CODES AND TOOLS TO INVESTIGATE SUB-CRITICAL ACCELERATOR-DRIVEN SYSTEMS

Yu.A.Korovin, A.Yu.Konobeyev, V.N.Sosnin
Institute of Nuclear Power Engineering
1 Studgorodok,
249020 Obninsk, Russia
korovin@iate.obninsk.ru

M.Vecchi
Ente per le Nuove Tecnologie, l'Energia e l'Ambiente,
40129 Bologna, Italy
vecchi@marcello1.arcoveggio.enea.it

ABSTRACT

Computer software elaborated for numerical studies of particle transport in complex heterogeneous media is described. The software includes the CASCADE code for simulation of high energy particles (with energies above 20 MeV), the MCNP-4B module for tracking of low-energy neutrons (below 20 MeV) to thermal energies, routines providing interface between high-energy and low-energy transport codes and routines for data preparation and description of special features incorporated in physical modelling (geometry and composition, α-particle pre-compound spectra, description of angular distributions, etc.). Analysis of sensitivity of the models to the variation of model parameters, to the approximations and the uncertainty of input parameters was performed. Results of calculations performed for sub-critical reactor are presented.

1. INTRODUCTION

Monte-Carlo codes such as well known HETC [1], CASCADE [2], etc. were developed during previous decades to back-up measurements performed in different accelerator laboratories around the world. Calculations performed using such codes typically referred to fairly simple target compositions and geometry. However, the prospect of design of full-scale prototype sub-critical reactor prompted the development of more sophisticated computational instruments which could allow for numerical studies of complex heterogeneous media.

Computer code system CASCADE/INPE was recently developed for such purpose. The set of codes included in the package consists of the following principal parts

I. CASCADE code calculates the characteristics of high-energy particle interactions with matter and, subsequently, tracking of particles produced to low energies. Admissible mass numbers of projectile are within the range from 1 to 240, and mass numbers of target nuclei are from 2 to 240. The energy range for projectiles is from 20 MeV up to 10 GeV. The nuclear model takes into account continuous nuclear density distribution, "trailing"-effect and allows to describe the yields of nucleons, mesons and light fragments in nuclear reactions. The code has been elaborated in JINR [2] and was modified in the present work. Basic additions to the code include

- The module for particle transport calculations for arbitrary complex geometry, such as nuclear reactor core with detail description of fuel pins, cladding etc.
- The routine for calculation of the pre-compound spectra of α-particles playing important role in the accurate description of helium production rate and long-lived nuclide production for different types of heavy targets.
- The possibility to describe angular distributions of nucleons based on the empirical parametrization, which allows to achieve agreement between calculated and measured double-differential cross-sections for nucleons for the total range of emission angles.
- New phenomenological approach to describe fission product yields.
- The possibility to calculate pre-compound γ-emission spectra.
- The routine intended to perform calculations using evaluated data files compiled in the ENDF/B-VI format containing energy and angular distributions of secondary particles. The files available for use in simulations were compiled at the Obninsk Institute of Nuclear Power Engineering (for ^{12}C, ^{16}O, ^{23}Na, ^{28}Si, ^{39}K, ^{51}V, ^{52}Cr, ^{56}Fe, ^{208}Pb, ^{232}Th, ^{233}Pa, ^{233}U, ^{238}U, ^{239}Pu for the energies up to 50 MeV, for ^{235}U up to 300 MeV) [3] and at the LANL (for most important structural materials, lead and bismuth isotopes at the energies up to 150 MeV).

II. MCNP-4B code allows to perform calculations of particle transport, multiplication factors etc. in the low-energy region in arbitrary energy units

III. The routines providing interface between high-energy (CASCADE) and low-energy (MCNP) transport codes and allowing to process the results of calculations during the computer run.

Inter-comparison of different codes performed in Ref.[1] proved that the intranuclear cascade evaporation model realized in the CASCADE code and described above produces reliable results as compared with experimental data.

New computer code package CASCADE/INPE has been elaborated to investigate sub-critical accelerator driven systems. With the help of this package the basic features of accelerator driven reactor systems were investigated. Sensitivity of calculations of reactor parameters to the choice of calculation models, approximations and uncertainty of input parameters was examined.

The principal layout of the sub-critical reactor consists of accelerator, target, core and system for heat removal.

In the present study, the concept of a sub-critical reactor is examined with core submerged in a volume filled with liquid metal coolant. The target and the coolant are composed of molten Pb-Bi alloy. Reactor vessel is a cylindrical container entailed by hemisphere with radius of 3 m and height of the cylindrical part equal to 5,85 m. The horizontal mid-plane of the active region is located at the distance of 13,3 cm below the point of beam penetration in the target. The beam pipe radius is equal to 9,75 cm. The geometry of the target and the core corresponds to that cited in [4].

The fuel composition under investigation is U-Pu MOX fuel irradiated in "Superfenix" reactor. A316 stainless steel is chosen for the analysis as a structural material.

All calculations were performed for 600-MeV protons interacting with Pb-Bi target. The accelerator current was taken to be equal to 3,0 mA, which is close to the value chosen for the EAP-80 [4].

2. SENSITIVITY OF CALCULATIONS OF REACTOR PARAMETERS TO THE CHOICE OF CALCULATION MODELS, APPROXIMATIONS AND UNCERTAINTY OF INPUT PARAMETERS

Following values characterizing the processes in the sub-critical unit were investigated. Total number of neutrons with energies below 20 MeV fed to MCNP per one incident proton is equal to

$$N_{n/p}= N_{src}/N_p. \tag{1}$$

Here N_p is the total number of primary protons, and N_{src} is the number of neutrons with energies below 20 MeV produced by CASCADE code, the so-called "source" neutrons.

Relative amount of neutrons produced in the matter (N_n) per "source" neutron is defined as follows

$$M_{src} = N_n/N_{src} \tag{2}$$

The source criticality factor k_{src} is equal to

$$k_{src} = 1 - 1/M_{src} \tag{3}$$

The calculations were performed for the number of incident protons N_p in the CASCADE simulations equal to 2,000. This number of incident proton events chosen for the CASCADE simulation corresponds to 25,000-31.000 particle histories simulated in the MCNP runs.

All calculations presented in this Section were performed for homogeneous assemblies. The variant of the core with 120 elements is considered. The length of active part of the fuel pin is taken to be equal to 87 cm.

2.1 VARIATION OF LEVEL DENSITY PARAMETER IN THE DESCRIPTION OF PARTICLE INTERACTIONS WITH NUCLEI FOR ENERGIES ABOVE 20 MeV

Calculations were performed using intranuclear cascade evaporation model described above and also in Ref [5]. Level density parameter was set to be equal to $a=A/10$, $A/20$ and $A/5$. The results produced are given in Table 1.

The explanation of variation of the $N_{n/p}$ value shown in Table 1 is following: increase of the level density parameter leads to the decrease of the "nuclear temperature", which, consequently, results in the increased number of particles emitted during the equilibrium stage of the reaction per one incident proton. The value of source criticality factor remains practically the same for all three cases.

2.2 CORRECTION OF ANGULAR DISTRIBUTIONS OF NUCLEONS IN NUCLEON-NUCLEON INTERACTIONS

The calculations described below were performed using Kalbach's empirical systematics [6] for description of angular distributions of nucleons escaping from nuclei. Application of the above systematics allows to reproduce more accurately experimental values of double-differential cross-sections for nucleons for different, mainly big angles. The resulting values of $N_{n/p}$ and k_{src} are presented in Table 1.

2.3 APPLICATION OF EVALUATED NUCLEAR DATA FILES AT THE ENERGY RANGE BELOW 150 MEV

Calculations were performed using evaluated neutron data from Ref [3]. The files were extended to the above mentioned neutron cut-off energy of 150 MeV. The model applied to evaluate double-differential cross-sections included calculations based on the modified geometry-dependent hybrid exciton model to obtain non-equilibrium spectra realized in the ALICE/ASH code [7]. Equilibrium spectra were calculated using super-fluid nuclear model to obtain nuclear level density [8]. Corrections were made in the calculated results to fit them to the existing measurements.

Evaluated data for ^{208}Pb and ^{209}Bi for energies below 150 MeV were used in the present calculations. Level density parameter was taken to be equal to $a = A/10$ to describe interactions at energies exceeding 150 MeV.

The definition of "source" neutrons given above remains unchanged. The source criticality factor calculated and the $N_{n/p}$ value are given in Table 1. Comparison of the data obtained with respective values described in Sec.2.1 and 2.2 demonstrates relatively small changes in k_{src} values.

2.4 UNCERTAINTY OF DESCRIPTION OF PRE-EQUILIBRIUM ENERGY SPECTRA OF NUCLEONS

Following calculations were performed to assess sensitivity of calculated k_{src} values to the method of description of non-equilibrium processes. It was assumed herewith, that neutrons with energies above 20 MeV are not formed in the nuclear interaction of incident proton with medium. This means that contribution of non-equilibrium processes in the spectra is virtually missing. Such calculation performed using the INC model with $a = A/10$ gives the result presented in Table 1.

The $N_{n/p}$ value is naturally decreased as compared with other results. The difference between the results obtained above indicates that contribution of non-equilibrium processes of incident interacton with medium in the integral value of production of neutrons with energies above 20 MeV is significant. It is interesting to note here, that k_{src} value remains practically unchanged.

2.5 SENSIBILITY TO THE CHOICE OF NEUTRON DATA LIBRARIES

All preceding calculations were performed using neutron data from ENDF/B-VI library for energies below 20 MeV. For the sake of comparison calculation was performed taking neutron data for ^{208}Pb and ^{209}Bi from the ENDL85 data library. Following values of spallation neutron multiplicity and source criticality factor were produced

$$N_{n/p} = 14.63, \qquad k_{src} = 0.900 \pm 0.002$$

Table I. Number of neutrons with energies below 20 MeV per initial proton, $N_{n/p}$, and source criticality factor, k_{src} calculated using different approximations and approaches. The error for k_{src} value is equal to 0.002 for each case.

Type of calculations	$N_{n/p}$	k_{src}
INC model, $a=A/10$	14.63	0.9307
INC model, $a=A/20$	12.67	0.9291
INC model, $a=A/5$	15.60	0.9278
INC model+Kalbach systematics, $a=A/10$	14.69	0.9282
INC model, $a=A/10$ + evaluated data files up to 150 MeV	13.75	0.9294
No pre-equilibrium phase in the first interaction, $a=A/10$	6.386	0.9286

Comparison of these results with those presented in Table 1 shows considerable drop in the k_{src}-value. This fact indicates sensitivity of neutron transport simulation to the choice of neutron data. Currently application of the data from the ENDF/B-VI data library seems to be most reasonable.

3. RESULTS OF CALCULATIONS

3.1. CALCULATION OF EFFECTIVE CRITICALITY FACTOR AND SOURCE CRITICALITY FACTOR FOR DIFFERENT DESIGN OF ACTIVE REGION

All calculations with the help of the MCNP code were performed for homogeneous hexagonal elements. ENDF/B-VI data at 300 K were used for the calculations.

Fig.1 shows the dependence of source criticality factor and effective criticality factor on the length of fuel pin for sub-critical reactor types with 120 and 132 assemblies. Also, Fig.1 presents the comparison between k_{src} and k_{eff}. One can see that for the fuel composition under consideration k_{src} and k_{eff} have close values. Fig.2 illustrates the power of reactor units with different number of assemblies depending on the length of the fuel pin. The power equal to 80 MW is observed for the unit with 120 elements and the fuel pin length equal to 115 cm and for the reactor with 132 elements and the fuel pin length equal to 105 cm.

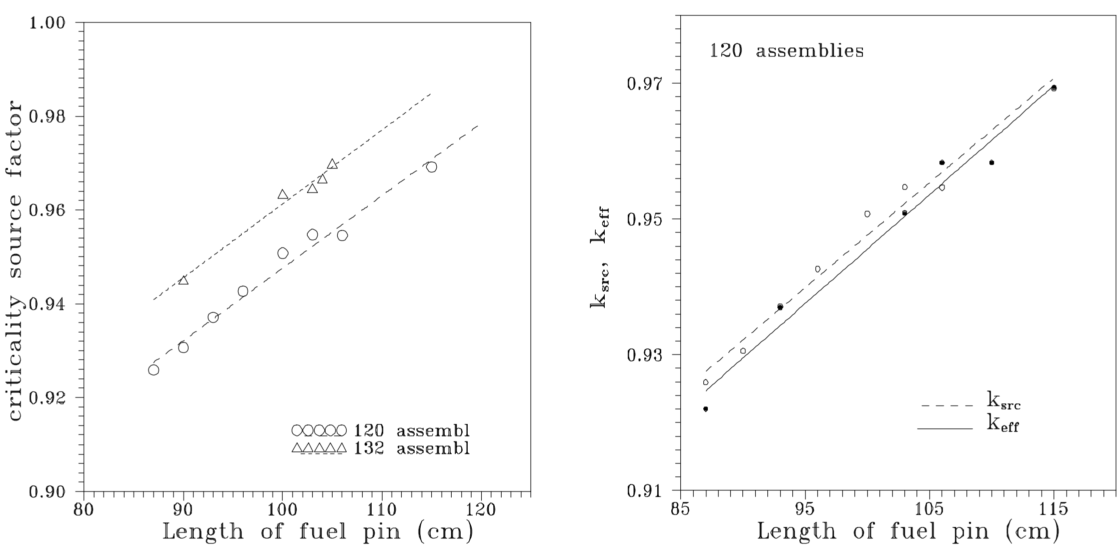

Fig.1. Dependence of source criticality factor k_{src} on the length of fuel pin for reactor core with 120 (circle) and 132 (triangle) assemblies (left) and comparison of k_{eff} (solid line) and k_{src} (dashed line) for different length of fuel pin for reactor core with 120 assemblies (right)

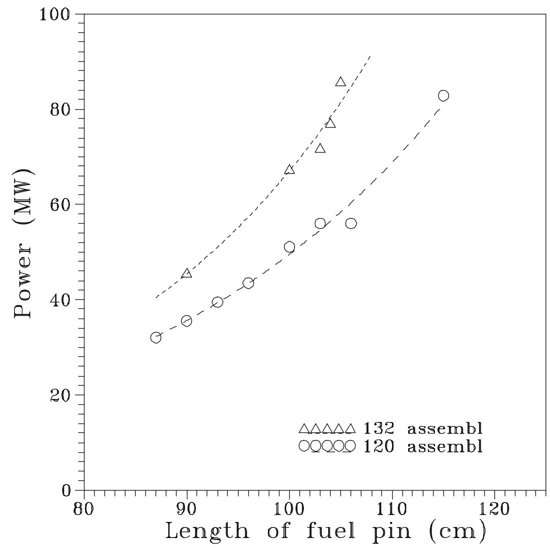

Fig.2 Power of the sub-critical unit for the core with 120 (circles) and 132 (triangles) assemblies for different length of fuel pin

3.2. NEUTRON SPECTRA INSIDE THE UNIT

Fig.3 shows neutron spectrum calculated and averaged for active region. The energy integrated neutron flux averaged for each "round" of hexagonal elements is shown in Fig.6. It can be seen that for 80 MW power unit the neutron flux is changed from 1.43×10^{15} to 0.67×10^{15} n/cm^{2}s depending on the distance from the beam axis. Near the point of primary beam penetration in Pb-Bi target the neutron flux is equal approximately to 1.8×10^{15} n/cm^{2}s.

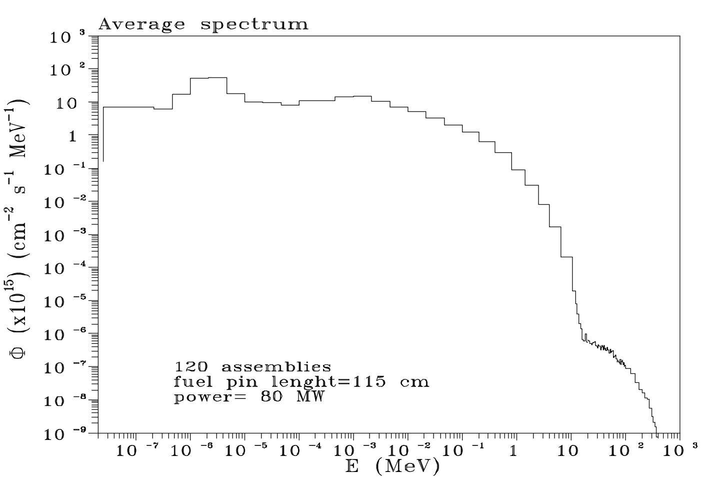

Fig.3 Average neutron spectrum for the reactor core with 120 assemblies and fuel pins length equal to 115 cm.

3.3 ENERGY DEPOSITION

Energy deposition has been calculated for the sub-critical unit with 120 and 132 fuel assemblies. Fig.4 shows typical energy deposition in units of kW/cm^3 (fuel) depending on the height of fuel pin with the total length of 115 and 105 cm. The values presented in Fig.4 correspond to the "round" of fuel elements exposed to the most severe operational conditions (closest to the beam axis).

Fig.5 illustrates energy deposition in the region of the target close to the point of primary beam penetration. The figure shows the energy deposition for primary beam and subsequent nuclear reactions in the matter induced by particles with energies above 20 MeV calculated with the help of the CASCADE code. Contribution of γ-rays produced in the interactions of such particles is presented separately. Fig.5 shows also the energy deposition due to nuclear reactions and γ-rays produced in the interactions of neutrons with energies below 20 MeV with matter calculated using the MCNP code.

There is a sharp jump in the value of the energy deposition for primary proton beam at the distance equal to the range of 600-MeV protons in Pb-Bi (30 cm). Similar jump was observed, also, in Ref [9].

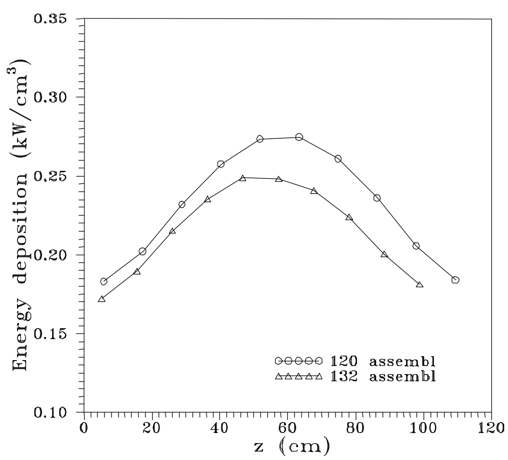

Fig.4 Z-distribution of energy deposition for the assembly close to the beam axis (third round) for the reactor core with 120 (circle) and 132 (triangle) assemblies in kW/cm^3 (fuel). For both cases total power is equal to 80 MW.

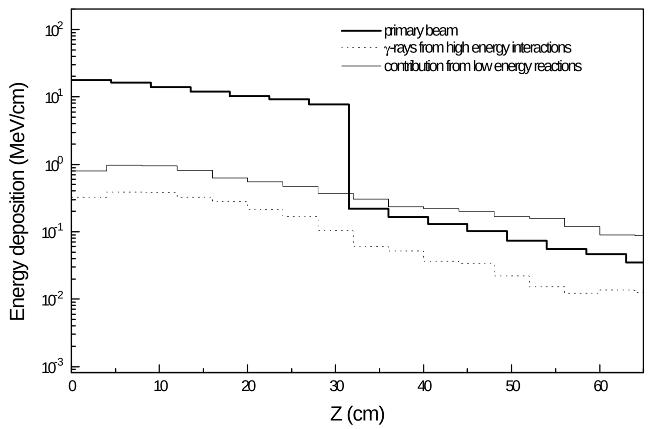

Fig.5 Z-distribution of energy deposition for the target area of the 80-MW unit(Mev/cm). Contributions: ionization losses in the matter produced by primary proton beam and charged reaction products with energies above 20 MeV (thick solid line); same for γ-rays produced in the reactions induced by particles with energies above 20 MeV (dashed line); energy yield from nuclear reactions and γ-rays produced in the interactions of neutrons with energies below 20 MeV (thin solid line).

3.4 COMPARISON OF MULTIPLICATION FACTORS OBTAINED USING DIFFERENT DATA LIBRARIES

The value of the effective neutron multiplication factor has been calculated with the help of MCNP/4B code for the EAP-80 facility using different neutron data libraries. The details of the calculations are given in Ref [5].

The configuration of the reactor was the same as that described in Refs [4,5]. The calculations were performed for hexagonal homogeneous elements. Neutron data for MCNP runs were prepared in the present work with the help of the NJOY/94 code.

The values of k_{eff} obtained are given in Table II.

The comparison of the data presented in Table II shows considerable discrepancies in the k_{eff} -values calculated with the help of different data libraries. For this reason the choice of appropriate data library for neutron transport calculations is a very important problem to be solved in future.

Table II. The k_{eff} -value calculated with the help of different data libraries

Library	Full data set is used for calculation	Data for Pb and Bi isotopes are taken from below mentioned libraries, other ones are from ENDF/B-VI
ENDF/B-VI	0,918 ± 0,001	
ENDF/B-V	0,896 ± 0,001	
BROND-2.2	0,906 ± 0,001	0,921 ± 0,001
ENDL-85	0,865 ± 0,001	0,889 ± 0,001
JENDL-3.2	0,913 ± 0,001	0,911 ± 0,001

3.5 CALCULATIONS OF NEUTRON YIELD FROM LEAD TARGET

Total neutron yield has been calculated for thick lead target with the help of the CASCADE/INPE code to compare with calculations of other authors and experimental data. The primary proton energy is equal to 0.8 and 1.6 GeV. The size of the target is D20×L60 cm for 0.8 GeV-proton irradiation and D20×L120 cm for 1.6 GeV-proton irradiation. Results of calculations are given in Table III.

Table III. Neutron yield from lead target irradiated with 600-MeV incident protons

Origin of data	Primary proton energy	
	0.8 GeV	1.6 GeV
Measured by slowing technique approach [10]	16.6	33.5
Measured by threshold technique approach [10]	18.9	37.8
"CASCADE/INPE" code	18.28	38.96
ANSALDO [11]	10.525	
ENEA [11]	19.573	
LANL [11]	17.954	
KFK [11]	16.566 16.916 16.673	
"MARS-10" code [10]	22.0	45.6

4. CONCLUSIONS

The computer software discussed is a universal tool for numerical studies of nuclear reactor incorporating particle beams within wide energy range. The software incorporates well-proven Monte-Carlo transport codes. It allows to perform calculations of parameters of particle transport in the medium of complex geometry and composition including all conceivable reactor materials. Particle transport can be simulated using different data libraries. Calculations performed show reasonable agreement with similar results produced by other groups.

REFERENCES

1. R.Michel, P.Nagel, P. "International Codes and Model Intercomparison for Intermediate Energy Activation Yields", NEA OECD/OCDE, NSC/DOC(97)-1, NEA/P&T No 14, Paris, 1997.

2. V.S.Barashenkov, Le Van Ngok, L.G.Levchuk et al, Preprint of Joint Institute for Nuclear Research, Dubna, JINR R2-85-173, 1985.

3. Yu.A.Korovin, A.Yu.Konobeyev, P.E.Pereslavtsev et al, "Evaluation and Test of Nuclear Data for Investigation of Neutron Transport, Radiation Damage and Processes of Activation and Transmutation in Materials Irradiated by Intermediate and High Energy Particles", Proc. Int. Conf. Nuclear Data for Science and Technology. Trieste, Italy, May 1997, p.851

4. "Energy Amplifier Demonstration Facility Reference Configuration", Report ANSALDO, EA B0.00 1 199 Rev.0, 22.12.1998

5. A.Yu.Konobeyev, Yu.A.Korovin, V.N.Sosnin, M.Vecchi, "Study of Accelerator-Driven Reactor Systems", *Kerntechnik*, **64**, pp.284-293 (1999).

6. C.Kalbach, "Systematics of continuum angular distributions. Extensions to higher energies", *Phys. Rev.*, **C37,** pp.2350-2370 (1988).

7. A.Yu.Konobeyev, Yu.A.Korovin, P.E.Pereslavtsev, "Code ALICE/ASH for Calcualtion of Excitation Functions, Energy and Angular Distributions of Emitted Particles in Nuclear Reactions" INPE, Obninsk, February 1997.

8. A.V.Ignatyuk, K.K.Istekov, G.N.Smirenkin, *Yadernaja Fizika* **29,** p.875 (1979); A.V.Ignatyuk, J.L.Weil, S.Raman, S.Kahane, *Phys. Rev.* **C47,** p.1504 (1993).

9. V.I.Belyakov-Bodin, V.D.Kazaritsky, A.L.Povarov, et al, *Nucl. Instr. Meth.* **A295,** p.140 (1990).

10. E.I.Yefimov, S.V.Ignatiev, “Spallation Product Formations and Secondary Neutron Yields from ADS Targets Irradiated by High-Energy Protons”, Proc. Int. Conf. Nuclear Data for Science and Technology, Trieste, Italy, 1997, p.1537.

11. “OECD: Thick Target Benchmark for Lead and Tungsten”, Report NSC/DOC(95)2, 1995.