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OPTIMIZATION STUDY OF ULTRACOLD NEUTRON SOURCES AT TRIGA REACTORS USING MCNP

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1 Introduction

The development of high intensity cold and very cold neutron sources is one of the important problem in condensed matter neutron research and in fundamental investigations with neutrons [1]. Ultracold neutrons (UCN) (energies below $\sim 2 \cdot 10^{-7} eV$) have proven to be useful instruments in several important experiments in low energy elementary particle physics [2]: the search for the neutron electric dipole moment, precise measurement of the neutron lifetime, the planned measurement of correlations in neutron decay, and possible experiments with unprecedentedly high sensitivity to the energy and momentum changes in UCN scattering and deviation under the influence of external forces.

These experiments have one feature in common — the time diagram of the experiment. It generally consists of three parts: in the first part the storage volume is filled with neutrons, in the second, the stored neutrons are kept in the storage chamber for a long period of time, and in the third, the storage chamber is emptied and the neutrons that remain are counted with the detector. The experimenter needs neutrons from the moderator only during the first short interval. TRIGA pulse reactors, which are able to produce the high intensity pulses at intervals of $10 - 20 min$ are most suitable for this kind of experiments.

Due to the very low mean reactor power in this mode of operation, it is possible to use for cold neutron production the most promising moderators: very cold solid methane, deuterium, and heavy methane, which can not be used at high flux reactors because of their low heat conductivity at low temperatures and low radiation stability. From the many different and partly used methods of producing UCN [3] only two are in use now: extraction of UCN at stationary reactor from small-sized liquid hydrogen moderator through vertical neutron guide (Serebrov's group at Gatchina) [4] and Steyerl's turbine at ILL [5]. De[illegible]es of UCN achieved in experimental volumes are around $10 cm^{-3}$. To increase the precision and sensitivity of the experiments, the UCN density is of crucial importance.

2 Geometry and method of calculation

The geometry of the reactor and moderator is shown in fig.1. As a typical TRIGA reactor, we took the exact geometry of the reactor core and the graphite reflector of TRIGA reactor of the Atomic Institute of Austrian Universities (Vienna). To simplify the calculations we use a homogeneous model reactor core composition (instead of heterogeneous): $U - 11.5kg$, $(20\% \ ^{235}U)$, $Zr - 130.8kg$, $H - 1.475kg$, $H_2O - 20.52kg$. The volume of the core: $\phi = 49.5cm * 35.56cm$.

Graphite reflector around the core: radial thickness $30.5cm$, height $56cm$.

The solid methane moderator ($T = 20K$) is placed in this model calculations inside the graphite reflector at three different distances from the core boundary: 0, 13, and $32cm$ in the median plane of the core. The aluminium cladding of the moderator and the graphite reflector was not taken into account in this optimization.

We aimed at realizing the optimal very cold (VCN) and UCN neutron sources in the sense of maximum efficiency for neutron production and the smallest heat load from reactor radiation. The cold source consists of two parts: a premoderator of very cold solid methane (the most efficient known cold neutron moderator) and a final stage moderator (VCN and UCN converter) of very cold solid deuterium [6, 7] or solid heavy methane CD_4. The advantage of deuterated converters in comparison with hydrogenous ones (in spite of their lower neutron cooling cross section) consists in the low capture cross section and the consequently large effective depth of the UCN (VCN) coming out of the converter. The purpose of the premoderator is to produce cold neutrons to irradiate the converter. The efficiency of the latter for VCN and UCN production is highest when it is irradiated with a cold neutron flux. The important criterion for the choice of the converter is the finest overlap of the incident cold neutron spectrum with the excitation spectrum of the converter (the main contribution of UCN (VCN) production in the converter comes from single downscattering events).

The Monte Carlo Neutron Photon (MCNP) [8] computer code, including a powerful three-dimensional geometry and source modelling capability, was used in our calculations of neutron transport and moderation beginning from the birth of the neutron in the fission event. Different forms and sizes of solid methane moderators were tried in order to choose the optimal one for the highest VCN and UCN production and the lowest radiation energy deposition.

3 Results of calculations of UCN (VCN) production

Figure 2 shows the calculated neutron spectra inside the graphite reflector (without a cold moderator and neutron guide channel) in three different positions of fig.1.b. Figures 3-5 show the calculated thermal and cold neutron spectra for different cross sections of the neutron guide in the vicinity of the solid methane moderators of three different forms (density of the moderator $n = 2.0 \cdot 10^{22} molecules/cm^3$). In view of the fact that the optimal deuterated VCN and UCN converter has a thickness of several cm, the form of the moderator of fig.5 is the preferable one. The calculations of cold neutron fluxes from the cold CH_4

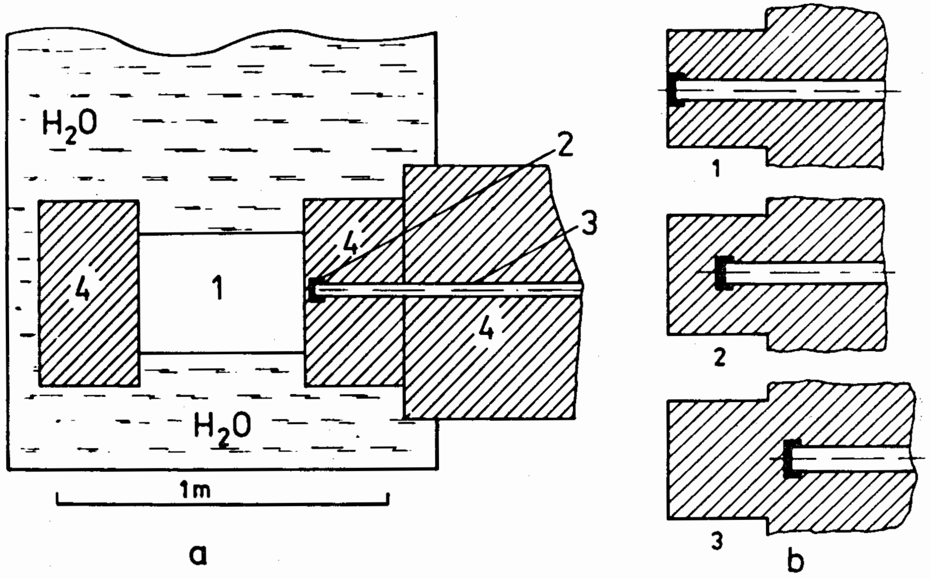

Fig.1.

- a. Reactor, cold neutron source, and neutron guide geometries:
  1. TRIGA core
  2. Cold solid methane moderator
  3. The first section of the neutron guide
  4. Graphite reflector
- b. Three positions of a cold methane moderator in a graphite reflector: distance from the core surface: $1 - 0cm$, $2 - 13cm$, $3 - 32cm$.

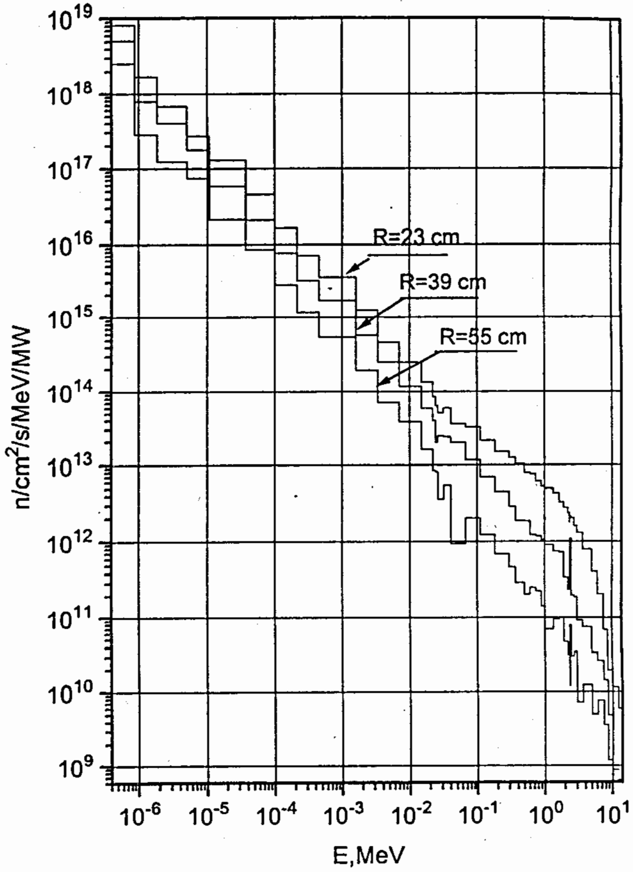

Fig.2. Neutron spectra (without moderator) in the three positions of fig.1.b inside the graphite reflector. The figures show the distance from the core center.

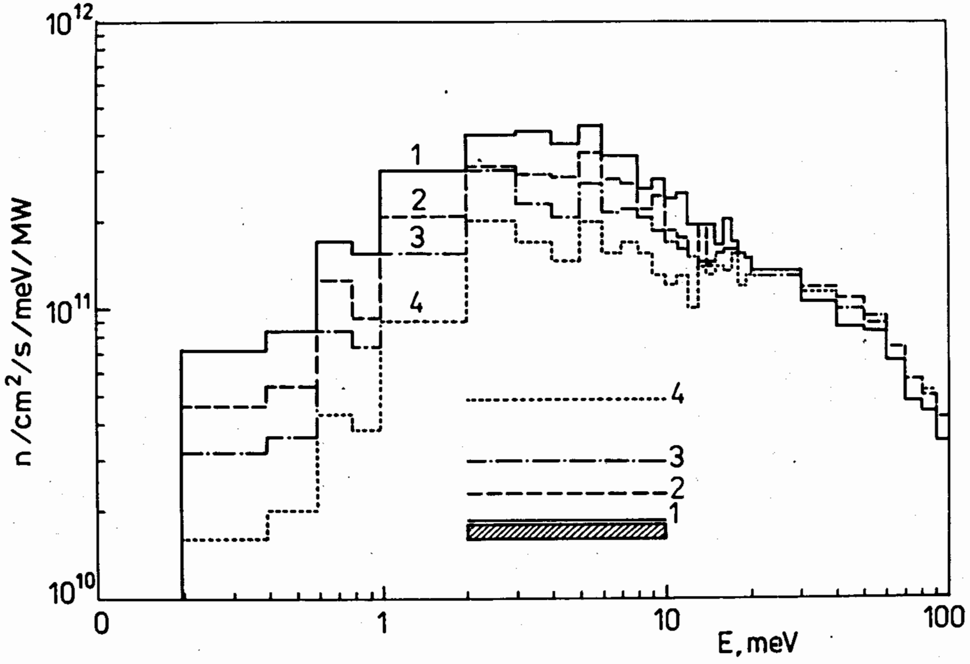

Fig.3. Cold and thermal neutron spectra from the flat cold methane moderator $\phi 10cm * 1cm$ in position 1 of fig.1b inside the graphite reflector, averaged over a $\phi 10cm$ area at different distances from the moderator surface: $1 - 0cm$, 2- 1.5cm, 3-3cm, 4-6cm.

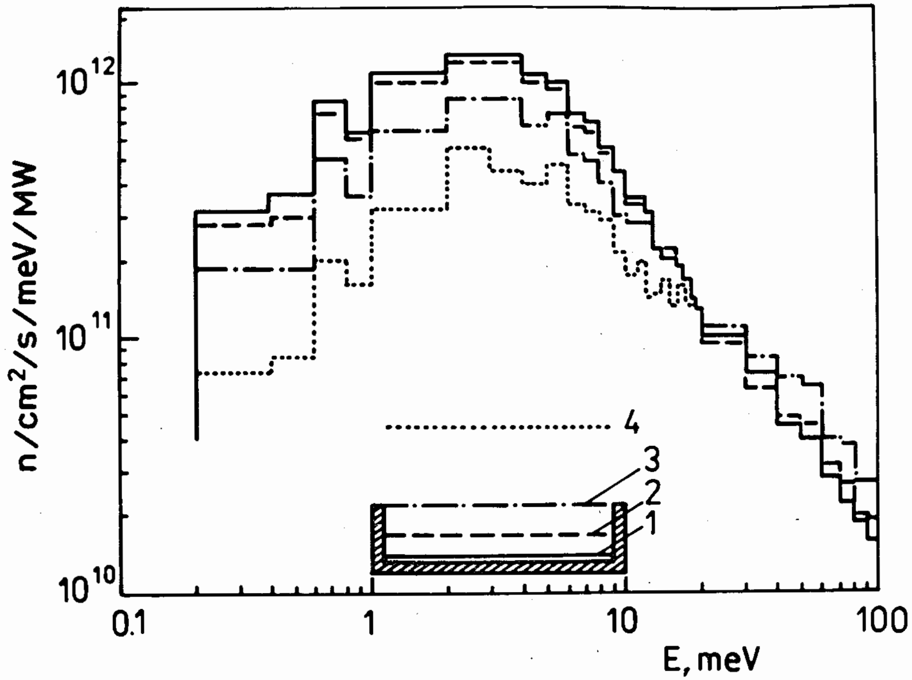

Fig.4. The same as in Fig.3 for the case where the methane moderator has the form of a cup $\phi 10cm * 4cm$ with a wall thickness of $1cm$.

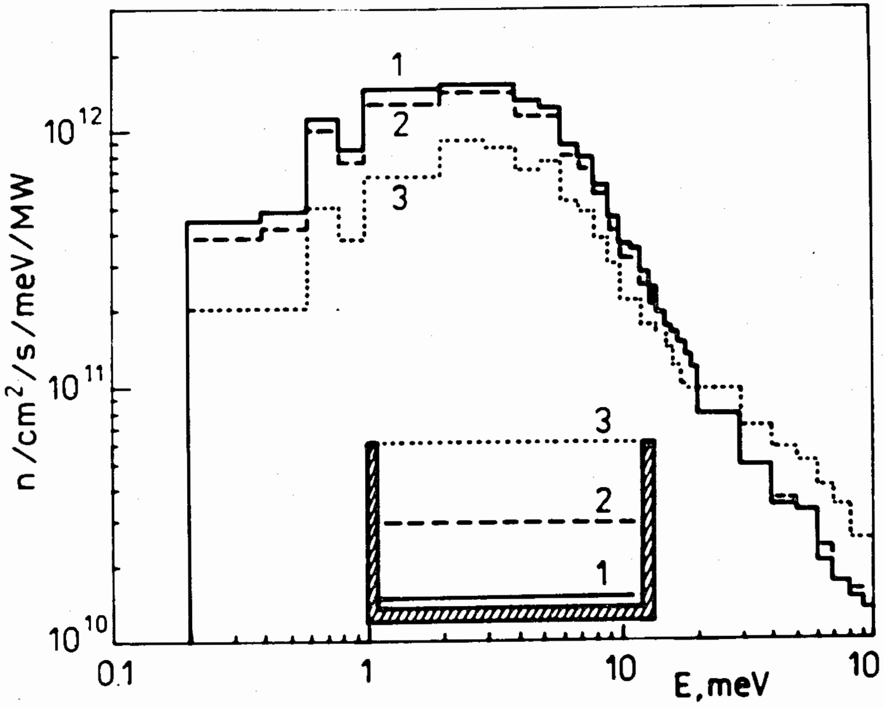

Fig.5. The same as in Fig.3 for the case where the methane moderator has the form of a cup $\phi 10cm * 7cm$ with a wall thickness of $1cm$ for distances from the moderator bottom: 1-0cm, 2-3cm, 3-6cm.

moderators, having the form of fig.5, but with different thickness, gave the following flux ratios: 1.0/0.93/0.92/0.78, respectively, for moderators with thickness $1.0, 2.0, 3.$, and $4.0cm$. From the consideration of highest cold neutron flux and lowest energy deposition, a moderator thickness of $1cm$ was chosen. Figure 6 shows the cold and thermal neutron spectra at the exit window of the "cup" methane moderator in the three different positions of fig.1.b of the moderator inside the graphite reflector. In any of the calculations of figs.3-5 we did not take into account the additional moderation and cooling of neutrons in the volume of the solid D_2, or CD_4 converter because of absence of kernels for these substances at low temperatures in ENDB/F library files. In reality, moderation in the converter volume will increase the UCN (VCN) flux.

Usually, for calculating the UCN and VCN production, the so-called gain factor $G(T_s, E_n)$ is used [9, 10, 11], which may be defined as the ratio of UCN yield from the particular "thick" (compared to the VCN mean free path) and simultaineously "thin" (in the sense that it does not influence the incident neutron flux) moderator at a given temperature T_s in a given incident neutron spectrum, and the yield from one consisting of light water (or polyethylene) at normal temperature in equilibrium with the neutron spectrum. The latter case corresponds to a Maxwellian low-energy tail flux at 300 K. The gain factor is proportional to the UCN (VCN) production (downscattering) cross section σ_{ds} and is inversely proportional to the cross section of UCN (VCN) losses in the moderator σ_{loss}:

$$G(T_s, E_n) \sim \sigma_{ds}/\sigma_{loss}. \qquad (1)$$

The VCN loss cross section consists of three components:

$$\sigma_{loss} = \sigma_c + \sigma_{ups} + \sigma_{el}^{inc}, \qquad (2)$$

where σ_c is UCN capture cross section for the nuclei of the converter, σ_{ups} is the cross section of UCN upscattering, σ_{el}^{inc} is the cross section of elastic incoherent scattering that decreases the UCN free path length in the converter. The influence of the last term may be diminished significantly by using UCN (VCN) reflector surrounding the converter and thereby improving the efficiency of the UCN extraction from the converter.

From the above expressions, the advantage of deuterated converters is evident: in spite of the fact that the nominator of (1) is larger for the hydrogenous converters, the low value of the denominator for deuterated ones significantly compensates this disadvantage.

In order to take into account the geometric peculiarities of the moderators, we used a more straightforward way in the present calculations directly calculating the UCN (VCN) production rate in the "realistic" neutron spectrum and separately simulating the VCN exit from the converters.

The VCN and UCN production rate into the unit energy interval $P(E_{UCN})$ in the convertor may be calculated according to the expression:

$$P(E_{UCN}) = n \int \Phi(E)\sigma(T, E \rightarrow E_{UCN})dE, \qquad (3)$$

where $\Phi(E)$ is the primary neutron flux density, $\sigma(T, E \rightarrow E_{UCN})$ is the cross section of downscattering on the nuclei of the converter for neutrons with energy E in the primary flux into the unit UCN energy interval, and n is the mean number of nuclei per cm^3 of the converter.

We used one-phonon incoherent approximation for calculating the downscattering cross section [12], and the Debye model of phonon state density with Debye temperature $T_D = 114K$ [13] for the **solid deuterium**. This calculation gives the value $2.5 \cdot 10^{-7} b$ for the downscattering cross section of neutrons with spectra of fig.5 into the energy interval $0.1 \mu eV$ in the vicinity of the final energy $E_f = 0.525 \mu eV$ (neutron velocity $10m/s$) for low temperature deuterium (this cross section almost does not depend on the

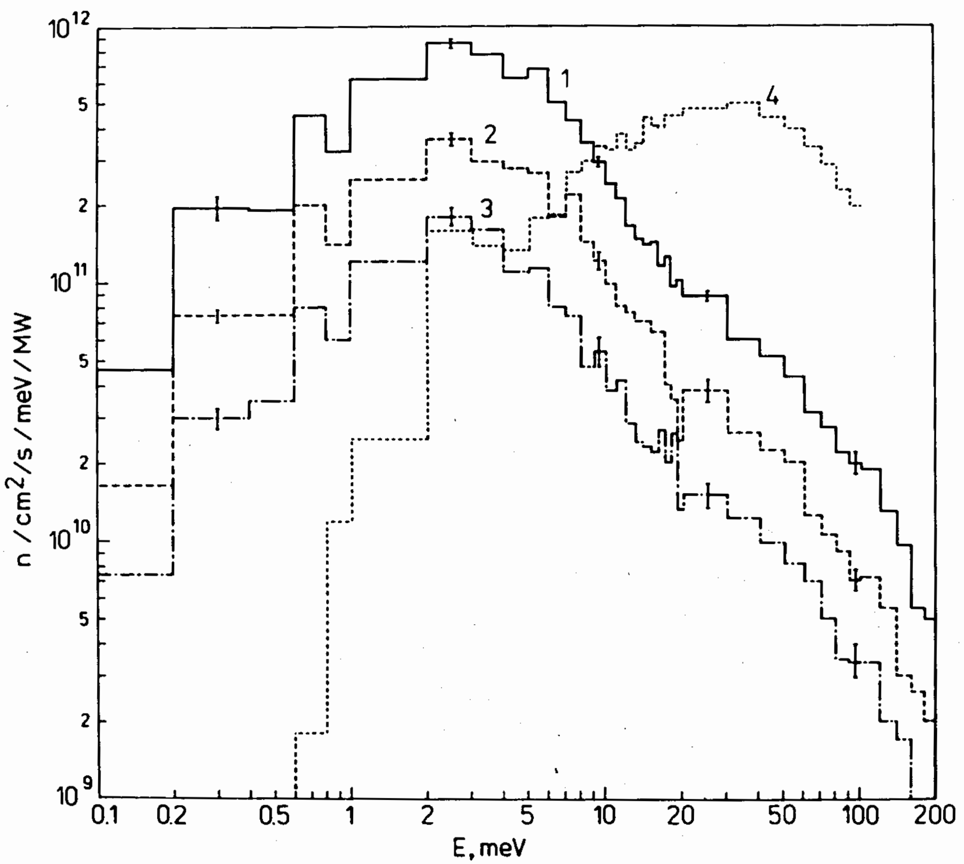

Fig.6. Cold and thermal neutron spectra from the "cup"cold methane moderator $\phi 10cm * 7cm$ with a cup thickness of $1cm$ in the three different positions of fig.1b inside the graphite reflector, averaged over an $\phi 8cm$ area at a distance $6cm$ from the moderator bottom. Dotted curve 4 shows thermal neutron spectrum in the position 1 of fig.1 without cold methane moderator.

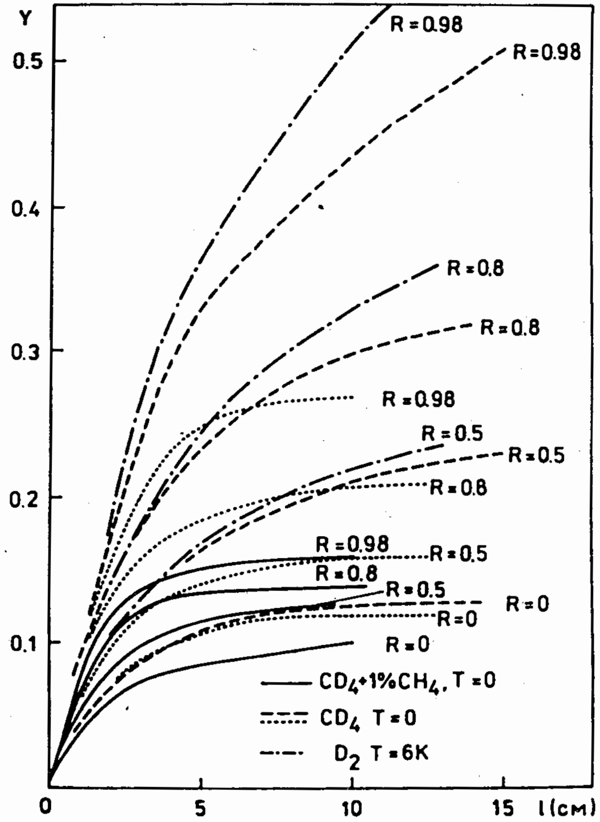

Fig.7. Exit probability of VCN with a vacuum velocity $v_{vac} = 10m/s$ from the converter $\phi = 8cm$ as a function of convertor thickness at different reflection coefficients of VCN from the side and bottom surfaces of the converter. For the case $CD_4 + 1\% CH_4$ and pure CD_4, VCN losses in the converter are determined by neutron capture by nuclei ($\sigma_a = 5.1b/molecule$ and $1.5b/molecule$ respectively), and incoherent elastic scattering σ_{el}^{inc}, decreasing VCN mean free path (this cross section is not known); we take $\sigma_{el}^{inc} = 4b/molecule$ (dashed curve) and $\sigma_{el}^{inc} = 10b/molecule$ (the dotted curve). For solid deuterium, $\sigma_{el}^{inc} = 4.05b/molecule$. The angular distribution of reflected neutrons obeyed the cosine law.

deuterium temperature below 20 K and is proportional to $E_f^{1/2}$). For the mean neutron flux of fig.5 (corresponding to the nearest position of the methane moderator to the reactor core) over the converter volume (density $n = 2.56 \cdot 10^{22} D_2 molecules/cm^3$), this gives a VCN production rate of

$$P = 1.3 \cdot 10^5 VCN/s/cm^3/0.1\mu eV/MW.$$

In pure solid deuterium at $T = 6K$ UCN (VCN) the capture cross section is approximately equal to the upscattering cross section, such that the neutron lifetime $\tau = n\sigma_{inel}v$:

$$\tau \simeq 0.04s.$$

This gives an equilibrium VCN density in the above mentioned-energy range of

$$\rho = P \cdot \tau = 5.2 \cdot 10^3 VCN/cm^3/0.1\mu eV/MW.$$

To the illustrate the reflector effect on UCN (VCN) yield, fig.7 shows the results of Monte Carlo simulation of the probability of VCN going out from converters as a function of its thickness. In these calculations, the neutron capture and elastic and inelastic (for the deuterium) scattering were taken into account. These results show the importance of having neutron reflector surrounding the convertor. This reflector may represent a supermirror layer covering the surface of the convertor or a sheet of substance with strong density irregularities and a high value of diffuse VCN reflectance. The most expedient material for the reflector is graphite, for which a significant (up to ~ 95%) albedo was measured for VCN [14].

Stationary VCN flux from the converter with volume V into the neutron guide with boundary energy E_b, taking into account the VCN losses in the converter during their going out from the converter into the neutron guide, is:

$$\Phi = P \cdot V \cdot Y \cdot \eta, \qquad (4)$$

where Y is the averaged over converter volume VCN exit probability, η is that part of the VCN phase space volume in the spherical layer $[0.475\mu eV \leq E_{VCN} \leq 0.575\mu eV]$, which is acceptable for guiding through neutron guide. At $E_b = 0.2\mu eV$, $\eta \simeq 0.18$.

For the converter size $\phi 8 * 6cm$, the VCN exit probability is $Y = 0.4$ if the VCN reflection coefficient from the side and bottom surface of the converter is equal to 0.98 (fig.7). The VCN flux emerging from the converter into the neutron guide with diameter $8cm$ and boundary energy $0.2\mu eV$ is:

$$\Phi_{VCN} = 2.8 \cdot 10^6 VCN/s/0.1\mu eV/MW.$$

At the reactor pulse with prompt energy yield $10MJ$, the VCN fluence into the neutron guide in the above-mentioned energy interval will achieve:

$$\Psi_{pulse} \simeq 3 \cdot 10^7 VCN/pulse.$$

The ratio of cold neutron intensities (and corresponding UCN (VCN) production rates) for hystograms 1, 2, and 3 of fig.6 (three positions of the cold moderator inside the graphite reflector) are **1/0.49/0.23.**

In the above calculation, we did not take into account additional contribution to the UCN (VCN) generation in the converter from incident neutrons with energies above $0.2eV$.

The most promising deuterated converters are not suitable for horizontal UCN guides because of their large boundary energy proportional to the scattering potential $E_b = (\hbar^2/2m)4\pi \sum_i N_i b_i$, which produces the low-energy cutoff for the emergent UCN spectrum. These boundary energies for solid deuterium and heavy methane are, respectively: $E_{D_2} \simeq 90neV$, and $E_{CD_4} \simeq 190neV$. In order to restore this part of the neutron energy spectrum in the storage, chamber it is necessary to use gravitational deceleration by introducing inclined or vertical neutron guide components between the UCN source and the storage chamber.

In addition to ordinary UCN losses in the converter due to nuclear capture, upscattering and incoherent elastic scattering, which decrease the VCN mean free path, additional important effect may cause a significant reduction of the UCN (VCN) current out of the converter. In disordered substance with strong coherent scattering substance, like deuterated compounds, elastic neutron scattering takes place from the fluctuations of scattering length density due to inhomogeneities of the density of the substance. Such elastic scattering may significantly decrease the VCN mean free path and, hence, the effective source thickness for the emergent neutrons. Recent measurements of UCN production in solid deuterium [15] did not show any significant influence of this effect on UCN yield. An investigation of this phenomenon in the solid heavy methane would be desirable.

There is no experimental information on the scattering kernel or frequency spectrum for heavy methane, which could be used for calculatong the VCN production rate. Nevertheless, we expect that heavy methane has a cumulative combination of the advantages of deuterium in comparison with hydrogen, due to its lower capture cross section, and the advantages of methane in over hydrogen [16] due to its larger density and, especially, due to the importance of low-frequency lattice vibrations and rotational modes in the production of UCN (VCN). Therefore, we hope that in spite the high value expected for elastic incoherent cross section of the heavy methane in comparison with deuterium (and a lower VCN mean free path in the converter), the UCN (VCN) production efficiency of heavy methane may be higher than that of deuterium.

4 Energy deposition in cold moderator

The Table shows the results of our calculations for reactor radiation energy deposition in a solid "cup" methane moderator (mass $130q$) and a solid heavy methane converter ($\phi 8 * 6 cm$, mass $200g$) in the three different positions of fig.1b.

Energy deposition in a solid methane moderator and in a solid heavy methane converter for the three positions of fig.1b.

Position	1	2	3
$W_{CH_4}(W/g/MW)$	0.44	0.056	0.011
$W_{CD_4}(W/g/MW)$	0.19	0.024	0.0043
$W_{tot}(W/MW)$	95	12	2.3

The calculated energy deposition values may be compared with experimental data on energy deposition in methane for the TRIGA reactor of Pennsylvania State University [17]. The measurements were performed in a vacuum vessel placed 19 cm from the core face. After extrapolation of their results to the core surface according to the coordinate dependence of the neutron flux density, we obtain $W_{CH_4} = 0.25W/g/MW$, the difference may be partly attributed to an unreliable extrapolation.

With the calculated energy deposition values for cold methane and taking into account the known values of the heat capacity of this substance for temperatures higher $10K$ [18] it is possible to evaluate the heating ΔT of the moderator after a reactor pulse with prompt energy release of $10MJ$. The results are:

$$\Delta T = 8.7K, \qquad 1.7K, \qquad 0.4K,$$

respectively, for positions 1, 2 and 3 of fig.1b.

At a pulse repetition rate equal to one reactor pulse ($10MJ$) every ten minutes, the mean energy deposition in a cold methane moderator would be:

$$\tilde{W} \simeq 0.16W.$$

The heat capacity of heavy methane is not known, but it should not differ significantly from the heat capacity of ordinary methane (similar to small difference between the heat capacities of cold solid deuterium and hydrogen). In this case, because the energy deposition in heavy methane is significantly lower than in methane, we may expect a lower increase in temperature in the heavy methane converter.

The energy deposition in a solid deuterium converter is small in comparison with that shown in the Table.

In above calculation, we did not take into account the energy deposition in the aluminium walls of the moderator. From the experience of the Dubna group in constructing large ($\simeq 1kg$) solid methane moderator at the JINR IBR-2 reactor [19], we may conclude that the energy deposition in all of the metallic details of the moderator will add approximately 30% to the total energy deposition in the cold moderator.

5 Radiation damage

In this section we rely entirely on the experience of Dubna group [19] which performed test runs of large cold solid methane moderator at the pulse reactor IBR-2 at the energy deposition rate in methane of $\simeq 0.14W/g$. They found that changes in cold neutron production with time were less han 0.2% after 15 hours of continuous operation. Hydrogen production and polimerization of the moderator substance are expected to be low according to [19] if to place the cold moderator after graphite moderator (e.g. position 2 of fig.1b).

6 Nonstationary transport and storage of UCN

In [20], the simple method for nonstationary UCN storage in experimental chambers was described using well-separated pulses from aperiodic pulse neutron sources. The possible installation includes a comparatively short neutron guide (several meters long) and a shutter at the entrance window of the storage chamber. The nonstationary UCN (VCN) transport and storage was rigorously simulated [21] for horizontal and vertical arrangements of neutron guides of different forms, with realistic characteristics of neutron losses due to imperfections in the surface of the guides. It was shown that for the neutron guides of practical lengths (5–7 m) and typical surface quality, the UCN (VCN) flux decreases 3–5 times during transport.

Several important advantages of the proposed method of UCN storage at aperiodic pulse reactors are evident:

1. Low mean power of the reactor: if the intervals between pulses are about $10min$, the mean neutron flux is only $\simeq 2 \cdot 10^{10} n/cm^2/s$. This means low radiation heating of the cooled moderator and converter, which is important at very low temperatures and low thermal conductivity [6, ?].
2. Low radiation damage and decomposition of the moderator [19].
3. Very low neutron background during UCN storage and measurements.
4. Possibility of using short neutron guides (several meters) due to the low mean power of the reactor. This will permit large losses of UCN to be avoided during their spreading along the neutron guide.

7 Acknowledgments

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Покотиловский Ю.Н., Рогов А.Д. E3-97-127
Численная оптимизация источников очень холодных
и ультрахолодных нейтронов для реакторов типа ТРИГА

Проведена численная оптимизация источников холодных и ультрахолодных нейтронов для реакторов типа ТРИГА. Потоки тепловых и холодных нейтронов для различных положений и конфигураций холодных метановых замедлителей моделировались с применением программы MCNP. Оценена генерация очень холодных и ультрахолодных нейтронов для наиболее перспективных конечных замедлителей — очень холодного твердого дейтерия и дейтерированного метана. Для оптимизированных замедлителей вычислено радиационное энерговыделение.

Работа выполнена в Лаборатории нейтронной физики им.И.М.Франка ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна, 1997

Pokotilovski Yu.N., Rogov A.D. E3-97-127
Optimization Study of Ultracold Neutron Sources
at TRIGA Reactors Using MCNP

We performed Monte Carlo simulation for the optimization of ultracold and very cold neutron sources for TRIGA reactors. The calculations of thermal and cold neutron fluxes from the TRIGA reactor for different positions and configurations of a very cold solid methane moderator were performed with using the MCNP program. The production of neutrons in the ultracold and very cold energy range was calculated for the most promising final moderators (converters): very cold solid deuterium and heavy methane. The radiation energy deposition was calculated for the optimized solid methane-heavy methane cold neutron moderator.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna, 1997