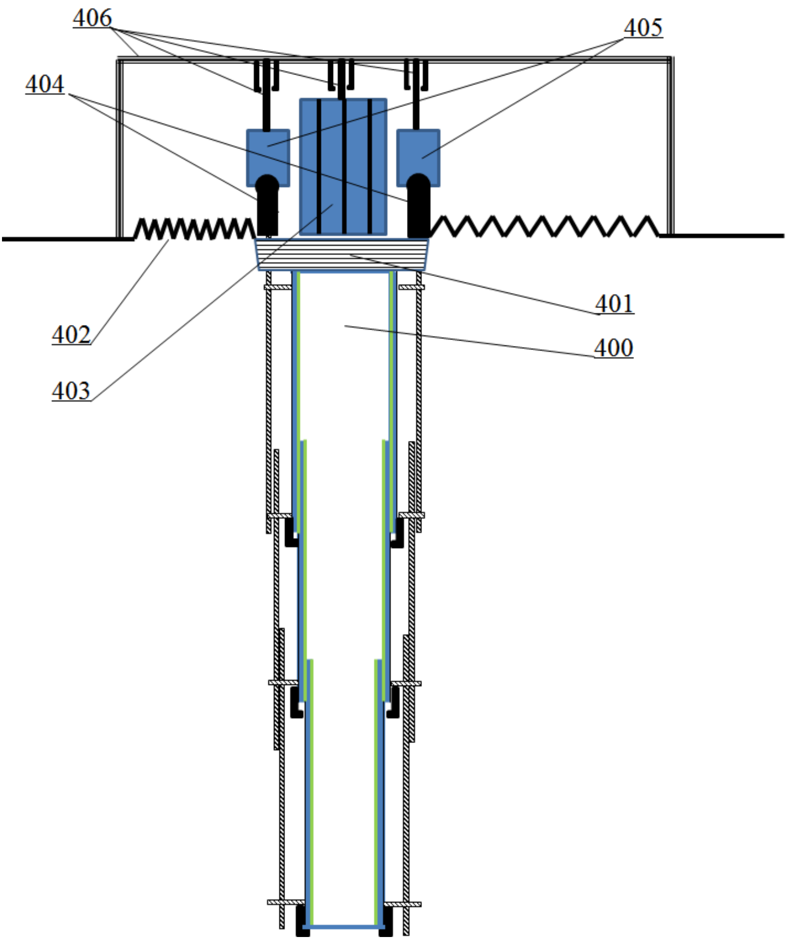
Dominika Hunik

Sławomir Tadeja

Michał Smolis

Thank You
for attention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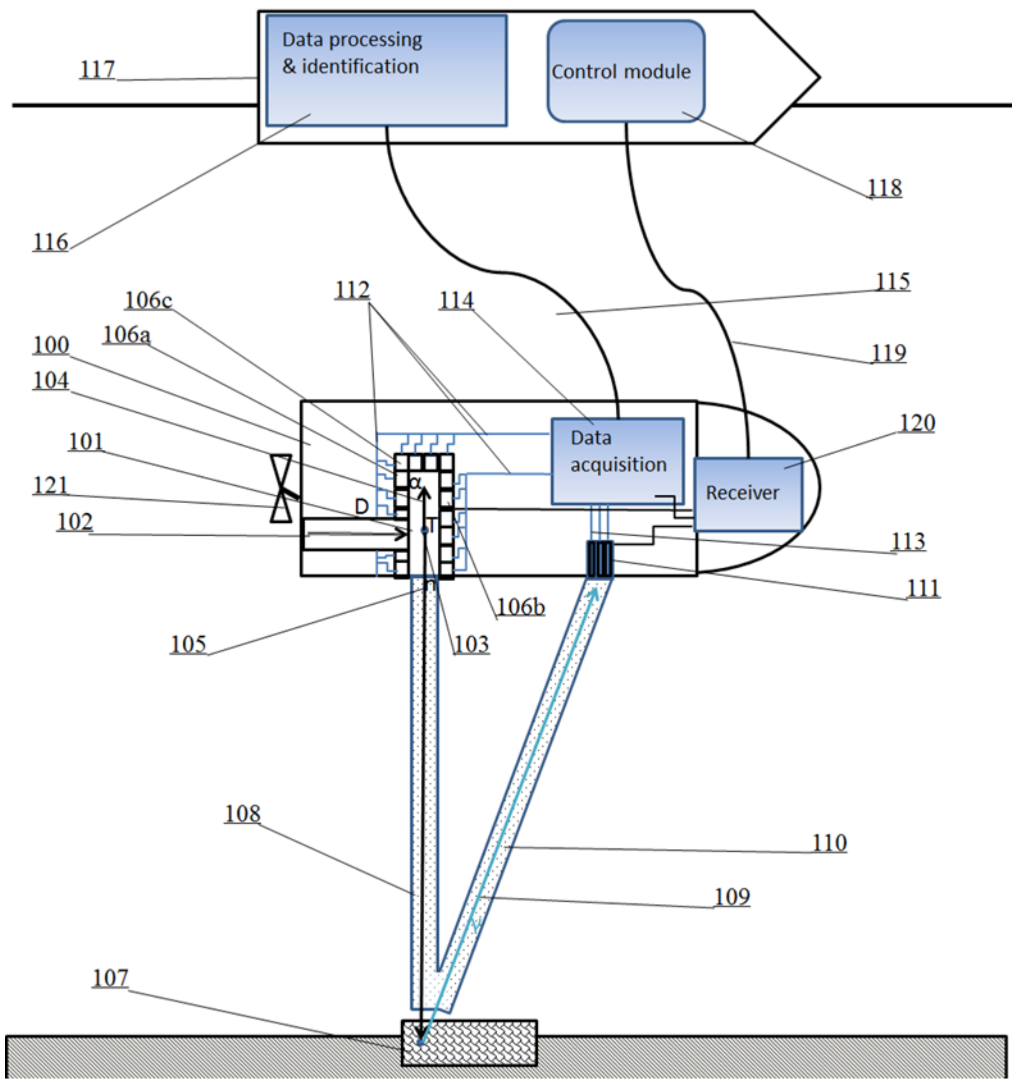
Data processing
& identification
Control module
117
118
116
115
106c
112
114
119
100
106a
104
120
101
Data
acquisition
121
Receiver
D
α
T
102
113
111
n
106b
105
103
108
110
109
107

Place of interaction

(L substances with N_l atoms in molecule)

$$P(x) = 1 - exp(-\mu_{tot} x) \Leftrightarrow x = -\frac{ln(1 - F(x))}{\mu_{tot}}; F(x) \in [0, 1)$$

(F ≡ Cumulative distribution function of x pdf generated with constant probability)

$$\mu_{tot} = \sum_{i=1}^{N} K_i \sigma_i(E_{neut});$$

$$\left(k_{il} = \frac{S_i}{\sum_{j=1}^{N_l} S_j} \frac{\rho_l N_A}{\sum_{j=1}^{N_l} S_j M_j};\ K_i = \sum_{l=1}^{L} k_{il} u_{Vl} \text{ or } K_i = \sum_{l=1}^{L} k_{il} \frac{u_{ml}}{\rho_l \sum_{i=1}^{L} \frac{u_{mi}}{\rho_i}} \right)$$

k_{il} – concentration of i^{th} atom in l^{th} substance

S_i – i^{th} stochiometric coeficient (number of i^{th} atoms in molecule [**DB**]

M_j – molar mass of j^{th} element [**DB**]

ρ_l – density of l^{th} substance [**DB**]

u_{Vl} and u_{Ml} – volume and mass fraction of l^{th} substance, respectively [**CF**]

$\sigma_i(E_{neut})$ – total cross section [**MT = 1**] for interaction with i^{th} element [**DB**]

T **F**

$x < x_{max}$

neutron propagated to x_{max}

Element

$$P(i) = \frac{K_i \sigma_i(E_{neut})}{\sum_{i=1}^{N} K_i \sigma_i(E_{neut})}$$

Elastic scatering [MT=2]

$$E'_{neut} = E_{neut}$$

[**DB**] neutron angular distibution ⇒ new neutron direction

Process

(M processes chosen by user in the Config File)

$$P(p) = \frac{\sigma_p(E_{neut})}{\sum_{i=1}^{M} \sigma_i(E_{neut})} \text{ or } P(p) = \frac{\sigma_p(E_{neut})}{\sigma_{tot}(E_{neut})}$$

σ_i – cross section for the process i [**DB**]

Fission

n+$A \rightarrow A' + A''$ [**MT=19**] (total neutron energy deposition)

n+$A \rightarrow n' + A' + A''$ [**MT=20**]

n+$A \rightarrow 2n' + A' + A''$ [**MT=21**]

n+$A \rightarrow 3n' + A' + A''$ [**MT=38**]

Neutron(s) energies⇐[**DB**]

[**DB**] neutron angular distibution ⇒ new netron direction

Leading to the nuclei excitation

$n + A \rightarrow n' + A'^* \rightarrow n' + A' + \gamma$ [MT=51-91]

n+$A \rightarrow p + A'^* \rightarrow p + A' + \gamma$ [MT=601-649]

n+$A \rightarrow d + A'^* \rightarrow d + A' + \gamma$ [MT=651-699]

n+$A \rightarrow T + A'^* \rightarrow T + A' + \gamma$ [MT=701-749]

n+$A \rightarrow {}^3He + A'^* \rightarrow {}^3He + A' + \gamma$ [MT=751-749]

n+$A \rightarrow \alpha + A'^* \rightarrow \alpha + A' + \gamma$ [MT=801-849]

Radiative Capture: $n + A \rightarrow A'^* \rightarrow A'\gamma$ [MT=102]

Excited level

(Z levels chosen by user in the Config File)

$$P(e) = \frac{\sigma_{ep}(E_{neut})}{\sum_{i=1}^{Z} \sigma_{ip}(E_{neut})}$$

σ_i – cross section for excitiation of level i [**DB**]

List of $\gamma's$ [**DB**] or sequensional calculations of $\gamma's$ energies ⇐ levels energies [**DB**]

$$E'_{particle} = \frac{(E_{neut} + M_A)^2 - M^2{}_{A'} + m^2{}_{particle}}{2(E_{neut} + M_A)} - \sum_{i=1}^{N} E_{\gamma i}$$

[**DB**] particle angular distibution ⇒ particle direction

N gamma quanta with energy E_γ [**DB**] and direction ⇐ γ angular distribution [**DB**] (usually homogeneous)

$M_A / M_{A'}$, $m_{particle}$ –mass of initial/final nuclei and final particle, respectively [**DB**]

Leading to one particle in the final state

n+$A \rightarrow p + A'$ [MT=600]

n+$A \rightarrow d + A'$ [MT=650]

n+$A \rightarrow T + A'$ [MT=700]

n+$A \rightarrow {}^3He + A'$ [MT=750]

n+$A \rightarrow \alpha + A'$ [MT=800]

$$E'_{particle} = \frac{(E_{neut} + M_A)^2 - M^2{}_{A'} + m^2{}_{particle}}{2(E_{neut} + M_A)}$$

[**DB**] particle angular distibution ⇒ particle direction

$M_A / M_{A'}$, m_p –mass of initial/final nuclei and final particle, respectively [**DB**]

Leading to more particles in the final state

n+$A \rightarrow 2n + A'$ [MT=16]

n+$A \rightarrow 2n + A' + \gamma$ [MT=876]

n+$A \rightarrow n + \alpha + A'$ [MT=22]

n+$A \rightarrow n + p + A'$ [MT=28]

n+$A \rightarrow n + d + A'$ [MT=32]

n+$A \rightarrow T + n + A'$ [MT=33]

n+$A \rightarrow {}^3He + n + A'$ [MT=34]

n+$A \rightarrow 2\alpha + A'$ [MT=108]

n+$A \rightarrow 2p + A'$ [MT=111]

n+$A \rightarrow \alpha + p + A'$ [MT=112]

n+$A \rightarrow d + p + A'$ [MT=115]

n+$A \rightarrow T + p + A'$ [MT=116]

n+$A \rightarrow \alpha + d + A'$ [MT=117]

n+$A \rightarrow 3n + A'$ [MT=17]

n+$A \rightarrow n + 2\alpha + A'$ [MT=29]

n+$A \rightarrow 2n + p + A'$ [MT=41]

n+$A \rightarrow n + 2p + A'$ [MT=44]

n+$A \rightarrow p + \alpha + n + A'$ [MT=45]

n+$A \rightarrow T + 2\alpha + A'$ [MT=113]

n+$A \rightarrow 4n + A'$ [MT=37]

n+$A \rightarrow 3n + p + A'$ [MT=42]

n+$A \rightarrow n + 3\alpha + A'$ [MT=28]

n+$A \rightarrow 3n + \alpha + A'$ [MT=25]

particle directions and energies have to be generated according to the phace space for M=1…4 particles in the final state (e.g. GENBOD)

Other potentially useful information

Neutron absorption

[MT=27; sum of MT=18 and MT=102 through MT=117]

Neutron disappearance

[MT=101; sum of MT=102-117]