PAUL SCHERRER INSTITUT

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UCN extraction from solid deuterium

10.05.2023 Workshop on UCN and VCN sources at ESS

Contents of this talk

Introduction:
UCN scattering in solid deuterium

Measurements at the
PSI UCN source

Simulations and parametrization
of elastic scattering

Implications for ESS

Purpose of this talk is to…

… comment on the ESS UCN in-pile source design goal of a 2 cm sD_2 compartment

… identify further requirements e.g. for the cooling system

… to achieve a high UCN extraction

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Introduction:
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Bulk and surface effects

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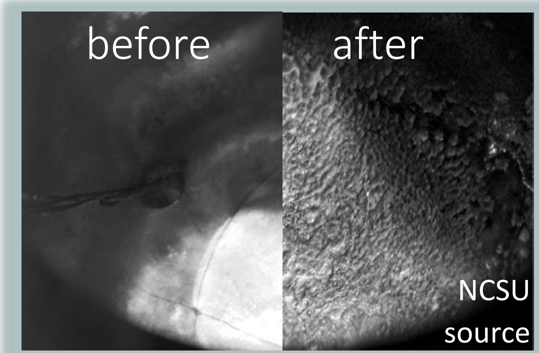
PSI UCN source

Simulations and parametrization
of elastic scattering

Implications for ESS

Scattering on sD_2 surface frost

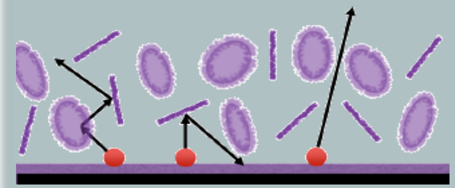
A. Anghel et. al, Eur. Phys. J. A 54 148 (2018)



Heat deposition during proton beam pulse causes sublimation from sD_2 surface

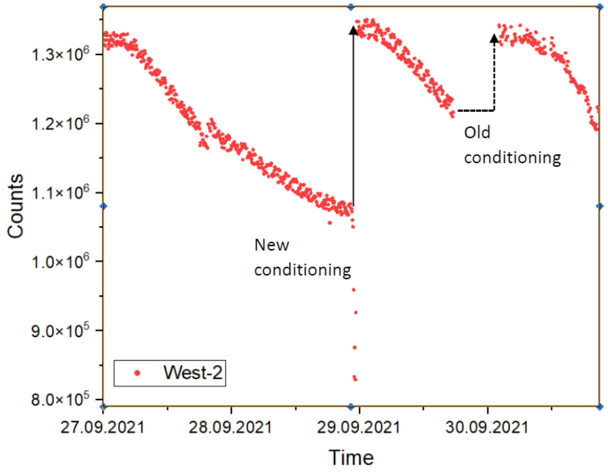
D_2 vapor freezes and forms frost on cold surface after pulse

Back-reflection on sD_2 frost reduces UCN extraction



Periodic surface conditioning is required to maintain high UCN yield

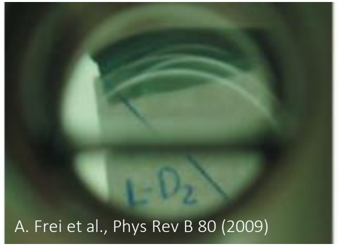
- (partial) melting and refreezing
- thermoelectric heating of surface
- **use heat deposition of p-beam**



Scattering on crystal defects

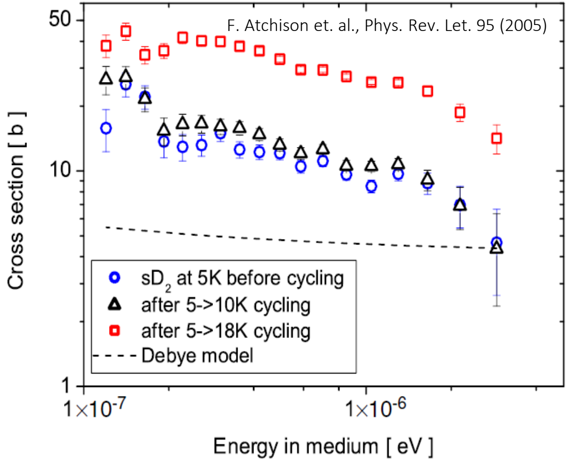
Elastic scattering on defects dominates the total scattering cross section at low sD_2 temperatures

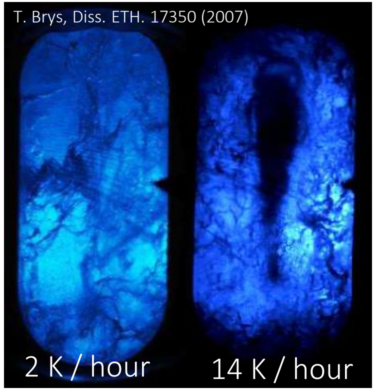
Thermal cycling and fast freezing / cooling increases the number of defects due to large volume contraction of sD_2



slow at 18.7 K

fast at 10 K





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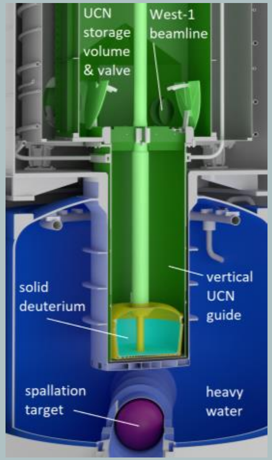
Measurements at the PSI UCN source

UCN yield
as a function of
sD_2 amount and cooling
procedure to determine the
UCN extraction efficiency



Simulations and parametrization of elastic scattering

Implications for ESS

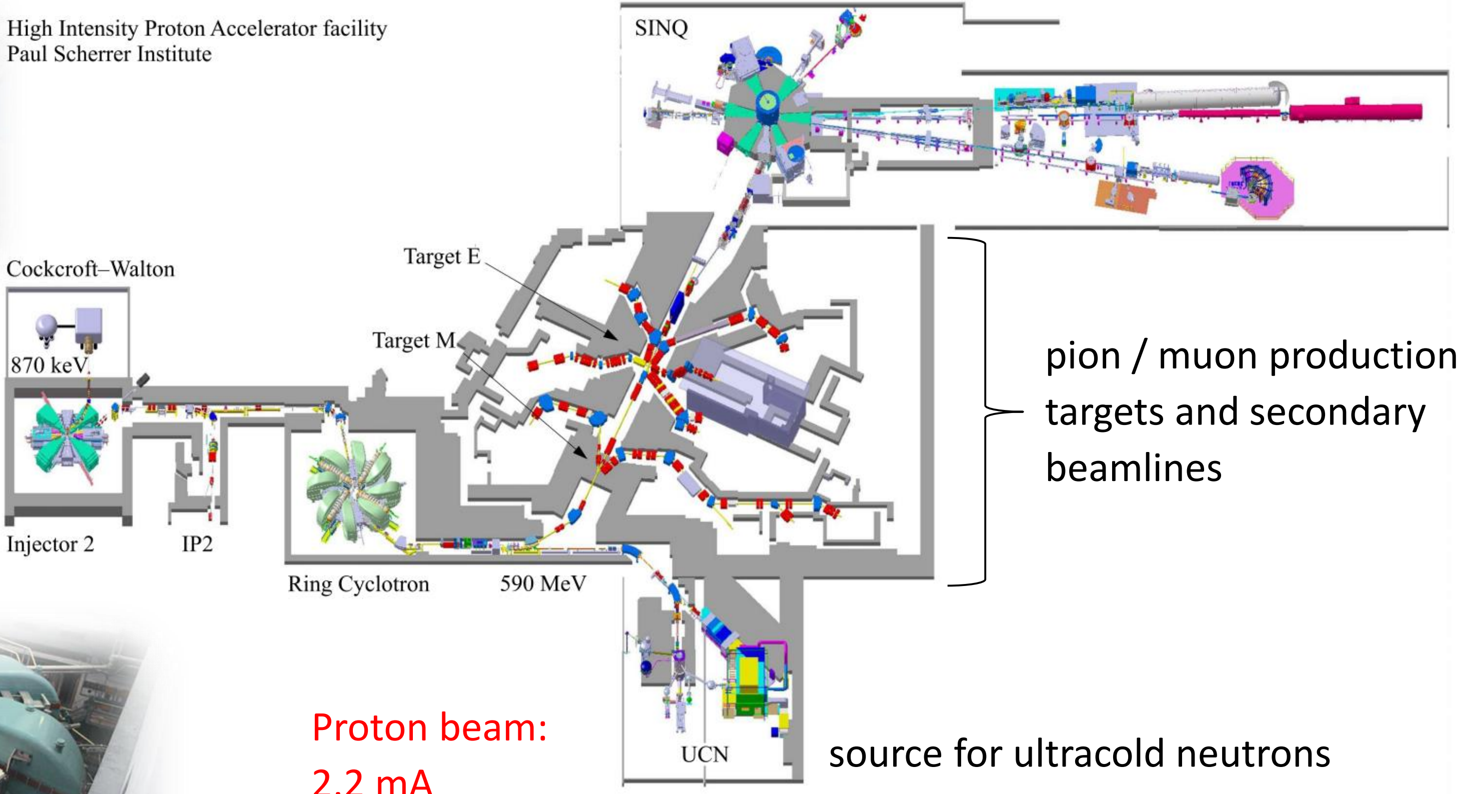
PAUL SCHERRER INSTITUT PSI

target and moderator station for thermal and cold neutrons and secondary beamlines

870 keV

72 MeV

590 MeV

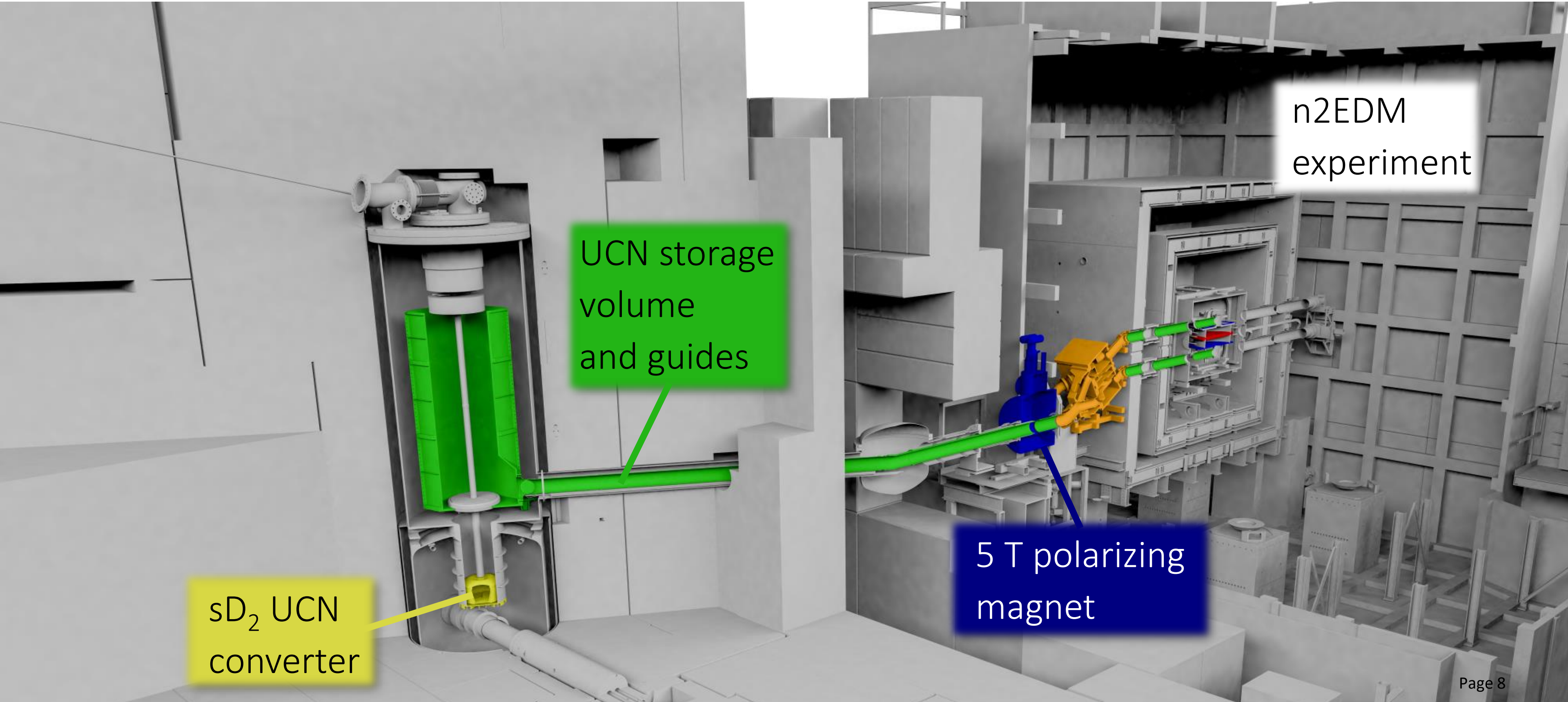


pion / muon production targets and secondary beamlines

source for ultracold neutrons

Proton beam:
2.2 mA
8 s long pulse every 300 s

PSI UCN source



Determine UCN extraction

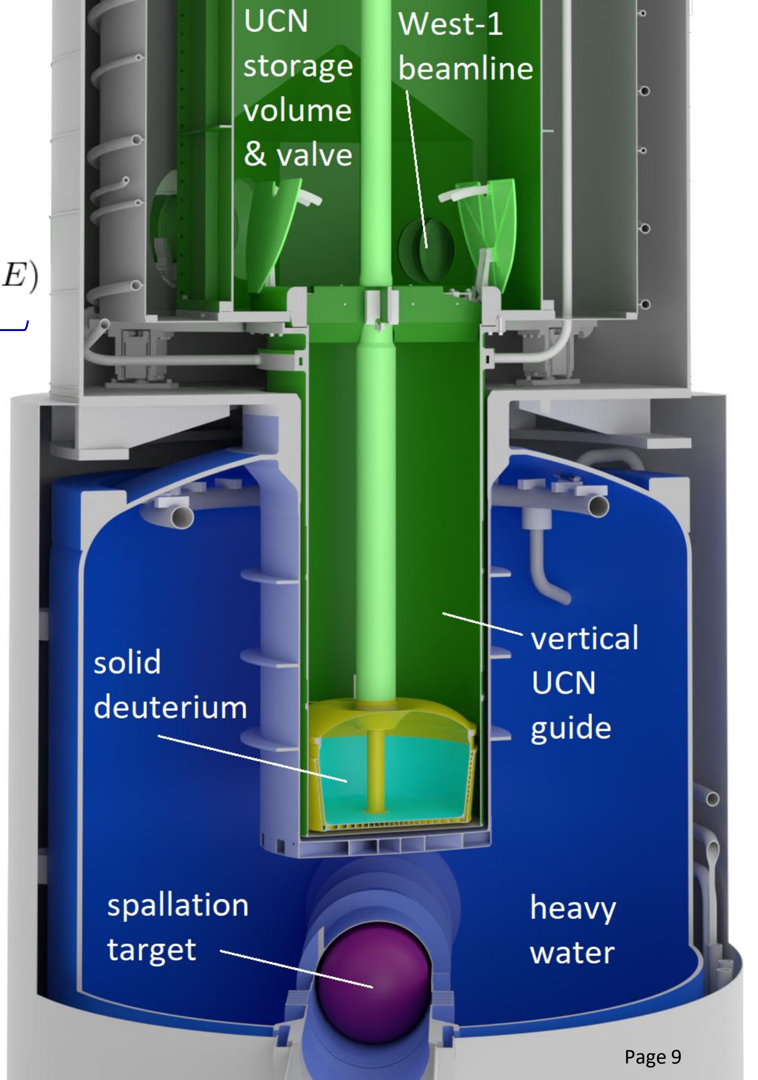
$$N(V) = \int_V \int_0^\infty \int_0^\infty \rho \, d^3\mathbf{r} \, dE \, dE_0 \, \frac{d\sigma}{dE}(E_0 \to E) \, \frac{d\varphi}{dE_0}(h, \mathbf{r}) \, \epsilon_{\mathrm{ext}}(E, \mathbf{r}) \, \epsilon_{\mathrm{t}}(E)$$

Method:

1. Calibrate UCN production and transport efficiency to beamports by measurements with thin sD_2 films where extraction efficiency $\epsilon_{\mathrm{ext}}(E) \approx 1$

2. Measure UCN yield $N(V)$ for increasing amounts (volume) of sD_2 to obtain the relative change of extraction efficiency

3. Parametrize elastic scattering in Monte Carlo simulations and fit the observed extraction efficiency



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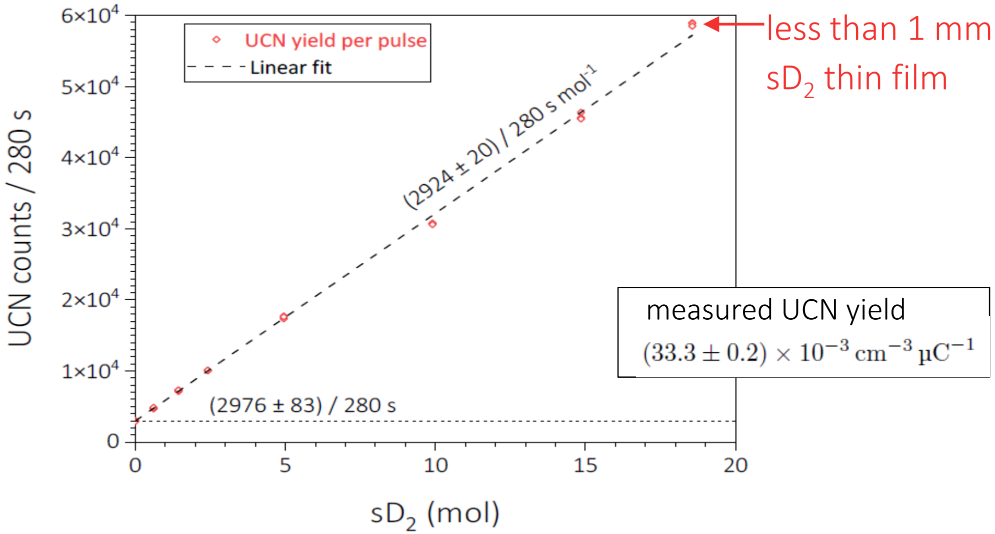
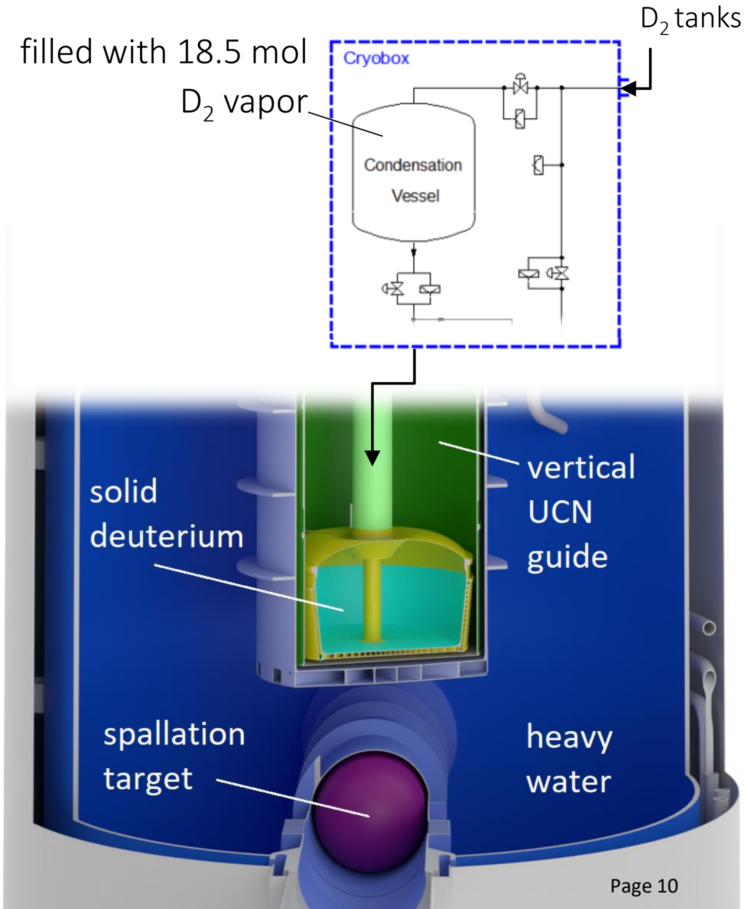
1. sD_2 thin film measurement

G. Bison et. al, Phys. Rev. C 107 (2023)

start with empty sD_2 vessel (< 0.01 mol D_2)

fill with known amount of D_2 vapor (± 0.1 mol) by monitoring condensation vessel pressure and measure UCN output





1. UCN losses

measured isomeric and isotopic purity of D_2 by Raman spectroscopy

- $C_{para} < 2.7$ %
- $C_{HD} < 0.2$ %

during operation < 1 % due to radiation induced para-to-ortho conversion

compute UCN lifetime in sD_2 at 5 K

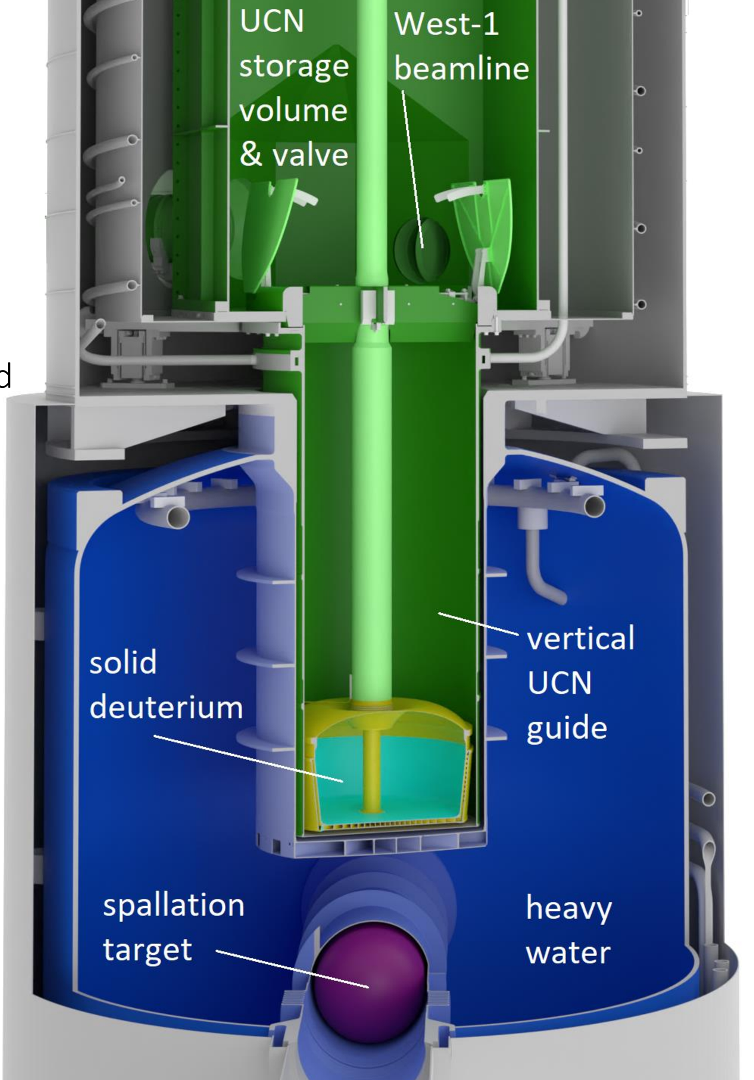
corresponding MFP = 9 cm much larger than sD_2 film thickness

$$\tau = \frac{1}{v}\left[c_{\text{para}}\ \Sigma_{\text{para}} + \Sigma_{\text{phonon}} + \Sigma_{\text{abs},D_2} + c_{\text{HD}}\ \Sigma_{\text{abs,HD}}\right]^{-1}$$

$$= \left[\frac{1}{56\,\text{ms}} + \frac{1}{168\,\text{ms}} + \frac{1}{146\,\text{ms}} + \frac{1}{269\,\text{ms}}\right]^{-1}$$

$$= 29\,\text{ms}$$

$$\Rightarrow \epsilon_{\text{ext}}(E) \approx 1$$

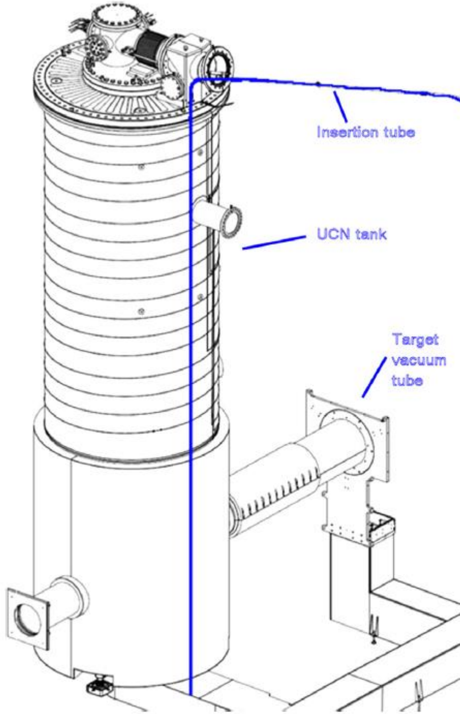


1. UCN production

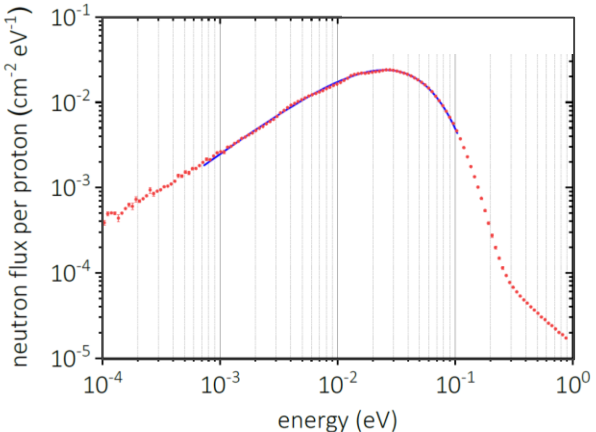
H. Becker et. al., NIM A 777 (2015)

evaluated downscattering cross section

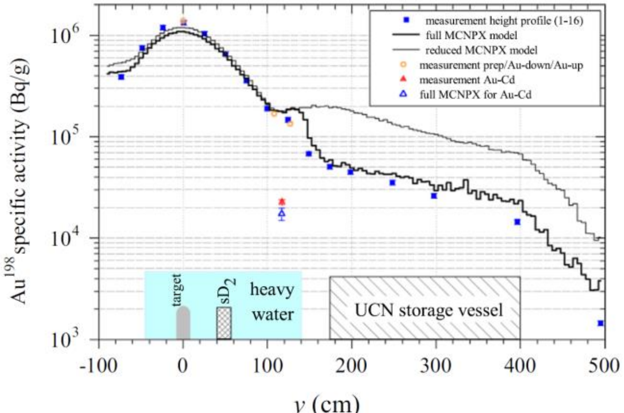
use thermal neutron spectrum from heavy water moderator



MCNP simulation of thermal flux ...



... confirmed by gold foil activation

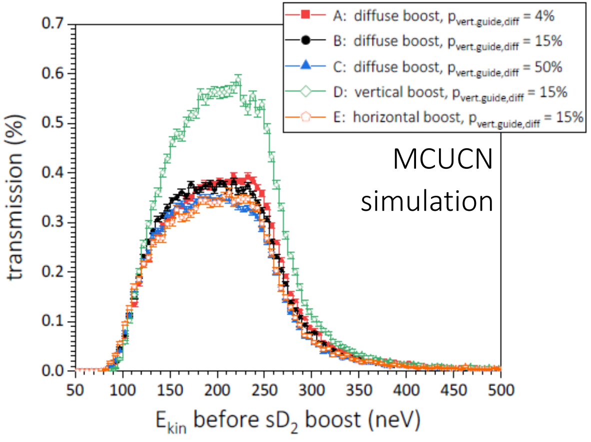


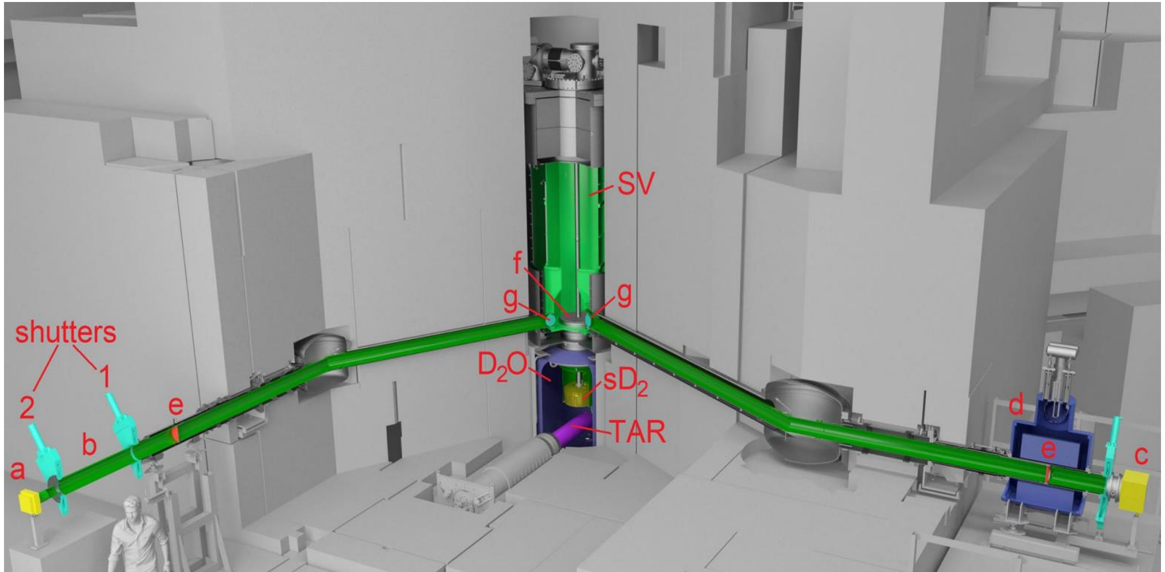
1. UCN transport efficiency

G. Bison et. al., Eur. Phys. J. A 56 33 (2020)
G. Bison et. al., Eur. Phys. J. A. 58 103 (2022)
G. Bison et. al., arXiv:2301.11668 (2023)

UCN transmission spectra calibrated by

- “ping-pong” transmission measurements
- storage time and time of arrival spectra
- UCN density measurements in storage bottles at different heights
- time of flight spectroscopy





modified for thin film source ($sD2$ distribution on cooled moderator surfaces from vapor deposition)

additional parameters scanned in wide range

1. UCN yield

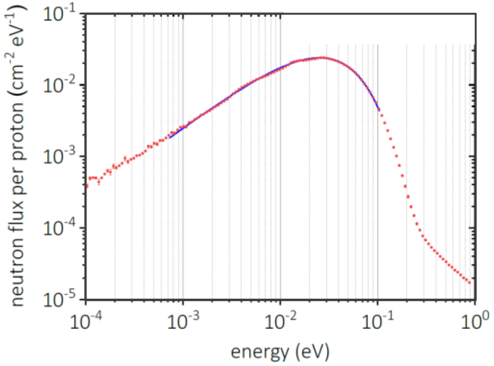
G. Bison et. al, Phys. Rev. C 107 (2023)

measured UCN yield

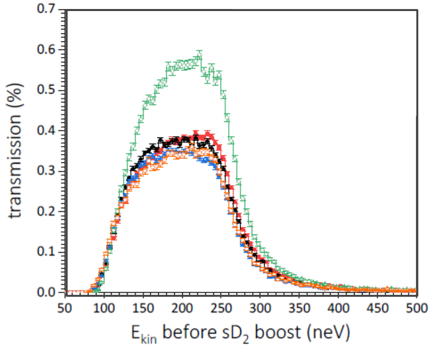
$$N(V) = \int_V \int_0^\infty \int_0^\infty \rho\, d^3\mathbf{r}\, dE\, dE_0\, \underbrace{\frac{d\sigma}{dE}(E_0 \to E)\, \frac{d\varphi}{dE_0}(h, \mathbf{r})}\, \underbrace{\epsilon_{\mathrm{ext}}(E, \mathbf{r})}_{\approx 1}\, \underbrace{\epsilon_{\mathrm{t}}(E)} = (33.3 \pm 0.2) \times 10^{-3}\,\mathrm{cm}^{-3}\,\mu\mathrm{C}^{-1}$$

characterized UCN production and transport efficiency

down scattering cross section



thermal flux from heavy water



UCN transport spectrum

Simulated UCN yield (10^{-3} cm^{-3} μC^{-1})	diffuse boost A	diffuse boost B	diffuse boost C	perpendicular D	perpendicular E
from base	36.3	34.6	29.8	48.3	-
from side walls	32.5	32.4	33.3	-	30.3
combined	34.1	33.3	31.9	37.7	

2. Measure extraction efficiency

increase sD2 filling level by deposition of D_2 vapor into cooled moderator vessel

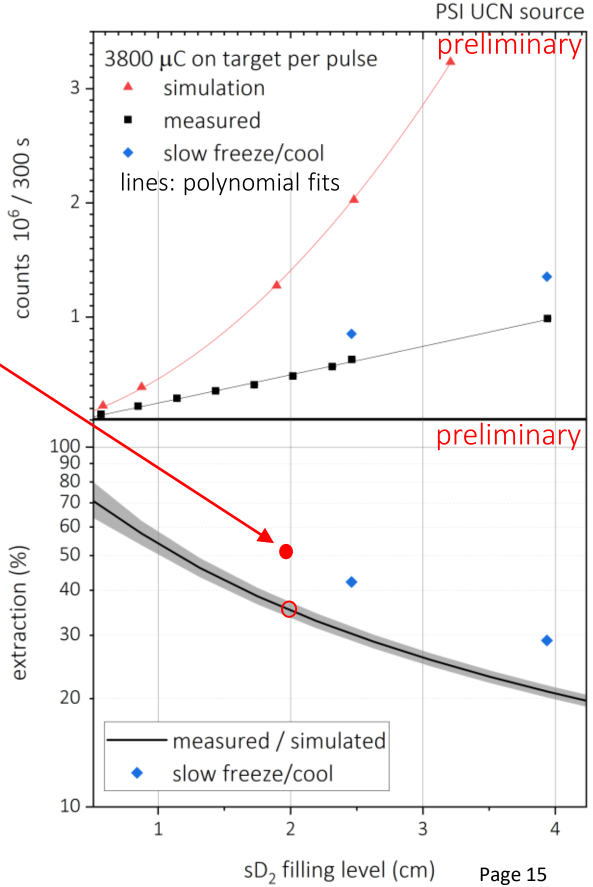
after deposition, remelt and freeze entire amount of D_2 to avoid surface frost

two freezing / cooling methods:
- fast (full cooling power)
- slow (0.25 K / hour)

compare to simulated UCN yield based on thin film calibration measurement

50 % extraction from 2 cm sD_2 converter is achievable …

… but requires slow freezing / cooling

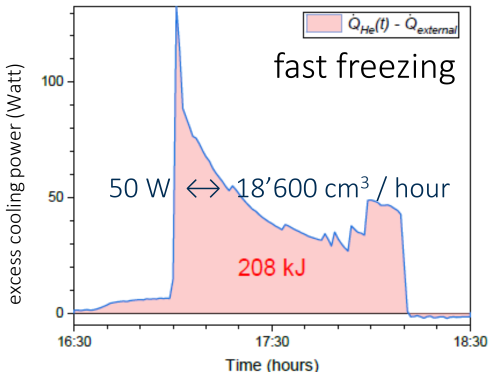


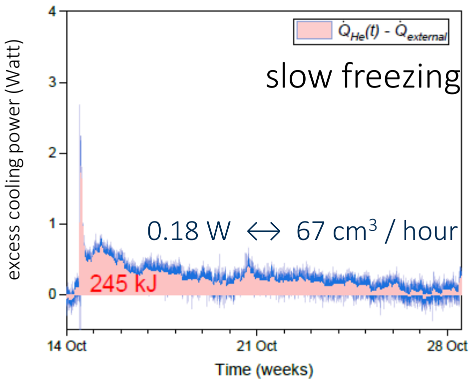
2. Slow vs. fast freezing of deuterium from the melt

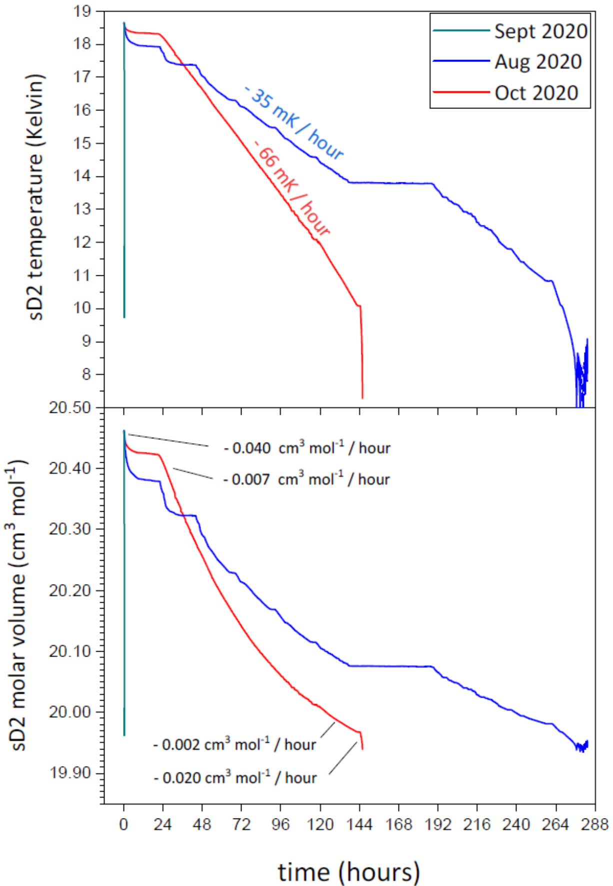
control helium cooling temperature on 10 mK level

monitor sD_2 crystal growth indirectly by the removal of latent heat, i.e. required excess cooling power (steady state power 12 W)

monitor sD_2 temperature by measuring the vapor pressure (or vessel lid temperature)







3. Parametrize elastic scattering

simulate UCN transport in sD_2

parametrize elastic scattering by total scattering cross section $\boldsymbol{\sigma}$

fit energy spectrum of extracted UCN to retrieve $\varepsilon_{\text{ext}}^{\sigma}(E, \boldsymbol{r})$

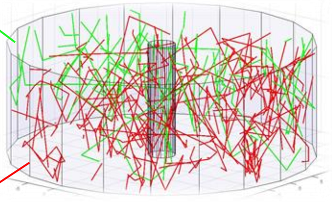
include $\varepsilon_{\text{ext}}^{\sigma}$ in computation of UCN yield to reproduce measurement

extracted

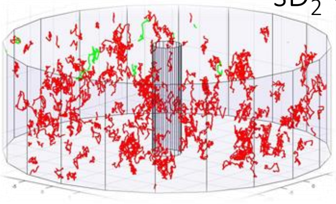
absorbed

up-scattered

sD_2 vessel

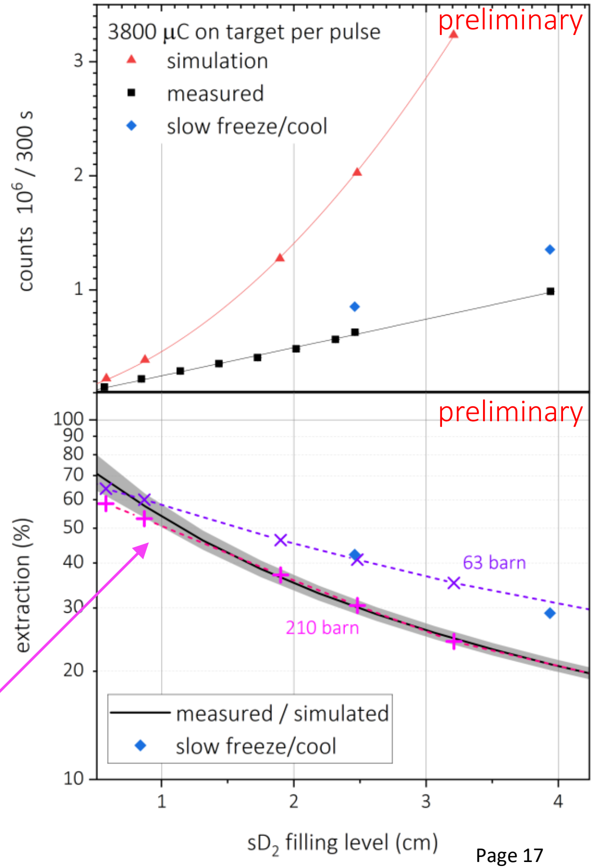


4.2 barn



210 barn

extraction model



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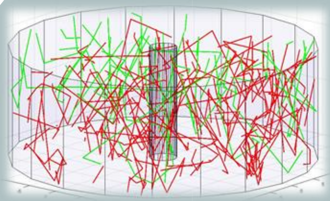
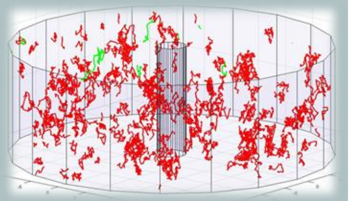
Measurements at the
PSI UCN source

Simulations and parametrization of elastic scattering

Cold neutron moderation

UCN production,
scattering and losses



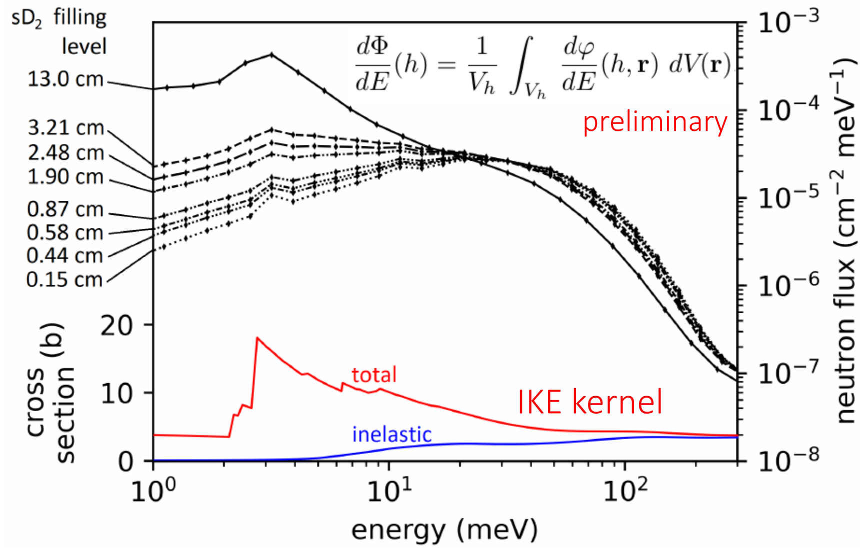


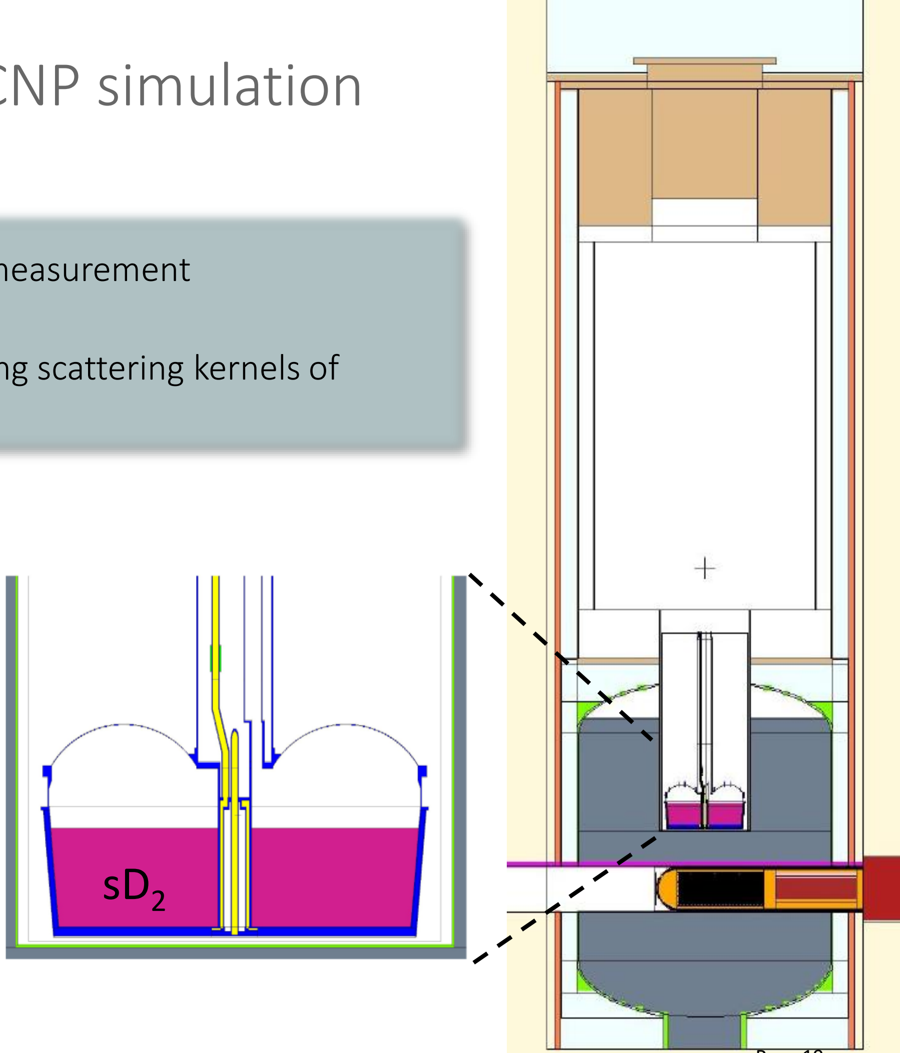
Implications for ESS

Cold neutron flux – MCNP simulation

same MCNP model as verified by gold foil activation measurement

added various amounts (filling levels) of sD_2 at 5 K using scattering kernels of W. Bernnat et. al., J. Nuc. Sci. Tech. 39, 124-127



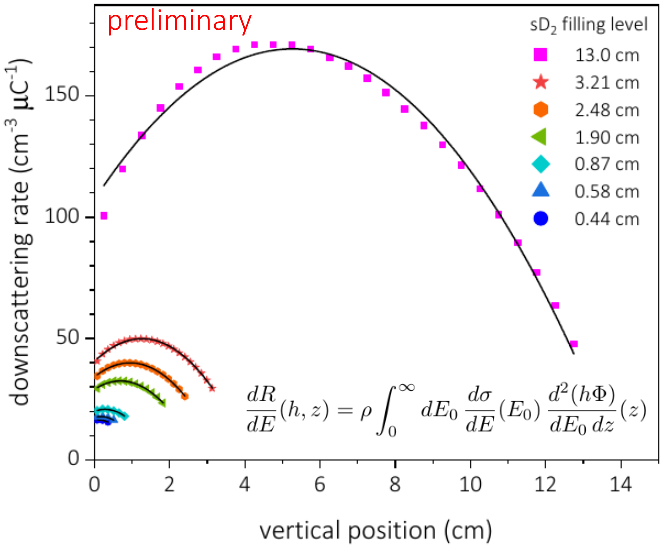


Cold neutron flux – spatial distribution

from MCNP cylindrical mesh tally compute vertical gradient of cold neutron flux

weighted by down scattering cross section to obtain UCN production rate at vertical position from surface

Option	Volume [liters]	P_{UCN} [cm^{-3} s^{-1}]	$\dot{N}_{UCN}$ [s^{-1}]	Heat [Watt]
		SD_2 thin slab in twister - location 1		
Fig. 5	1.81	3.1×10^5	5.6×10^8	760
Fig. 6	1.75	7.7×10^5	1.4×10^9	2910
Fig. 7	0.38	1.3×10^6	5.0×10^8	560
Fig. 9	0.13	1.7×10^6	2.2×10^8	520
		SD_2 thin slab in MCB - location 2		
Fig. 18a	0.91	3.8×10^4	3.4×10^7	159
PSI (upper 2 cm)	3.4	1.6×10^5	5.4×10^8	240 (total)



- integrated UCN energy range 0 – 250 neV
- typically 18000 **μC** per 8 s proton beam pulse
- 22000 cm^3 nominal sD_2 volume

Elastic scattering cross section

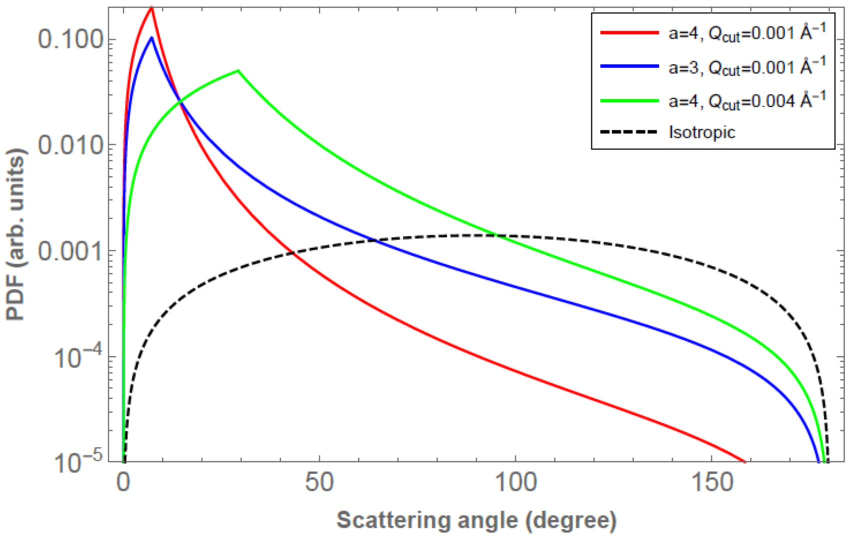
in-house UCN transport simulation
in sD_2 vessel

propagate UCN until random sample
of lifetime distribution in sD_2 is exceeded

elastic scattering cross section as free parameter(s)

- isotropic: one parameter σ
- spherical inhomogeneities in the high QR (Porod) limit:
  two parameters P, Q_{cut}

  (similar to T. Brys, Diss. ETH. 17350 (2007))



angular distribution of scattering angle

$$\frac{d\sigma}{d\Omega} = {b_{\rm coh}}^2 S(\mathbf{Q}) = {b_{\rm coh}}^2 (4\pi R^3 \delta\rho)^2 \left(\frac{j_1(QR)}{QR}\right)^2$$

QR ≫ 1: $\frac{d\Sigma}{d\Omega} = \frac{P}{Q^a}$ R > 10 nm for Q_{UCN}

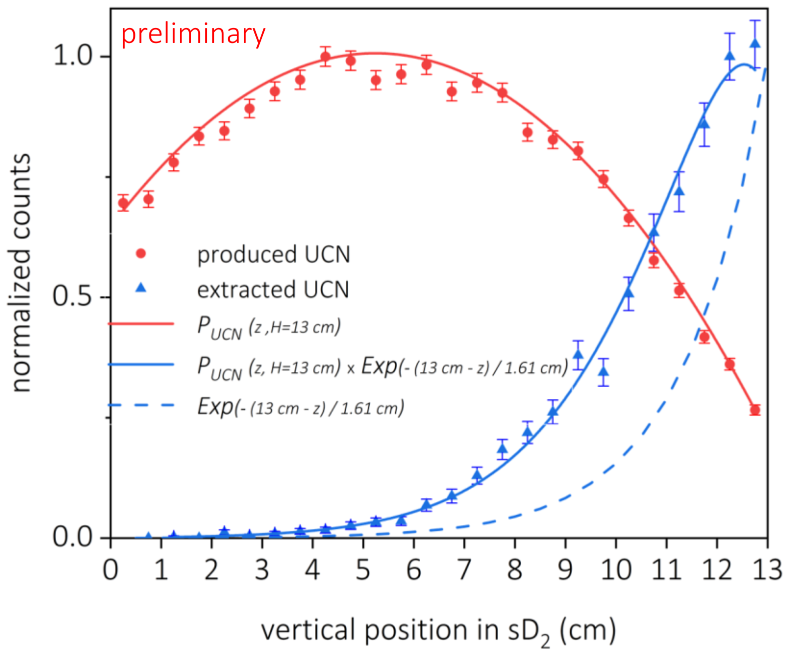
Extracted UCN: spatial distribution

tally starting position of extracted UCN

can be approximated by product of
exponential distribution and
cold neutron flux vertical gradient

extraction depth
(mean of exponential distribution)
1.6 cm from sD_2 surface

mean of total distribution
2.3 cm from sD_2 surface



isotropic scattering **σ = 63 barn**

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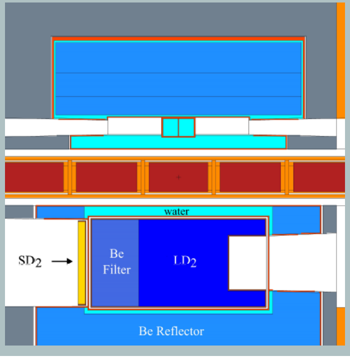


Implications for a sD_2 UCN source at ESS

measurements at PSI UCN source confirm that with 2 cm sD_2 compartment 50 % extraction is achievable

cooling system must be designed such that

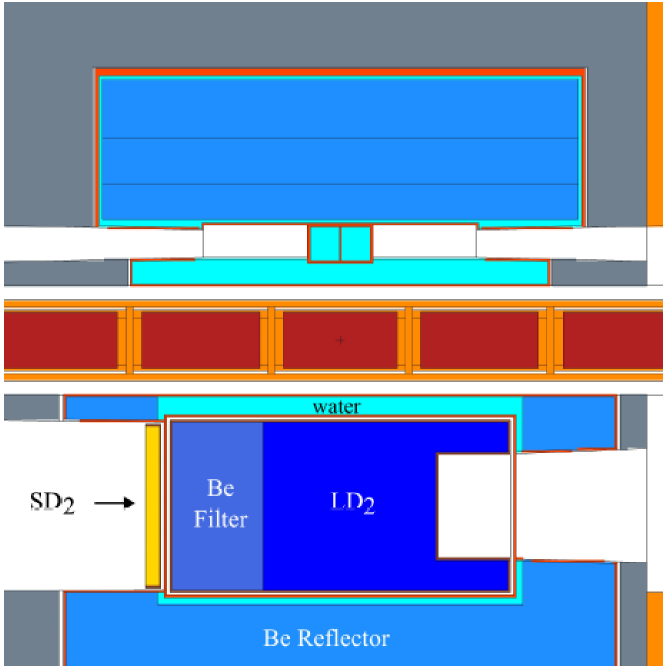
- slow freezing and cooling are possible
- keep sD_2 temperature at low temperature during operation

PSI: approx. 450 Watt at 5 K

geometry that allows for large sD_2 surface can optimize the volume-integrated UCN yield

PSI: 1600 cm^2

possible surface effects should be studied (ESS horizontal extraction vs. PSI/LANL/NCSU vertical extraction)



Thanks for your attention!