



Development of the high-brightness HEC-2 cold neutron source at the reactor PIK

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Physical properties of LH₂

Physical properties of LD₂

| | | | |
|--|--------|--|-------|
| Melting temperature* ,K | 13.9 | Melting temperature* ,K | 18.62 |
| Boiling temperature* , K | 20.4 | Boiling temperature* , K | 23.67 |
| Rotational energy level excitation (0 →1), meV | 14.7 | Rotational energy level excitation (0 →1), meV | 7.4 |
| Vibrational energy level ΔE, meV | 546 | Vibrational energy level ΔE, meV | 386 |
| Free scattering cross-section incoherent, barn | 20.052 | Free scattering cross-section incoherent, barn | 0.907 |
| coherent, barn | 0.397 | coherent, barn | 2.489 |
| *) Standart conditions | | *) Standart conditions | |

$$\sigma_{(n,\gamma)}^H = 0.332 \frac{V_0}{v}$$

$$\sigma_{(n,\gamma)}^D = 0.000506 \frac{V_0}{v}$$

$$V_0 = 2200 \text{ m} / c$$



$$s_H = 1/2$$



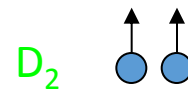
Ground state: L=0, S=0 - para
Antisymmetric spin arrangement

Excited state: L=1, S=1 - ortho

Normal condition (T=293 K):
Ortho:para = 3:1

T=20,3 K
Ortho:para = 0.2:99.8

$$s_D = 1$$



Ground state: L=0, S=0,2 - ortho
Symmetric spin arrangement

Excited state: L=1, S=1 - para

Normal condition (T=293 K):
Ortho:para = 2:1

T=20 K
Ortho:para = 98.1:1.9



$n + p, d$ Scattering

$$s_n = s_p = 1/2$$

$$J - \text{channel spin} = \mathbf{s}_n + \mathbf{s}_p + \mathbf{l}$$

Cold neutrons: $l = 0$

$$J = 0, 1$$

$$\psi(\mathbf{r}) \Big|_{r>r_0} = e^{ik_0 r} - a \frac{e^{ikr}}{r}$$

Scattering length

$$a_+ = a_t - J = 1$$

$$a_- = a_s - J = 0$$

$$a_{coh} = \frac{I+1}{2I+1} a_+ + \frac{I}{2I+1} a_-$$

$$a_{inc} = |a_+ - a_-| \frac{\sqrt{I(I+1)}}{2I+1}$$

$${}^1_1\text{H} - l=1/2$$

$$a_+ = 5.424 \pm 0.003 \text{ fm}$$

$$a_- = -23.749 \pm 0.008 \text{ fm}$$

$$a_{coh} = -1.869 \text{ fm}$$

$$a_{inc} = 12.632 \text{ fm}$$

$${}^1_1\text{D} - l=1$$

$$a_+ = 6.34 \pm 0.02 \text{ fm}$$

$$a_- = 0.65 \pm 0.03 \text{ fm}$$

$$a_{coh} = 4.44 \text{ fm}$$

$$a_{inc} = 2.68 \text{ fm}$$



We can only make scattering on H₂ and D₂.

Fermi pseudopotential

$$V(\mathbf{r}, \mathbf{R}_1, \mathbf{R}_2) = \frac{2\pi\hbar^2}{m} \sum_{i=1}^2 \left[a'_{i,coh} + \frac{2(a'_{i,+} - a'_{i,-})}{2I_i + 1} \mathbf{s}_i \cdot \boldsymbol{\sigma} \right] \delta(\mathbf{r} - \mathbf{R}_i)$$

$$a'_{+,-} = \left(1 + \frac{m}{M} \right) a_{+,-}$$

Born approximation is applicable.

Schwinger J., Teller E. Phys. Rev. **52**, 286 (1937)

$$\frac{d\sigma_{n,l \rightarrow n',l'}}{d\Omega} = \frac{4}{9} \frac{p}{p_0} \cdot c_{S \rightarrow S'} \times$$

$$\frac{1}{2l+1} \sum_{m,m'} \left| \int \exp\left\{ \frac{i(\mathbf{p}_0 - \mathbf{p})\mathbf{R}}{2\hbar} \right\} \Phi_{n',l',m'}^*(\mathbf{R}) \Phi_{n,l,m}(\mathbf{R}) d\mathbf{R} \right|^2$$

$$l, l' - \text{even}: S, S' = 0$$

$$l, l' - \text{odd}: S, S' = 1$$

$$c_{0 \rightarrow 0} = 3(a_+ + a_-)^2$$

$$c_{0 \rightarrow 1} = 3(a_+ - a_-)^2$$

$$c_{1 \rightarrow 1} = (3a_+ + a_-)^2 + 2(a_+ - a_-)^2$$

$$c_{1 \rightarrow 0} = (a_+ - a_-)^2$$

$$E_{n,\min} = 0.0137 [l'(l'+1) - l(l+1)] + 0.819(n'-n) \text{ [eV]}$$

For H₂ $E_{Qinel} = 0.0274 \text{ eV}$



Young and Koppel theory of inelastic scattering on H₂ and D₂ (Phys.Rev. **135**, 3A p.A603, (1964))

$$\sigma(E \rightarrow E', \mu) = \frac{\sigma_b}{2kT} \sqrt{\frac{E'}{E}} S(\alpha, \beta) \quad \alpha = \frac{E' + E - 2\sqrt{EE'}\mu}{AkT}; \quad A = M / m_n \quad \beta = \frac{E' - E}{kT}$$

$$S_{para}(\alpha, \beta) = \sum_{J=0,2,4\dots} P_J \times \frac{4\pi}{\sigma_b} \left[A_{para} \sum_{J'=0,2,4\dots} + B_{para} \sum_{J'=1,3,5\dots} \right] (2J'+1) \times S_f(w\alpha, \beta + \beta_{JJ'}) \times \sum_{\ell=|J'-J|}^{J'+J} 4j_\ell^2(y) C^2(J, J', \ell; 00)$$

$$S_{ortho}(\alpha, \beta) = \sum_{J=1,3,5\dots} P_J \times \frac{4\pi}{\sigma_b} \left[A_{ortho} \sum_{J'=0,2,4\dots} + B_{ortho} \sum_{J'=1,3,5\dots} \right] (2J'+1) \times S_f(w\alpha, \beta + \beta_{JJ'}) \times \sum_{\ell=|J'-J|}^{J'+J} 4j_\ell^2(y) C^2(J, J', \ell; 00)$$

$$\beta_{JJ'} = (E'_{J'} - E_J) / kT$$

$$y = (a/2) \sqrt{MkT\alpha}$$

$$S_f(\alpha, -\beta) = \frac{1}{\sqrt{4\pi\alpha}} \exp\left[-\frac{(\alpha - \beta)^2}{4\alpha}\right]$$

$$S_f(\alpha, \beta) = e^{-\beta} S_f(\alpha, -\beta)$$

$$w = \begin{cases} \frac{1}{2} - \text{H}_2 \\ \frac{1}{4} - \text{D}_2 \end{cases}$$

$$\sigma_b = 4\pi(a_c^2 + a_i^2)$$

a_c - coherent scattering length

a_i - incoherent scattering length

a – interatomic distance in the molecule

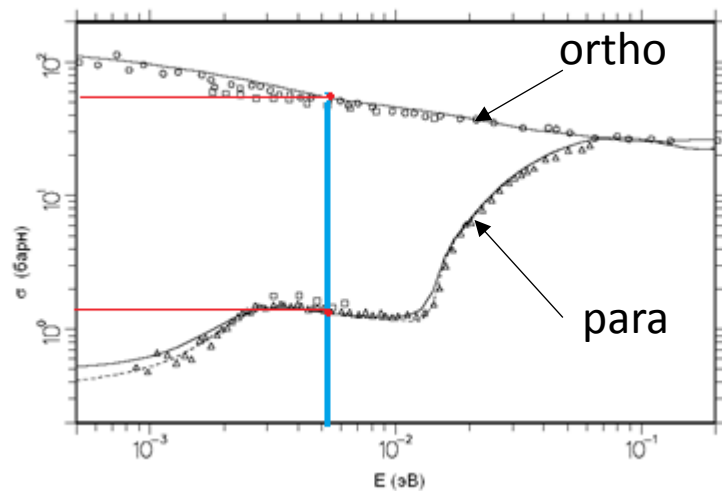
| | A (even) | B (odd) |
|---------|--------------------|--------------------|
| H para | a_c^2 | a_i^2 |
| H ortho | $a_c^2/3$ | $a_c^2 + 2a_i^2/3$ |
| D para | $3a_i^2/4$ | $a_c^2 + a_i^2/4$ |
| D ortho | $a_c^2 + 5a_i^2/8$ | $3a_i^2/8$ |



Cross-sections of inelastic scattering of neutrons on H and D



H_2

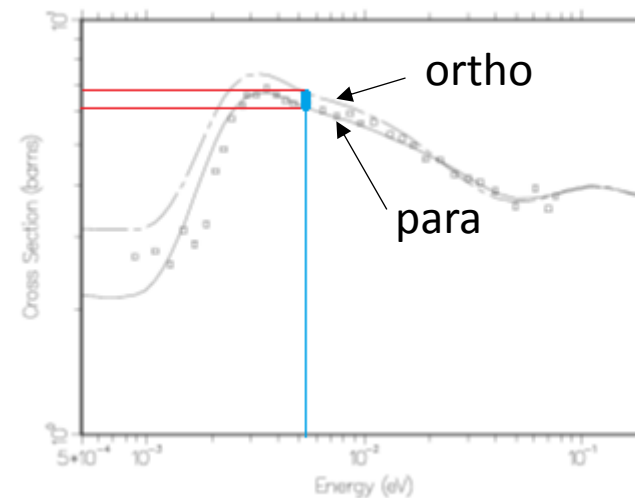


$$\lambda = 4 \text{ \AA} \longrightarrow E \cong 5.1 \text{ meV}$$

$$\sigma_{para} \cong 1.5 \text{ b} \rightarrow l \cong \mathbf{16} \text{ cm}$$

$$\sigma_{ortho} \cong 55 \text{ b} \rightarrow l \cong \mathbf{0.4} \text{ cm}$$

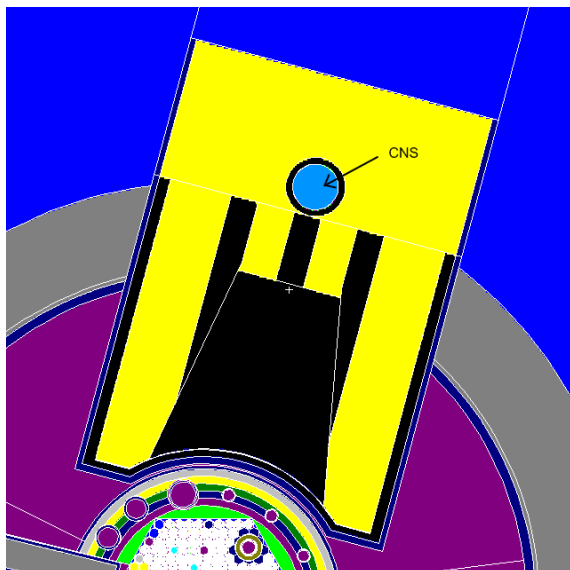
D_2



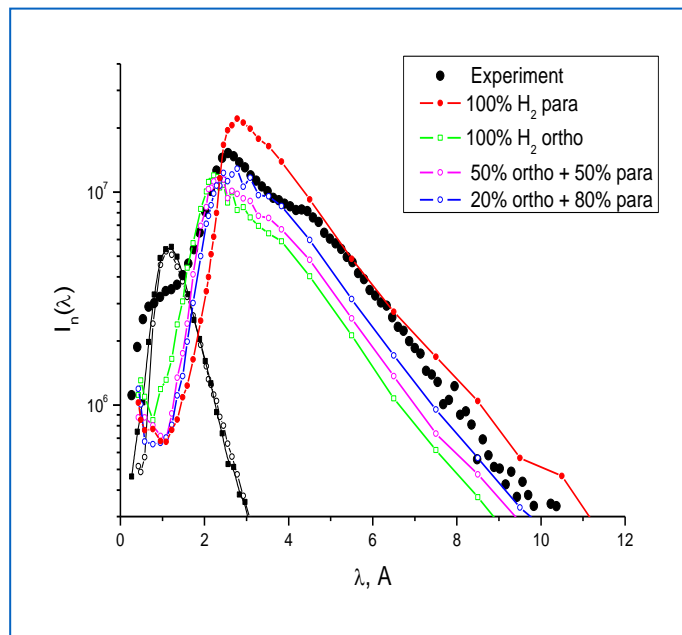
$$\sigma_{ortho} \cong 7 \text{ b} \rightarrow l \cong \mathbf{2.9} \text{ cm}$$

$$\sigma_{para} \cong 6 \text{ b} \rightarrow l \cong \mathbf{3.3} \text{ cm}$$

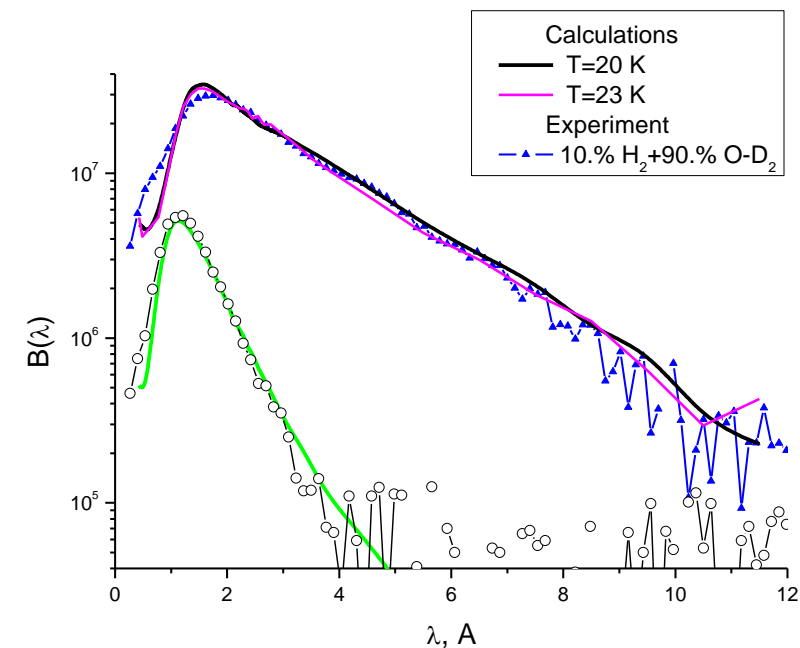
Chamber of 6L volume was situated in the reactor Thermal Column
A.P. Serebrov, V.A. Mityukhlyayev, A.A. Zakharov et al



Brightness of chamber filled with LH₂



Brightness of chamber filled with LD₂

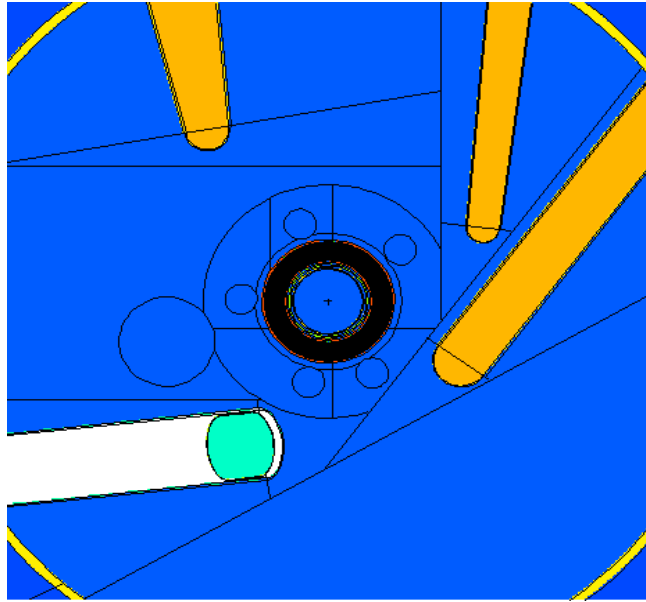


General conclusion:

CNS of large volume filled with LD₂ is more effective than chamber filled with LH₂ in mix spin state.



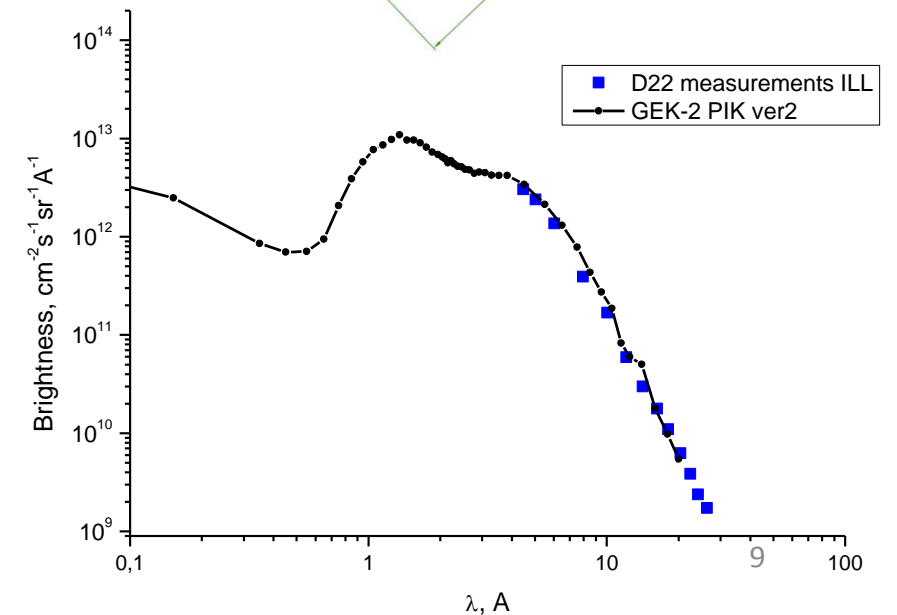
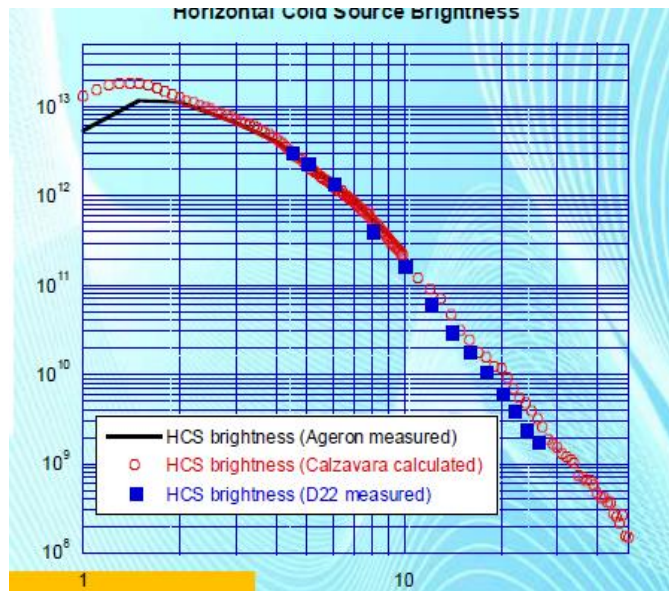
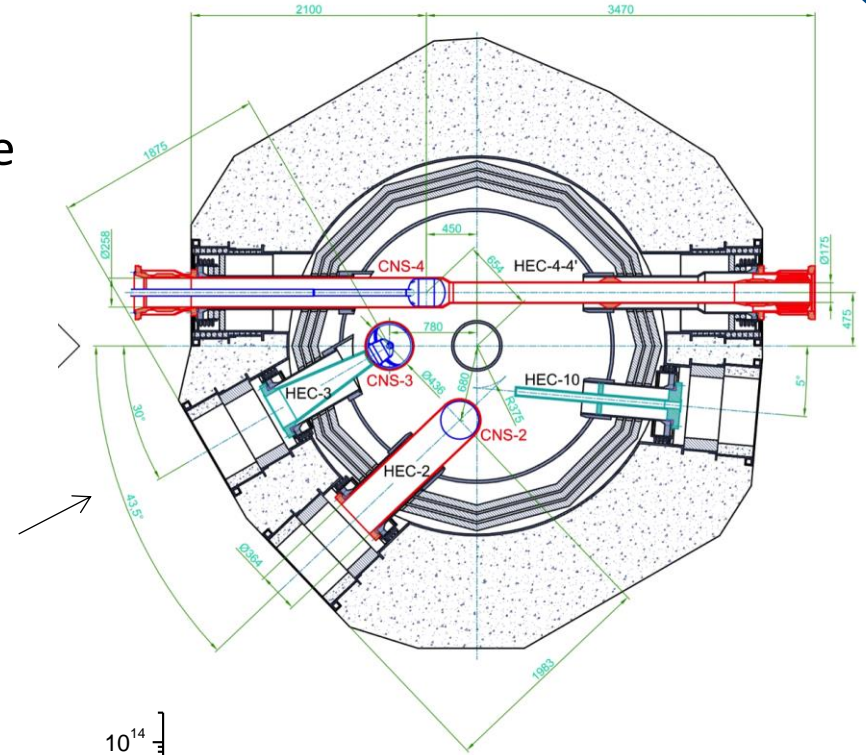
D₂ liquid CNS-2 (project)



← **ILL Horizontal cold source**
V = 5.2 l

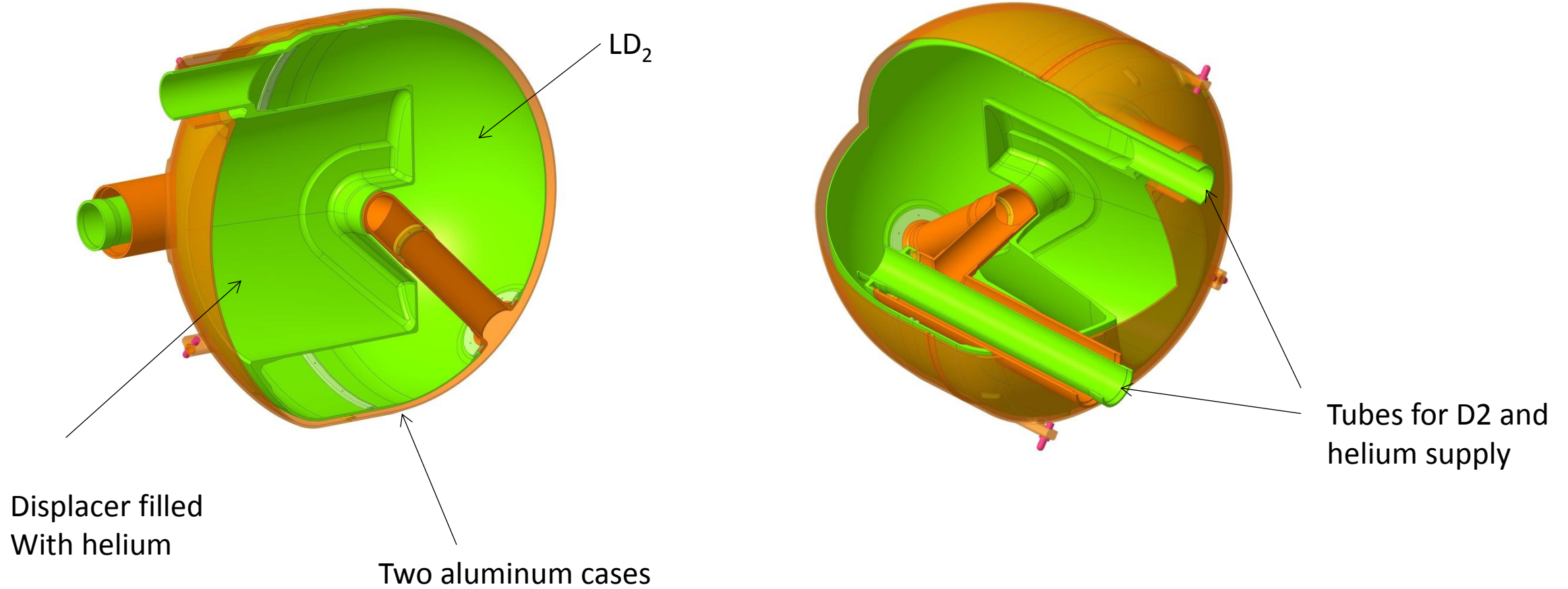
PNPI Cold neutron source 2
V = 14.8 l
Size - $\varnothing 330 \times 370$
Channel of maximal diameter – 380 mm

Distance from the centrum of the source to the centrum of the core – 694 mm





HEK-2 - CNS-2, LD₂ chamber. Project "Pribornaya basa"



Para-hydrogen for high-brilliant cold neutron sources

Low dimensional neutron moderators for enhanced source brightness

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²Hungarian Academy of Sciences, Wigner RCF, 1525 Budapest, Pf. 49, Hungary

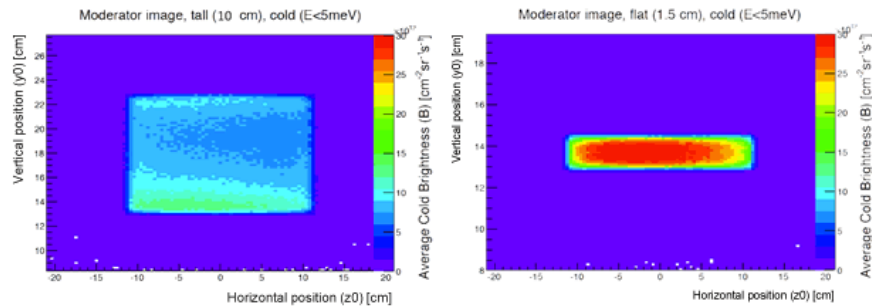
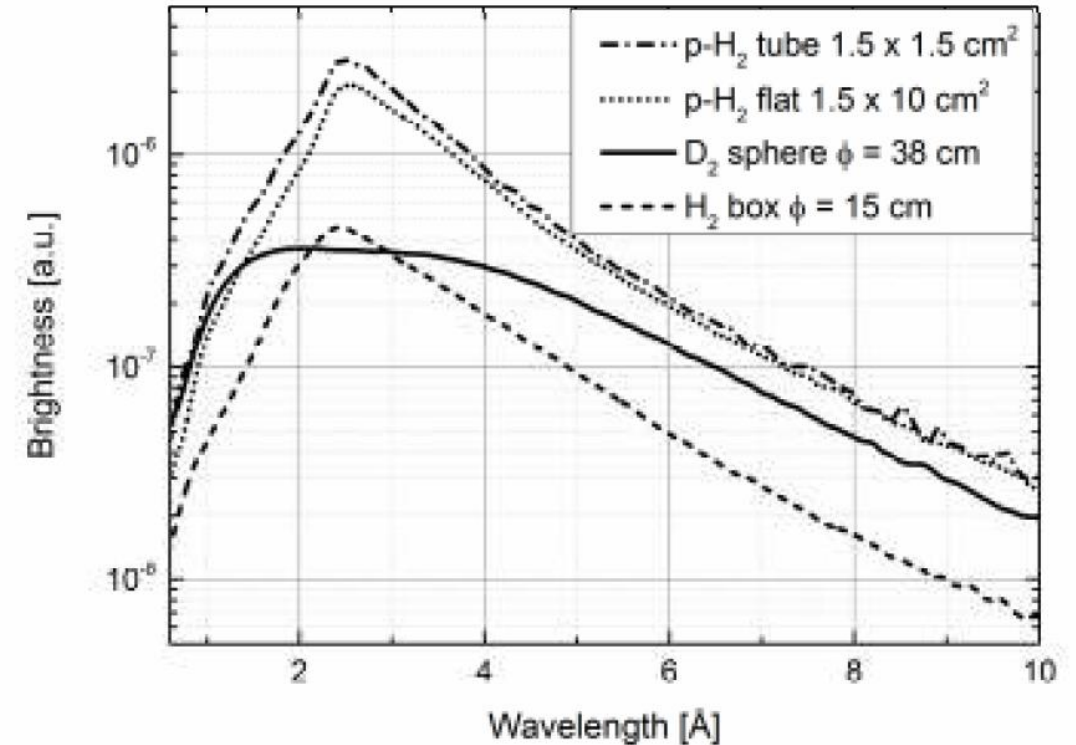
³DTU Nutech, Technical University of Denmark, DTU Risø Campus, 4000 Roskilde, Denmark

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(2014). *J. Neutron Res.* 17, 101–105.

Para-hydrogen is more convenient for spallation sources

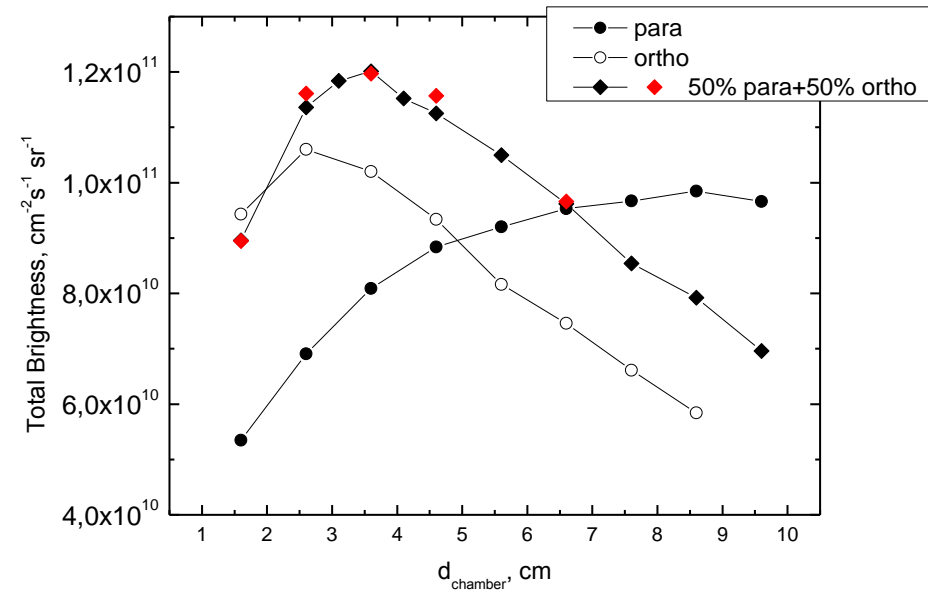
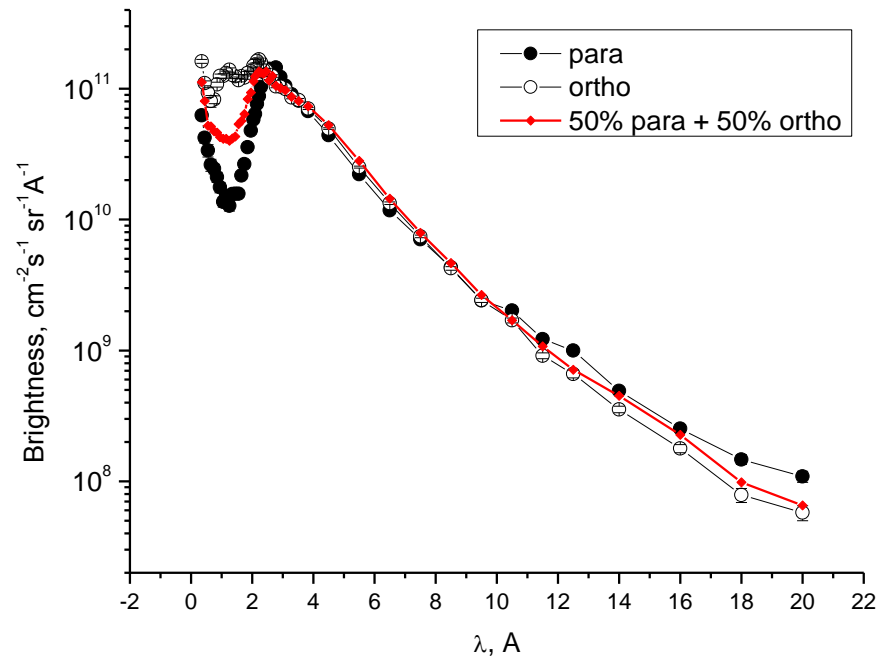
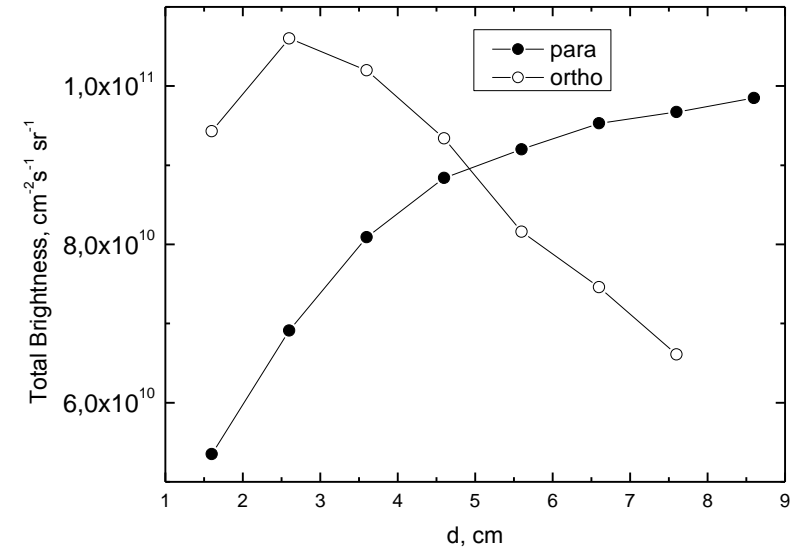
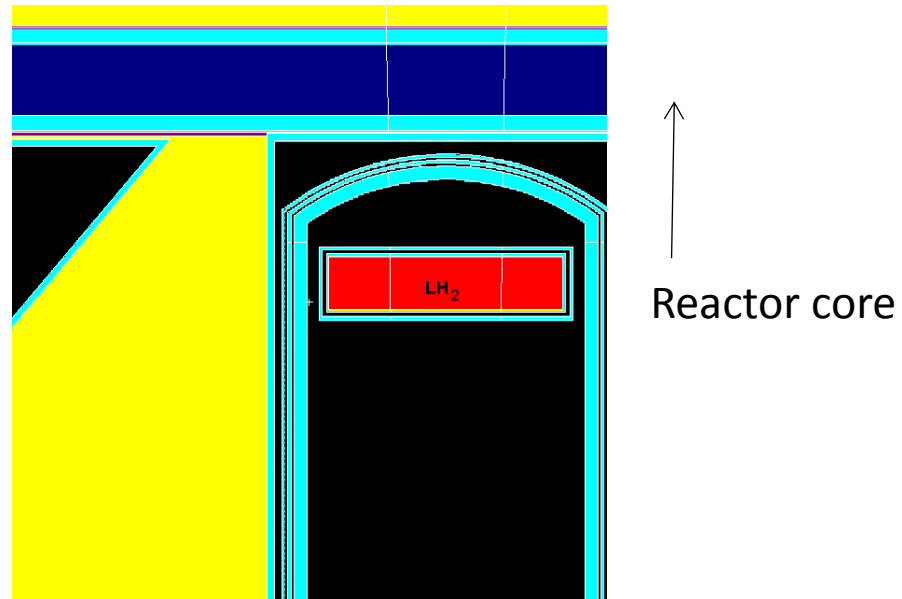
Low-dimensional Para-hydrogen CN source is plan to use on ESS.



Computer simulation for J_PARC source

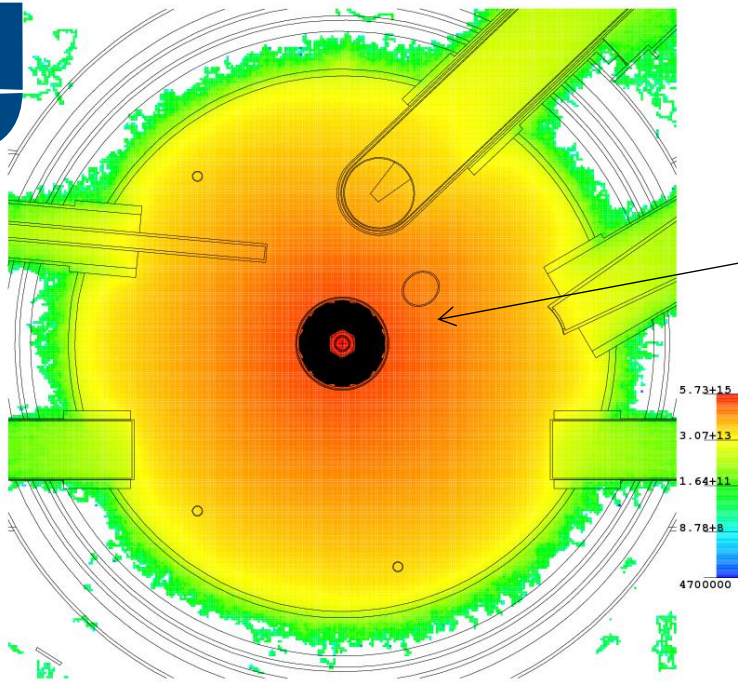


Liquid hydrogen chamber optimization for the reactor IR-8



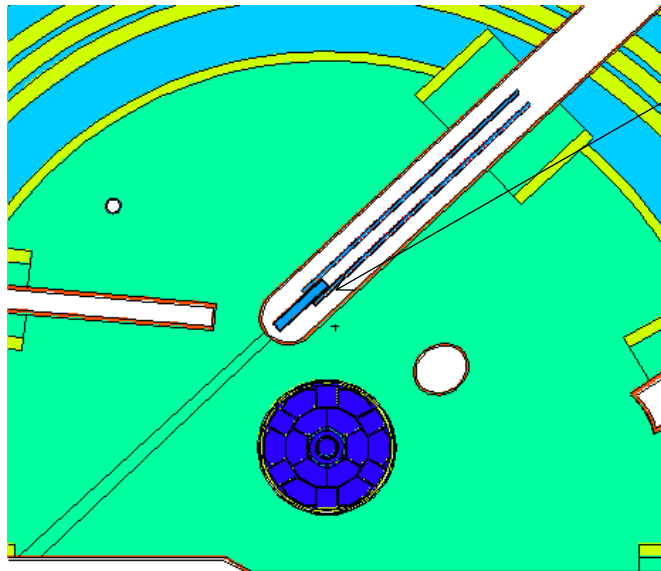
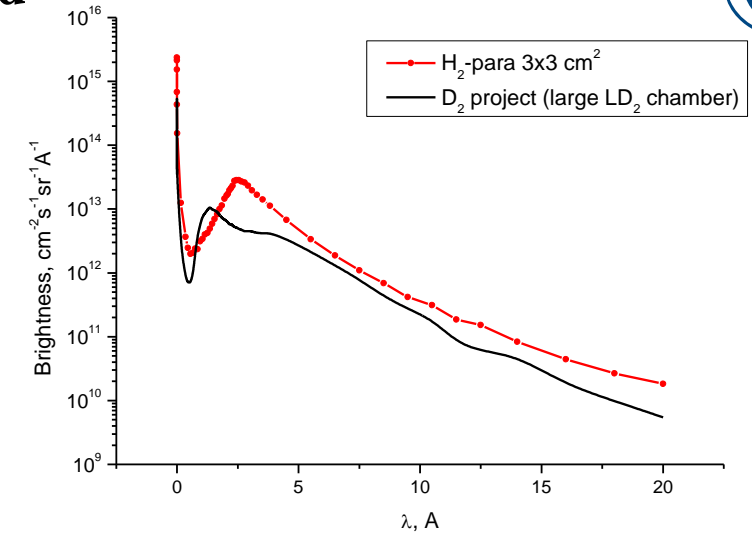


Comparison of para-hydrogen and Liquid deuterium sources



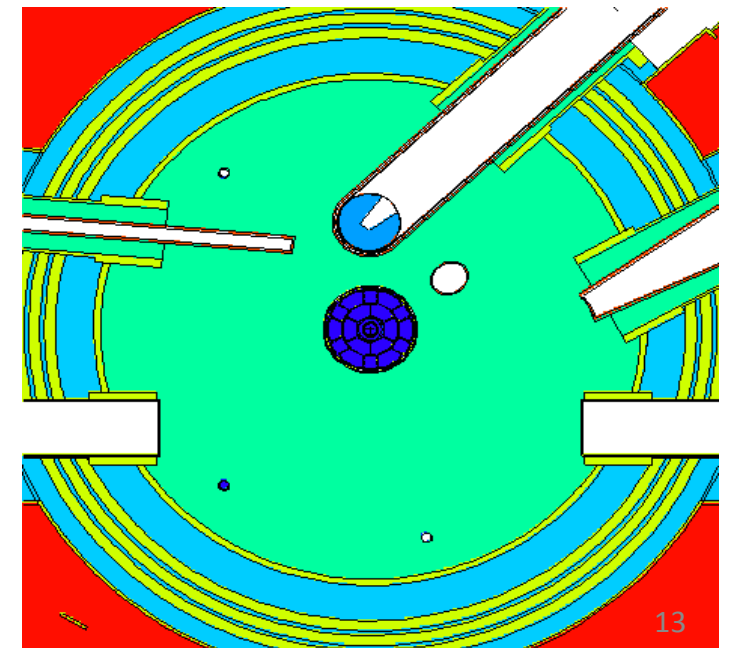
Field of cold neutron flux in heavy water reflector of reactor PIK

The problem of heat release



Para hydrogen source in HEC-2
F.Mezei, A.Ioffe, E.Vezhlev et al suggestion

Chamber size: 30x30x200 mm³





Flux field for cold neutrons. LD₂ chamber

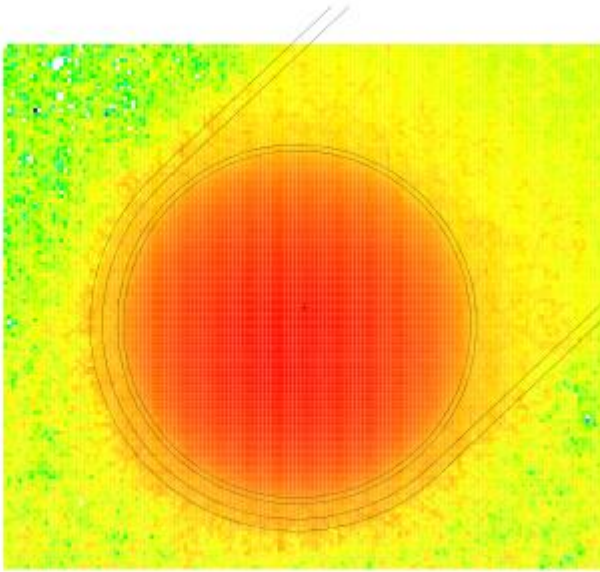


PIK HBT

```
basis: XY  
{ 1.000000, 0.000000, 0.000000 }  
{ 0.000000, 1.000000, 0.000000 }  
origin:  
{ 0.00, 52.50, 0.00 }  
extent = | 20.00, 20.00 }
```

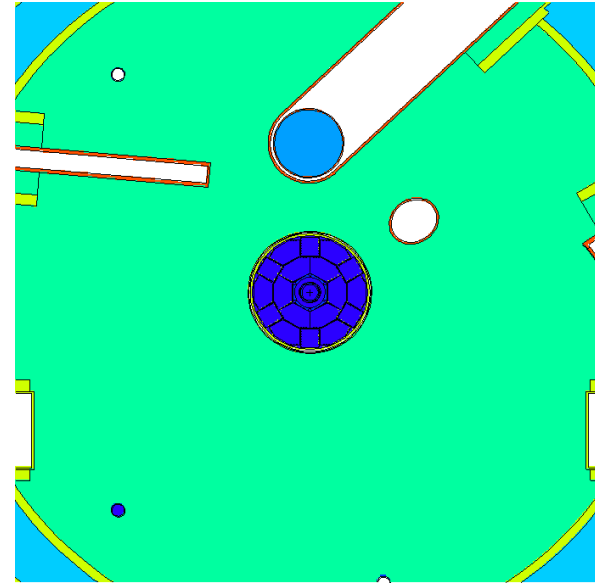
```
Mesh Tally 4  
npa 5000819  
runtpw = ../pcns2r  
dump 2
```

2.92E+14
2.41E+14
1.38E+14
9.88E+13
6.48E+13



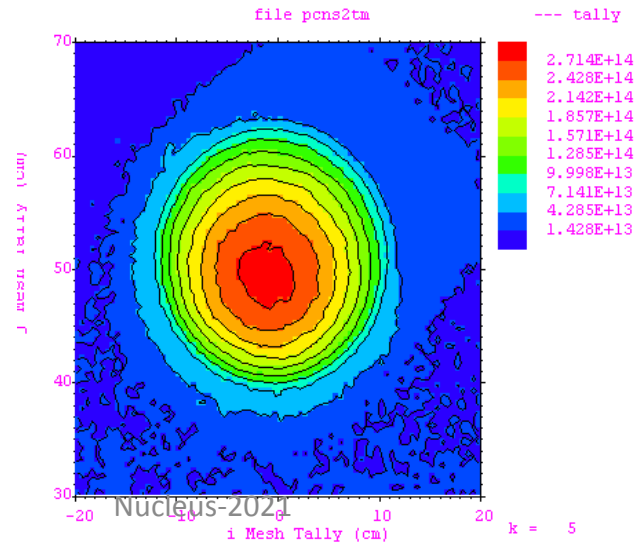
R=11.6 cm
V=6.5 l

Distance to the
core - 514 mm



Cold neutrons $\lambda > 4 \text{ \AA}$.

$$\Phi_{\text{cold max}} = 2.92 \cdot 10^{14} \text{ cm}^{-2}\text{s}^{-1}$$





Using displacer for increasing the flux of cold neutrons released from the chamber into the channel

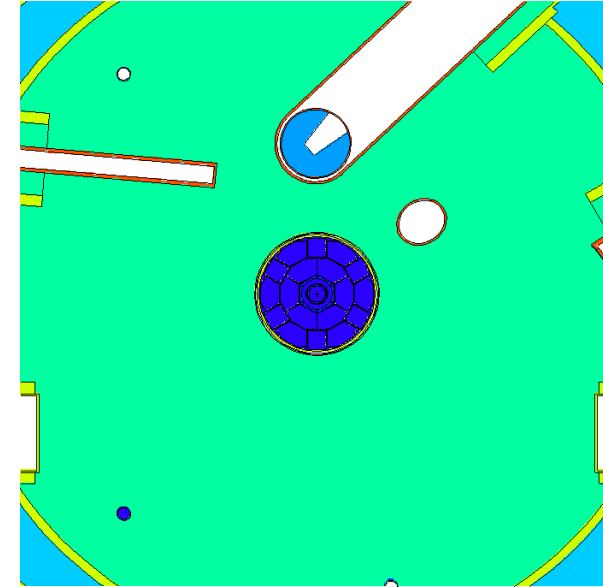
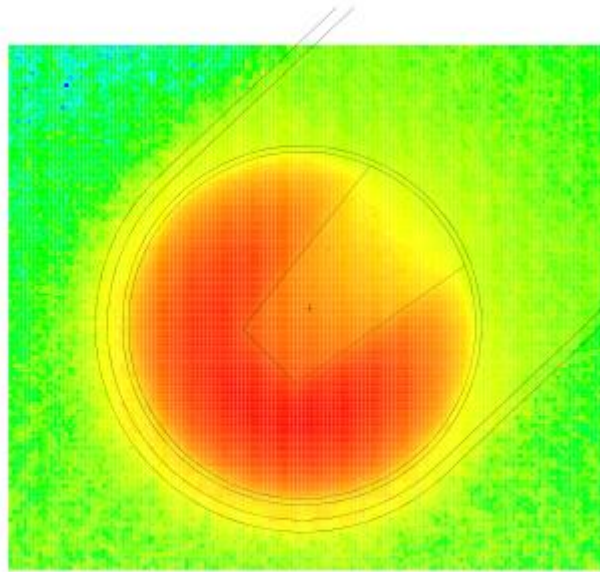


PIK HST

```
basis: XY  
{ 1.000000, 0.000000, 0.000000}  
{ 0.000000, 1.000000, 0.000000}  
origin:  
{ 0.00, 52.50, 0.00}  
extent = { 20.00, 20.00}
```

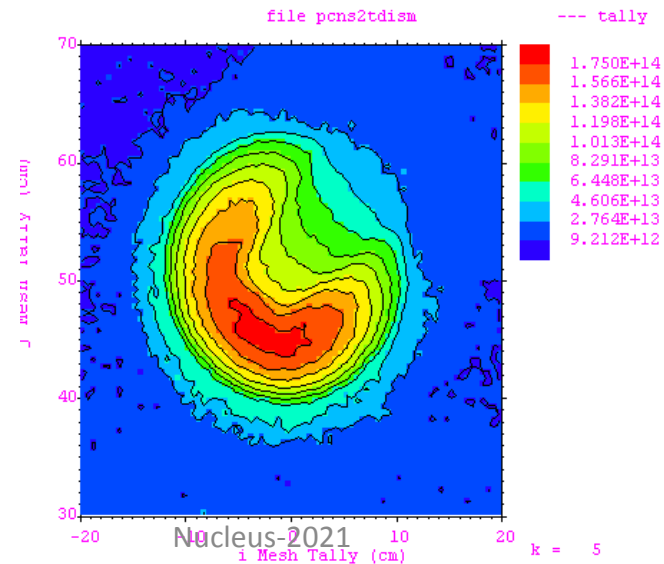
```
Mesh Tally 4  
nps 20002399  
runtime = ../pcns2dism  
dump 5
```

1.81e+14
4.32e+13
1.03e+13
2.48e+12
5.93e+11



$$\Phi_{\text{cold max}} = 1.81 \cdot 10^{14} \text{ cm}^{-2} \text{ s}^{-1}$$

38% decrease comparing to chamber without displacer

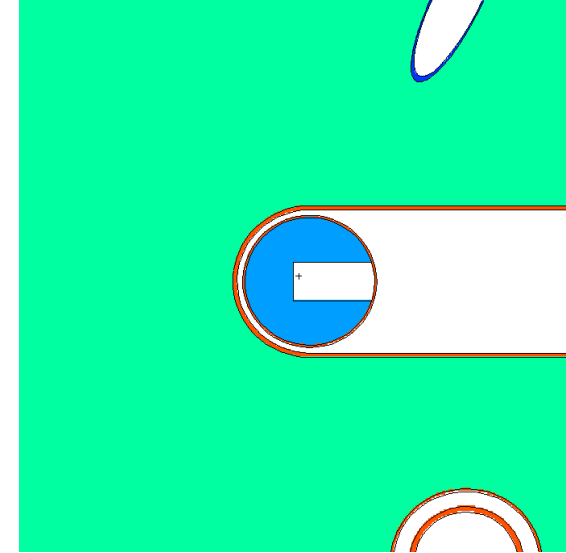
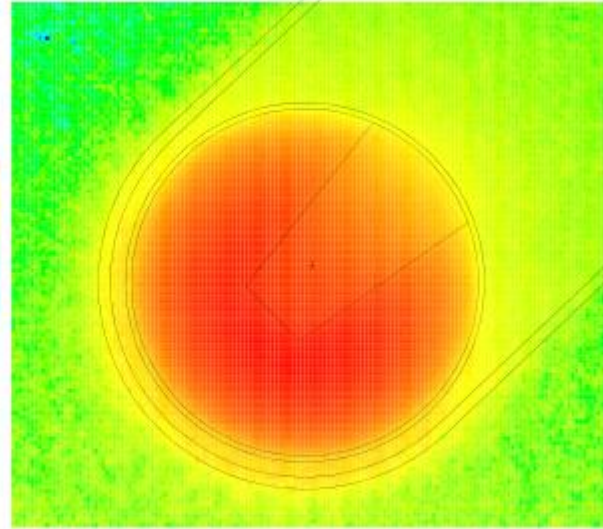




Optimization of displacer form

Displacer bottom have square form 60 x 70 mm²

```
PIK KEY  
  
basis: XY  
{ 1.000000, 0.000000, 0.000000}  
{ 0.000000, 1.000000, 0.000000}  
origin:  
{ 0.00, 52.50, 0.00}  
extent = { 20.00, 20.00}  
  
Mesh Tally 4  
nps 20002022  
runtime = ./pcns2dis2r  
dump 5
```



$$\Phi_{\text{cold max}} = 2.21 \cdot 10^{14} \text{ cm}^{-2} \text{ s}^{-1}$$

22% increasing



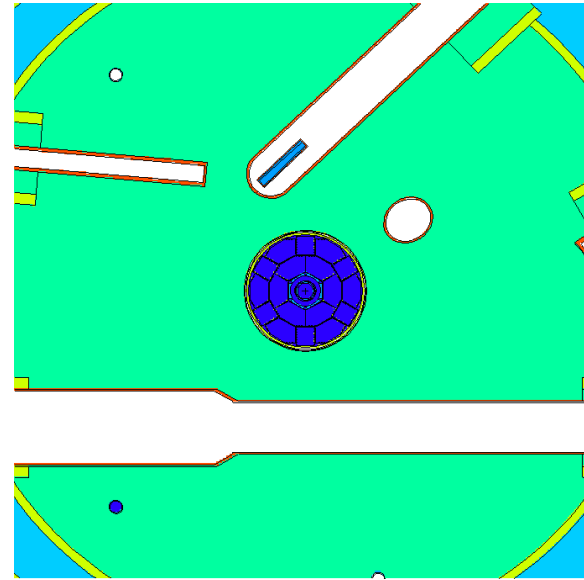
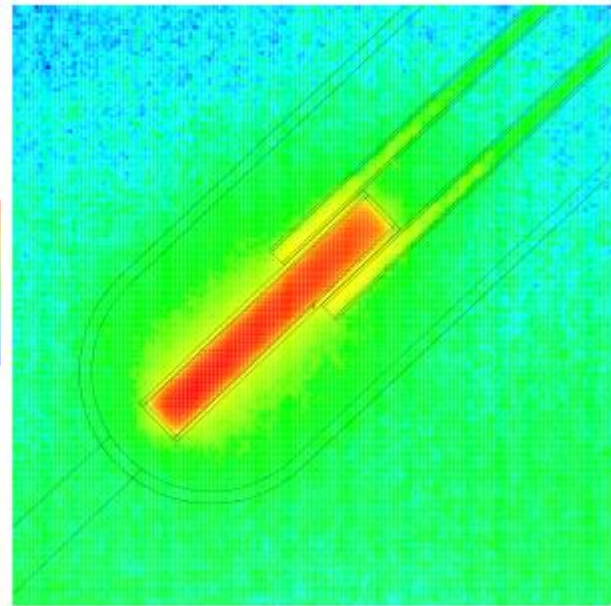
Ortho hydrogen

08/21/21 17:37:52
PIK HBT

```
prebid = 08/20/21 08:10:52  
basis: XY  
{ 1.000000, 0.000000, 0.000000 }  
{ 0.000000, 1.000000, 0.000000 }  
origin:  
{ -5.00, 45.00, -1.00 }  
extent = { 20.00, 20.00 }
```

```
Mesh Tally 4  
nps 49996577  
runtpw = ../port4cflxr  
dump 6
```

2.37e14
7.73e13
2.52e13
8.2e12
2.67e12



$$\Phi_{\text{cold max}} = 2.37 \cdot 10^{14} \text{ cm}^{-2}\text{s}^{-1}$$

Due to small mean free path of cold neutrons in ortho- hydrogen this variant is not optimal



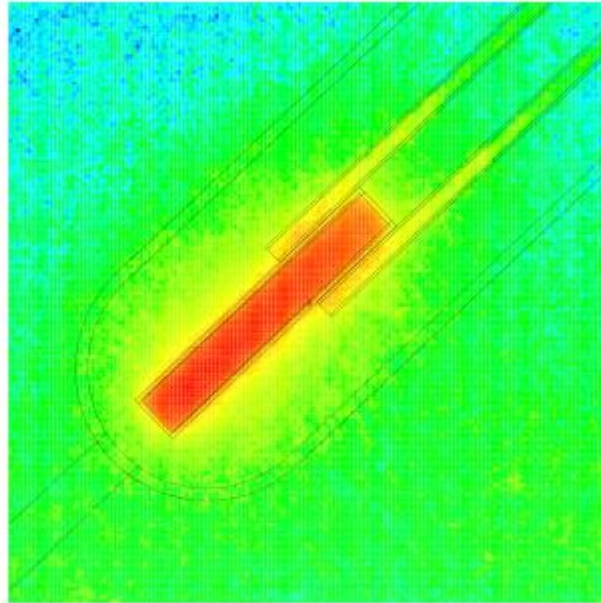
Para hydrogen

08/24/21 07:38:17
PIK HBT

```
prebid = 08/23/21 08:16:19  
basis: XY  
{ 1.000000, 0.000000, 0.000000}  
{ 0.000000, 1.000000, 0.000000}  
origin:  
{ -5.00, 45.00, -1.00}  
extent = { 20.00, 20.00}
```

```
Mesh Tally 4  
nps 50001377  
runtime = ../ppar4cflnr  
dump 6
```

1.1e+14
4.3e+13
1.7e+13
6.9e+12
2.7e+12

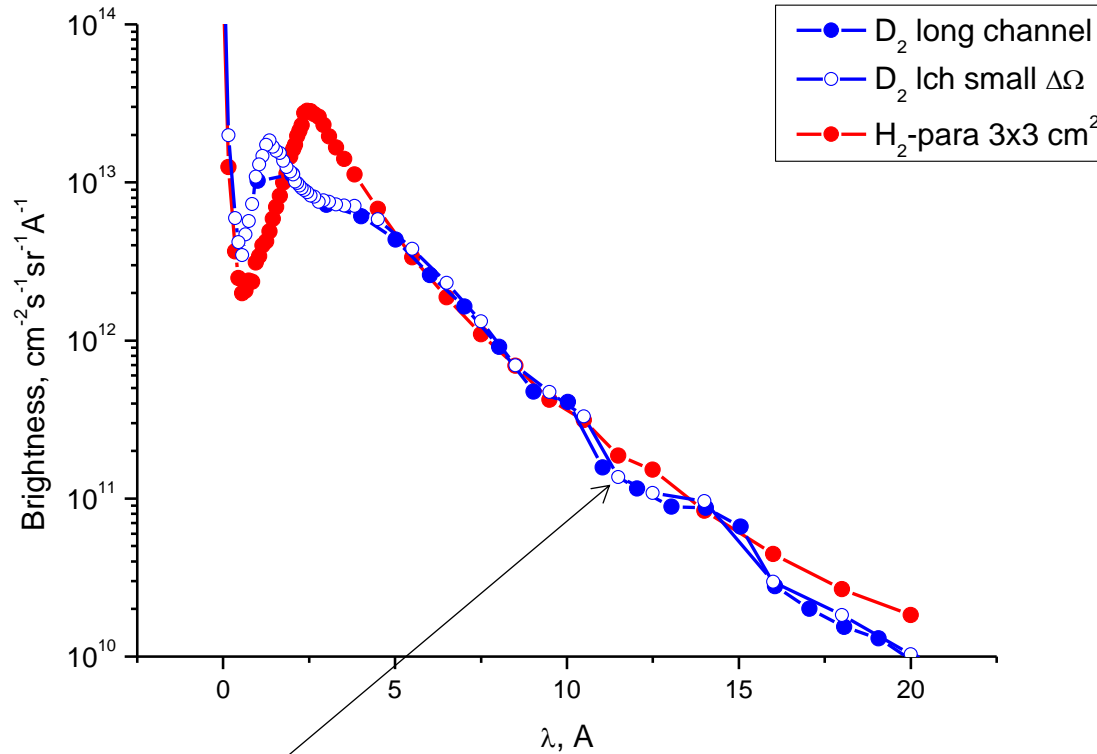


$$\Phi_{\text{cold max}} = 1.1 \cdot 10^{14} \text{ cm}^{-2} \text{ s}^{-1}$$

Large free path of cold neutrons in para hydrogen give the opportunity to collect all cold neutrons from the whole chamber length in the direction out of the reactor



Comparison of optimized para-hydrogen and liquid deuterium chambers



Brightness for the LD_2 chamber with 200 mm height displacer

| Variant | Integral Brightness $\lambda > 4 \text{ \AA}$ $\text{cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1}$ |
|-----------------------|---|
| Basic (project) | $9.8 \cdot 10^{12}$ |
| Para-hydrogen | $1.58 \cdot 10^{13}$ |
| LD_2 – long channel | $1.55 \cdot 10^{13}$ |



Conclusion and discussion

Para-hydrogen CNS and LD₂ CNS have comparable integral brightnesses of cold neutrons. At the same time there are different pro and contra for these two variants:

Para-hydrogen CNS

Pro

- Smaller heat release
- Small tritium production
- Easier to organize bi-spectral source

Contra

- Needed at least two chambers due to smaller shine surface
- Needings in operational control of the ortho-hydrogen content in the hydrogen contour
- Needings in catalytic conversion of ortho- to para- hydrogen during the CNS operation

Deuterium CNS

Pro

- Large shine surface
- Absence of additional systems
- Considerable background in creation

Contra

- Larger heat release
- Considerable tritium production
- It is more complicated to build bi-spectral source



Thank you for the attention!

