THE 7TH INTERNATIONAL CONFERENCE ON PARTICLE PHYSICS AND ASTROPHYSICS

Converters of very cold and ultracold neutrons: Monte Carlo simulation of their properties and specifics of available data libraries and software

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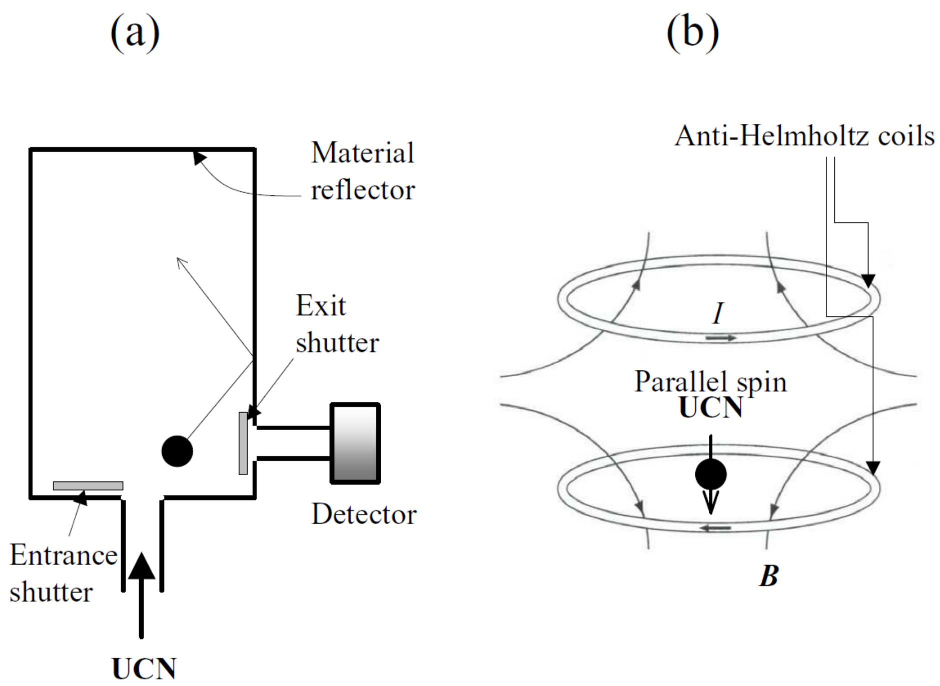
1. Introduction of VCN and UCN and their applications (1)

Type of neutron	E (eV)	T (K)	Λ (Å)	V (m/s)
Ultra cold	< 10^{-7}	≈(<) mK	> 800	< 5
Very cold	10^{-7} - 10^{-4}	10^{-2} - 10	800 - 30	5 - 130
Cold	(0.1 - 10) x 10^{-3}	10 - 120	30 - 3	130 - 1320
Thermal	(10 - 100) x 10^{-3}	120 - 1000	3 - 1	~ 1320 - 3950
Resonance	> 1		< 0.1	> 4 x 10^{4}

Ref.: G.V. Kulin (ISINN-29). The concept of an UCN source for a periodic pulsed reactor (2023).



Sketch of UCN traps: (a) A material trap using a material reflector, (b) A magnetic trap.

Ref.: Oh-Sun Kwon (2005), Sogang University. Quasi-elastic scattering of ultracold neutrons (Dissertation).

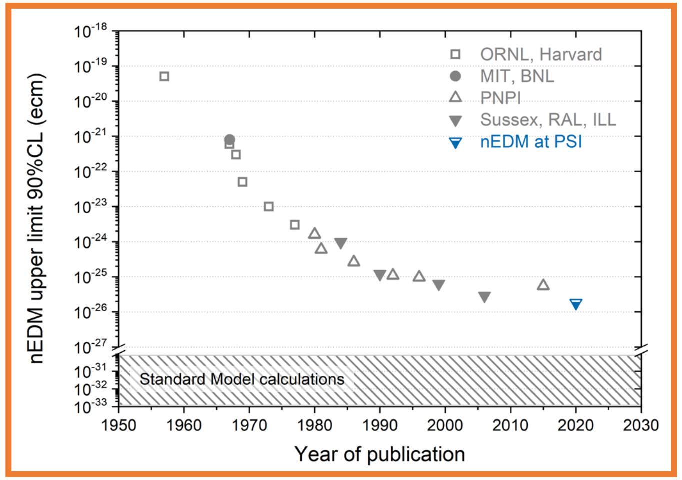
1. Introduction of VCN and UCN and their applications (2)

VCN

- For studying the structure and dynamics of materials via neutron scattering and imaging techniques
- For studying low-energy vibrational states
- Search for neutron-antineutron oscillation

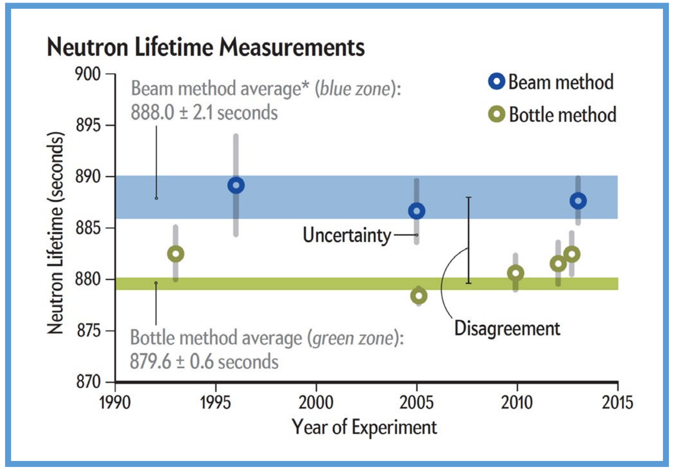
UCN

- Search for the neutron electric dipole moment (EDM)
- Measurement of the neutron lifetime
- Measurement of angular correlation coefficients of neutron beta decay
- Search for neutron-antineutron oscillations
- Quantization of neutron sates in gravitational field and search for new interactions
- Non-stationary quantum mechanics and neutron optics



The history of neutron EDM limits

Ref.: Abel, C.; et al. (2020)



Neutron lifetime measurements

Ref.: https://www.scientificamerican.com, modified

2. Some main tasks on the concept of low energy source

As part of the work on the concept of the source, priorities will be:

1. Simulation of the production of very cold neutrons (VCN) in various converters/materials for optimizing their parameters and increasing the efficiency of VCN extraction from the source.
2. Design and development of the required experimental equipment to carry out an experiment to measure the extraction efficiency of VCNs from a source with a specially designed reflector.
3. Analysis of possible candidate materials for use as UCN converter, considering the specifics of the planned source.
4. Modeling of the converter, calculation of the UCN output from it and optimization of its geometry.
5. Participation in the formation of technical requirements and in the design of a UCN converter unit.

3. Simulation implementation (1)

Thermal Scattering Law data (TSL)

- **h2o.7z**: H2O (H in H2O/ O in H2O)
- **ch.7z**: CxHx (C, H, O in Benzen, Ethanol, Mesitylene, M-Xylene, Toluene, Triphenylmethane, etc.)
- **cold.7z**: Para H, Ortho H, Para D, Ortho D

https://phits.jaea.go.jp/library.html

PHITS
Particle and Heavy Ion Transport code System

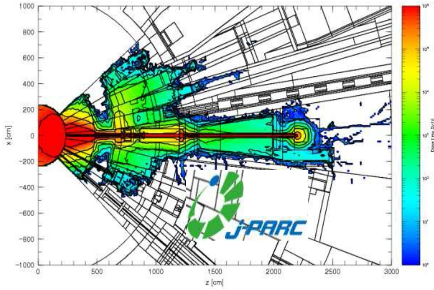
Particle and Heavy Ion Transport code System

Capability: Transport and collision of nearly all particles (neutron, proton, ions, electron, photon, etc.) over wide energy range (10^{-5} eV/n to 1 TeV/n) using Monte Carlo method

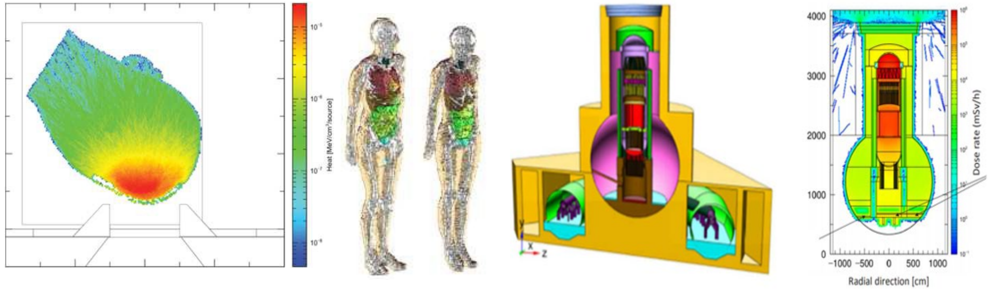
- sod2-05K: sD2 (at 5 K)

Developed by the spallation-physics-group
Link: https://git.esss.dk/spallation-physics-group/phits-tsl/-/tree/main/mixed/solid_deuterium?ref_type=heads

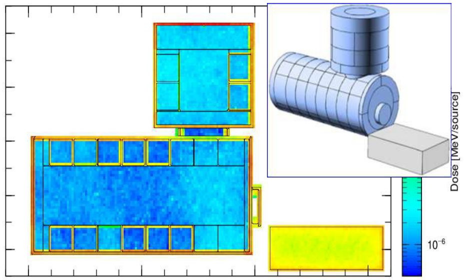
Version: PHITS 3.341
Library: JENDL-5 (ACE-J50) Library
Format of TSL files: ACE



Facility Design



Radiation Therapy & Protection



Space & Geoscience

https://phits.jaea.go.jp/library.html

3. Simulation implementation (2)

The sD_2 TLS library based on the neutron scattering kernel proposed by **Granada J.R.**

The main characteristics of Granada's model including:

- The lattice's density of states
- The Young-Koppel quantum treatment of the rotations
- The internal molecular vibrations
- The elastic processes involving coherent and incoherent contributions are fully described, as are the spin-correlation effects

$$S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{-i\omega t} \times \left\langle \sum_{l,l'}\sum_{\nu,\nu'} \overline{a^*_{l\nu} a_{l'\nu'}} \exp\{-i\mathbf{Q}\cdot\mathbf{R}_{l\nu}(0)\} \exp\{i\mathbf{Q}\cdot\mathbf{R}_{l'\nu'}(t)\} \right\rangle, \quad (1)$$

The intermediate scattering function $\chi(Q,t)$

The elastic term

$$\chi^{el}(\mathbf{Q},0) = 4b_c^2\, j_0^2(Qr/2)|F(\mathbf{Q})|^2\chi^{vib}(\mathbf{Q},0) \quad \text{(Elastic Coherent)}$$
$$+2(1+\alpha)\, b_i^2\chi^{vib}(\mathbf{Q},0) \quad \text{(Elastic Incoherent)} \quad (2)$$

The incoherent approximation for the inelastic term

$$\chi^{inel}(\mathbf{Q},t) = v(\mathbf{Q},t)\cdot I_s(\mathbf{Q},t)\cdot\chi^{vib}(\mathbf{Q},t) \quad (3)$$

Where:

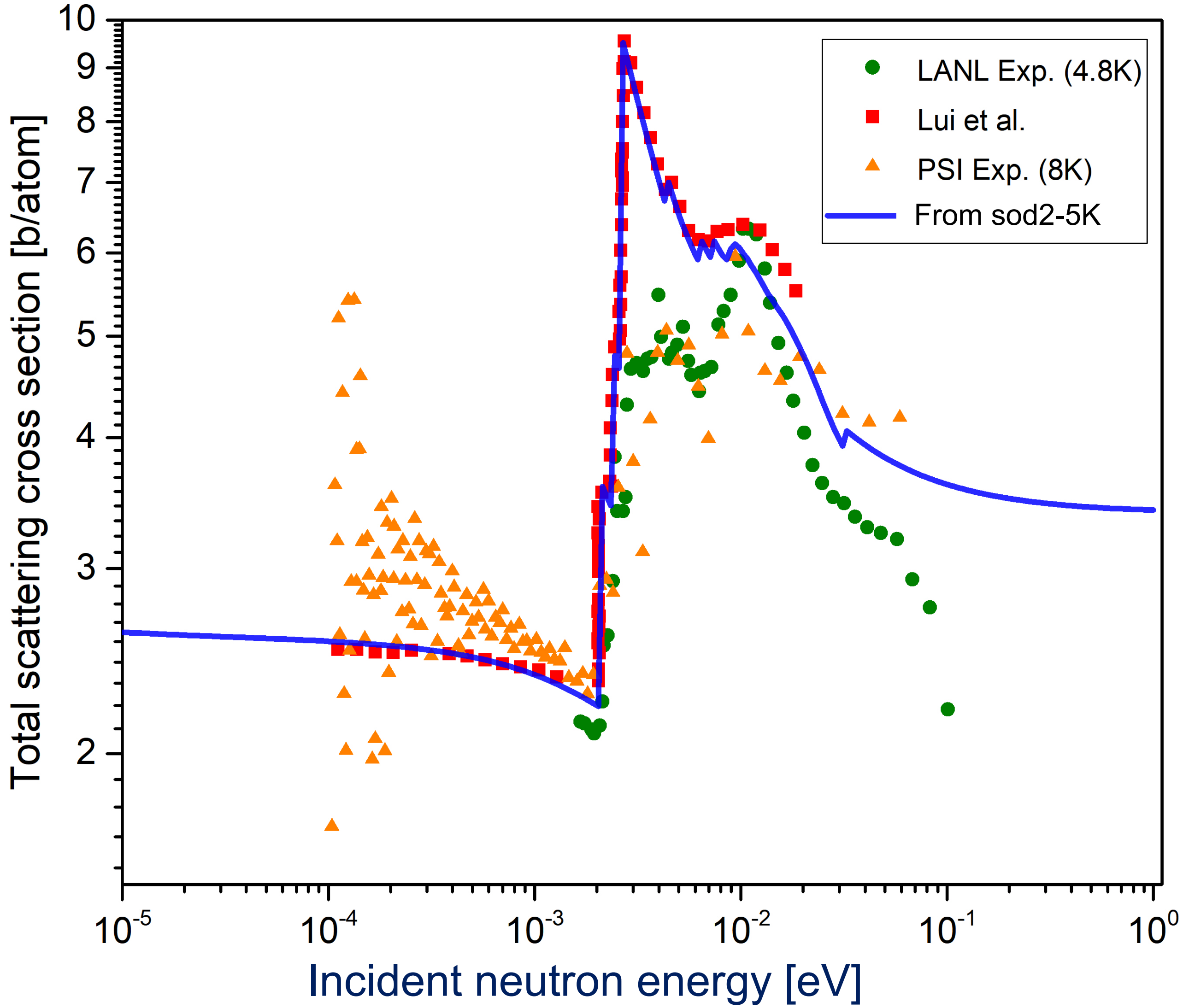
v(Q,t) contains all the complexity associated to **the molecular rotations** with definite parity for each (ortho, para) molecular species.

I_s(Q,t) is the self-contribution of the molecular centers determined by the dynamics of the lattice in the case of solid systems

|F(Q,0)| is the lattice structure factor corresponding to the arrangement of molecular centers

χ^{vib}(Q,0) is the Debye-Waller factor

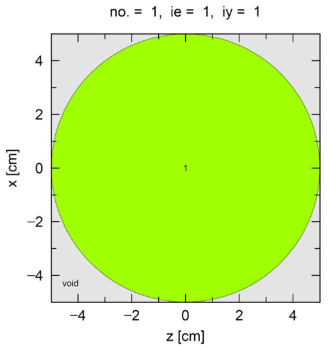
4. Simulation results (1/7)

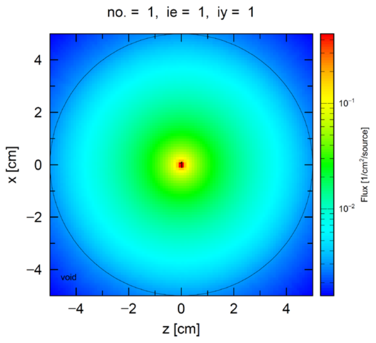


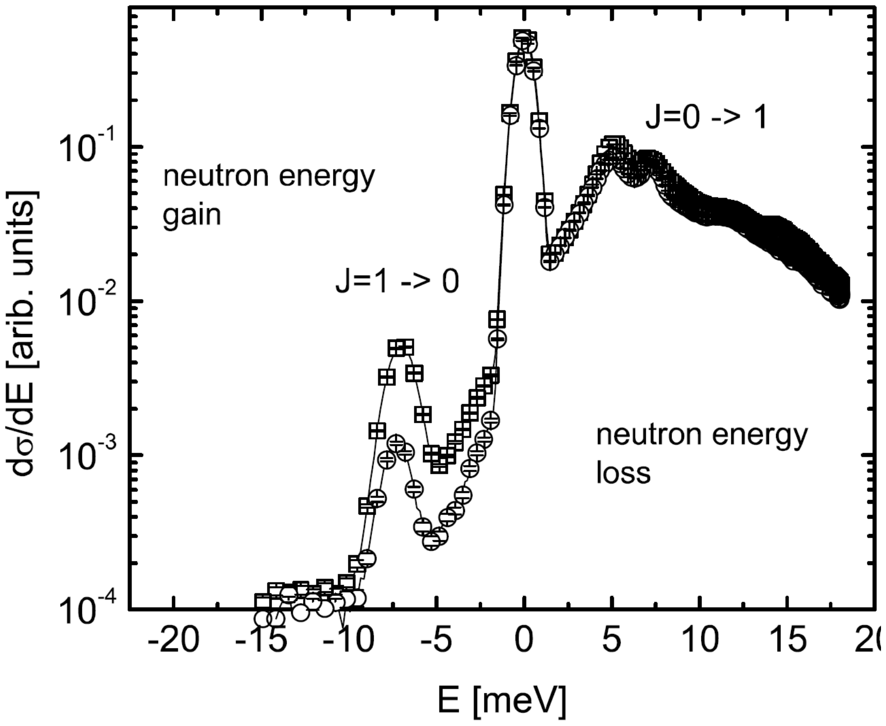
Total scattering cross section per atom for sD_2 at 5 K as a function of incident energy

4. Simulation results (2/7)

Simulation configuration	
Material	(Ortho) sD_2
Source type	Point isotropic
Sphere radius (cm)	5
Type of particle	Neutron
Initial energy (meV)	20.4
Temperature (K)	5

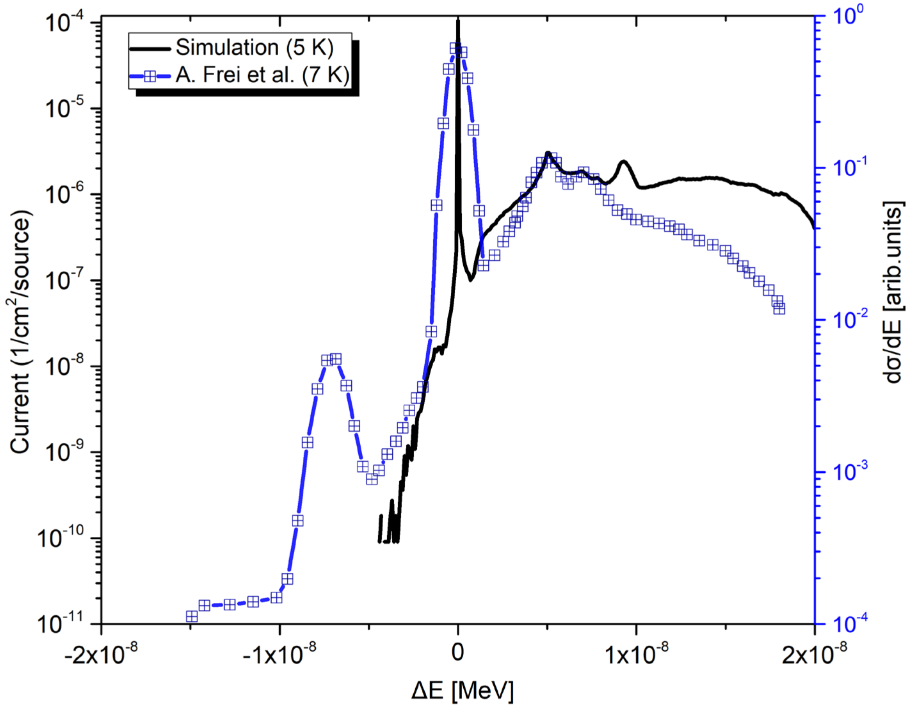






An example of a dynamical neutron cross-section of solid D_2 at T = 7 K. Comparison of two ortho-concentrations C_0 = 66.7% (□) and C_0 = 98% (○). Initial energy of the thermal neutrons is E_0 = 20.4 meV.

Ref.: A. Frei et al.. doi: 10.1209/0295-5075/92/62001



A comparison between simulation result with A. Frei's result.

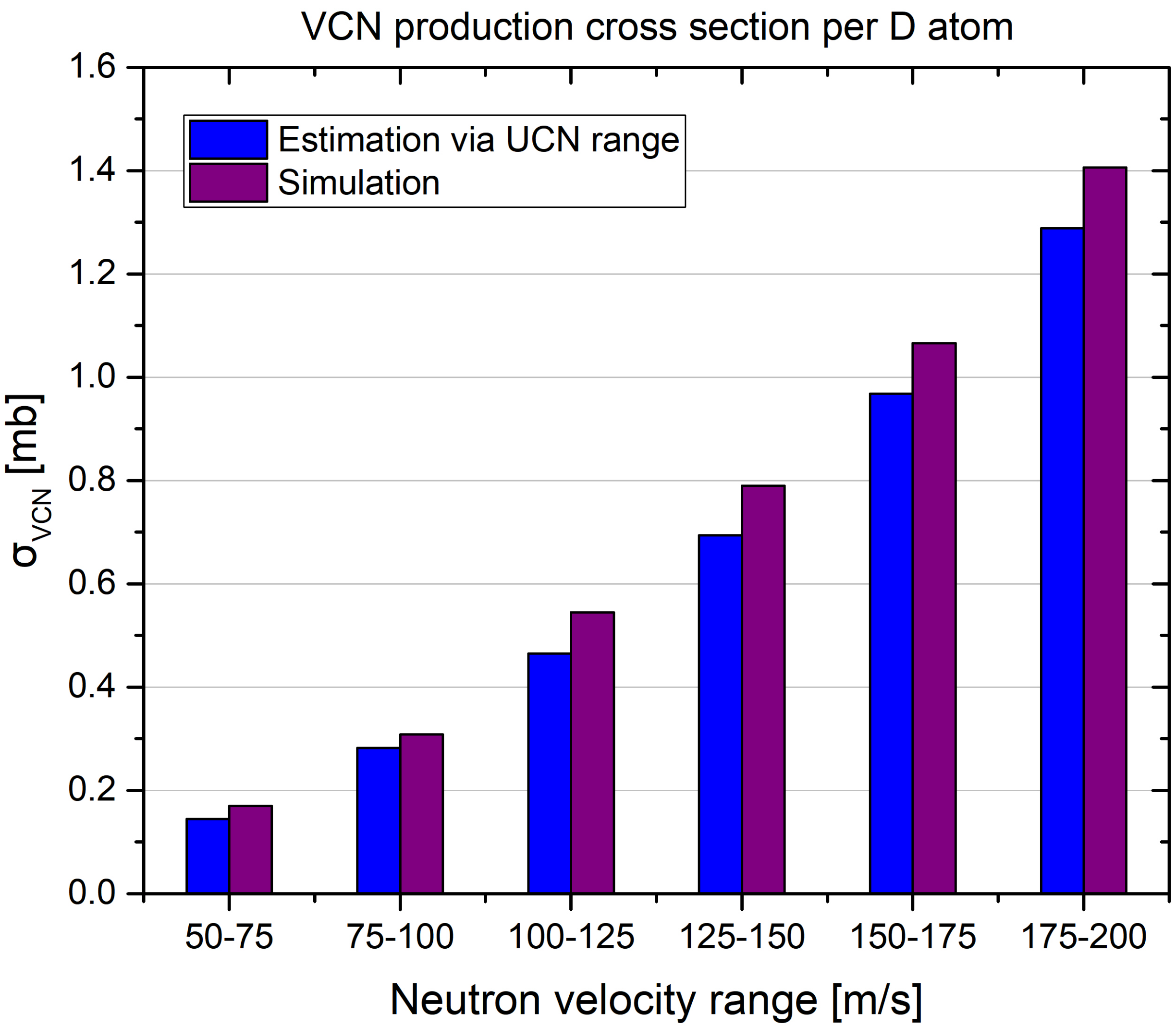
Note: The TLS library used for the simulation was developed for pure ortho-D_2 at 5 K

4. Simulation results (3/7)

E_0 (meV)	Velocities (m/s)	VCN production cross section (mb)
20.4	50 - 75	1.6991E-01
	75 - 100	3.0807E-01
	100 - 125	5.4464E-01
	125 - 150	7.9014E-01
	150 - 175	1.0660E+00
	175 - 200	1.4058E+00

VCN production cross-section approximation: $\sigma_{VCN} = \sigma_{UCN} \left(\frac{V_{VCN}}{V_{UCN}} \right)^3$

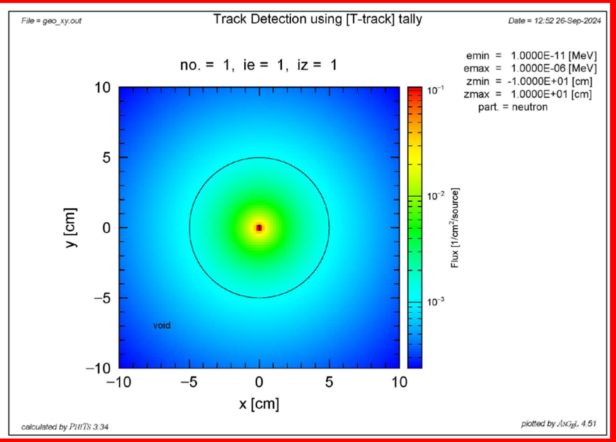
$V_{UCN} = \mathbf{5.3567}$ m/s (150 neV); σ_{UCN} = **0.75E-7** b.
[0, V_{VCN}] – the VCN production range.

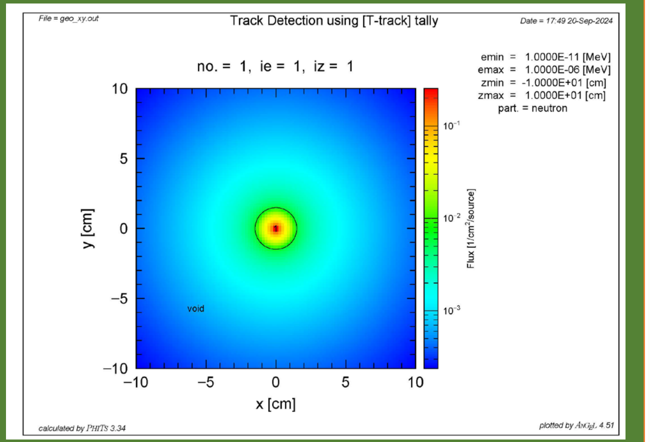


4. Simulation results (4/7)

Materials

№	Material	Density (g/cm3)	Temperature (K)
1	Solid Deuterium (sD_2)	0.206	5
2	Liquid Deuterium (lD_2)	0.1638	20
3	Parahydrogen	0.0708	20
4	Mesitylene	0.5184	20
5	Ice (H_2O)	0.9325	115





Incident neutron energy

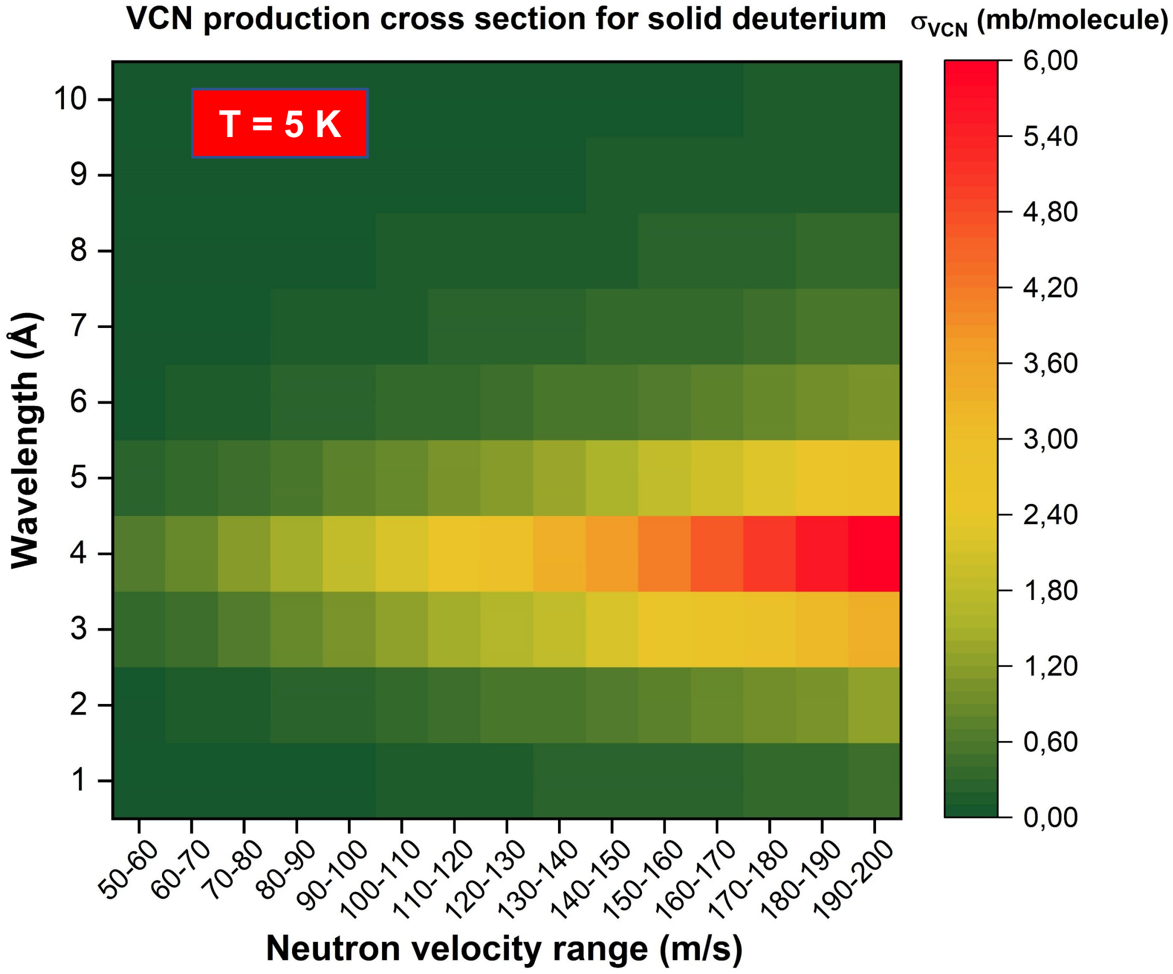
Wavelength (A)	Incident Energy (meV)
1	81,8042
2	20,45105
3	9,089355
4	5,112762
5	3,272168
6	2,272339
7	1,669473
8	1,278191
9	1,009928
10	0,818042
11	0,6760678
12	0,5680847
13	0,4840485
14	0,4173684
15	0,3635742
16	0,3195477
17	0,2830595
18	0,2524821
19	0,2266044
20	0,2045105

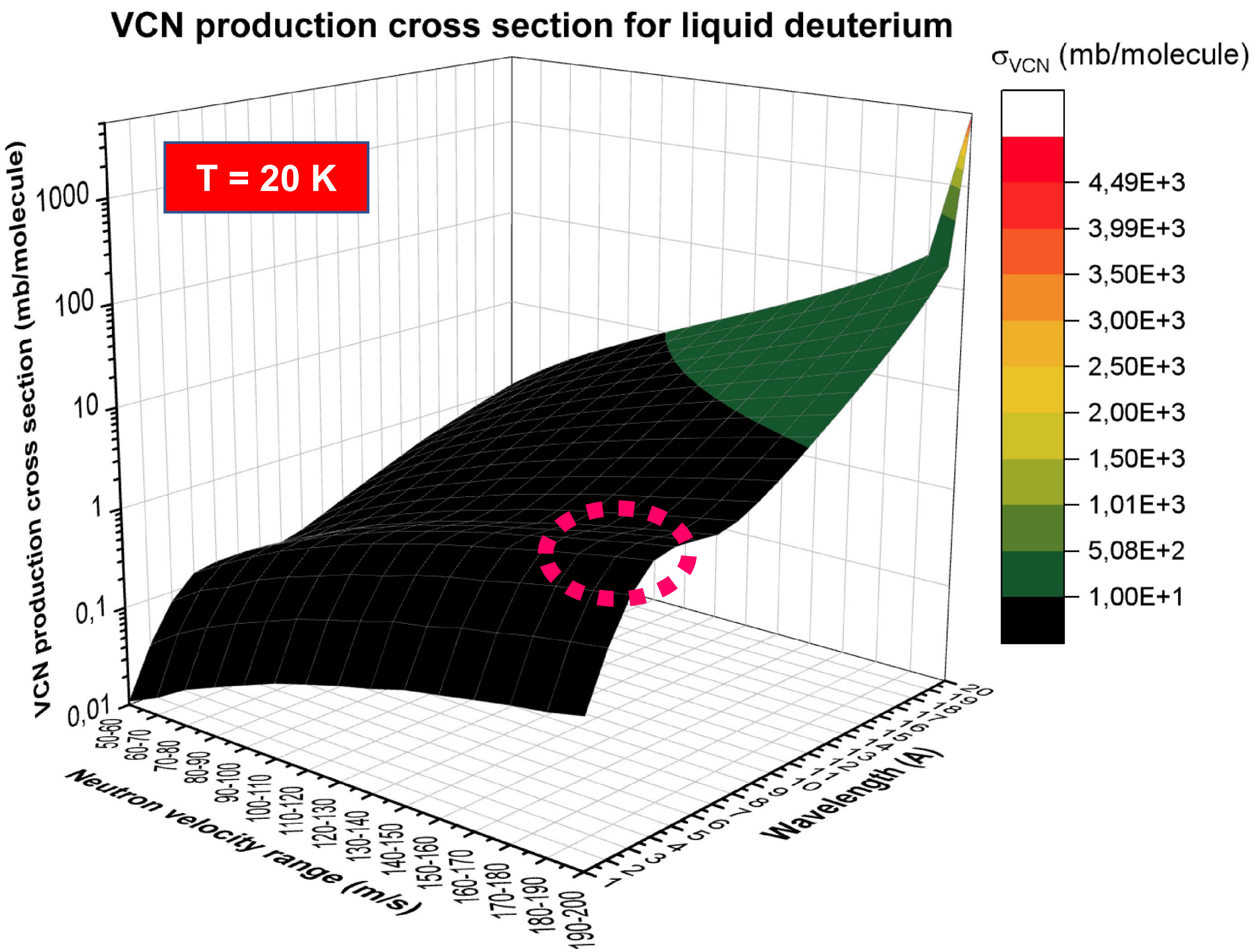
Neutron velocity range

Velocity (m/s)	E (meV)
50	0,01306759
60	0,01881733
70	0,02561248
80	0,03345304
90	0,042339
100	0,05227037
110	0,06324715
120	0,07526933
130	0,08833692
140	0,1024499
150	0,1176083
160	0,1338121
170	0,1510614
180	0,169356
190	0,188696
200	0,2090815

4. Simulation results (5/7)

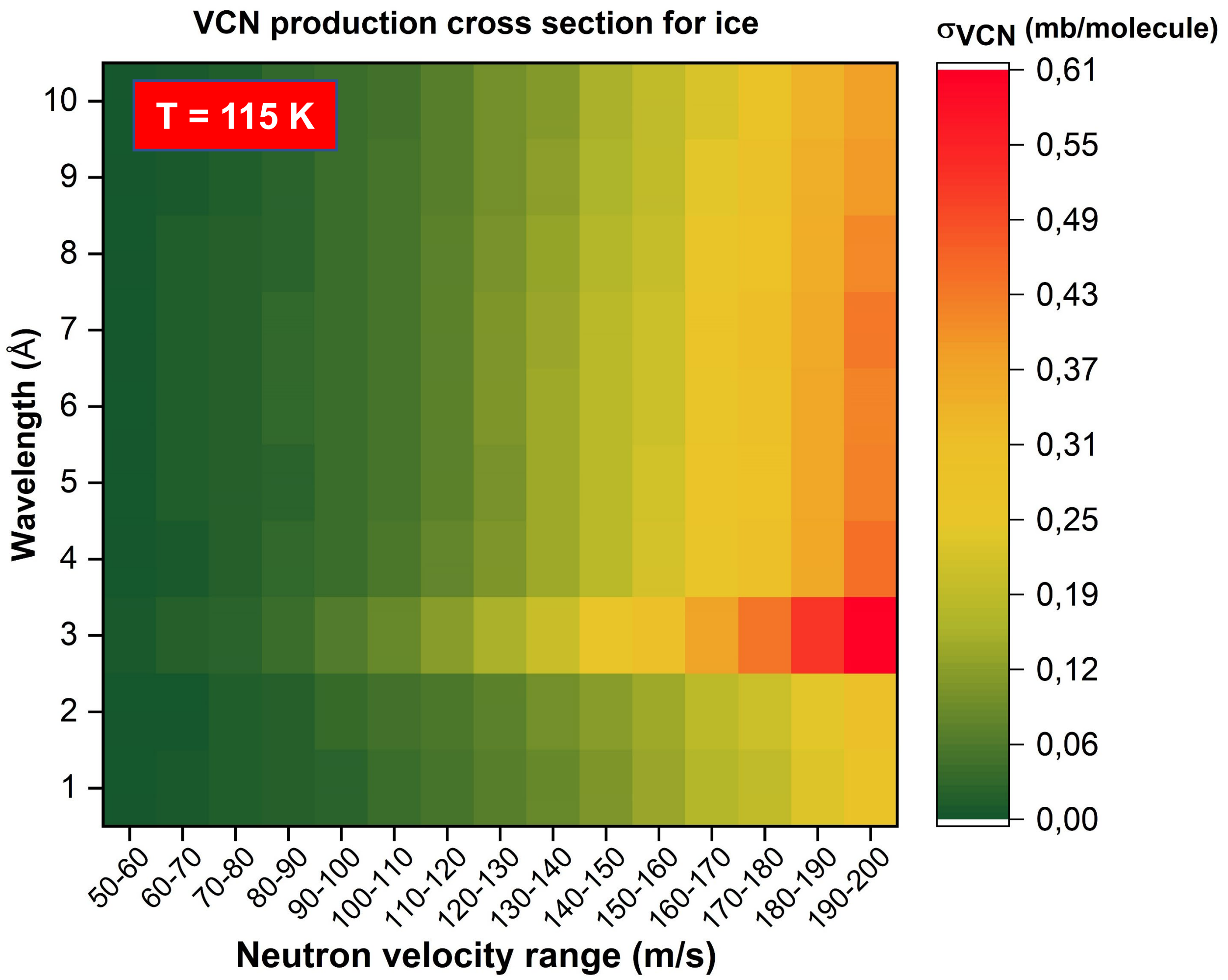
The VCN production cross section for solid deuterium and liquid deuterium

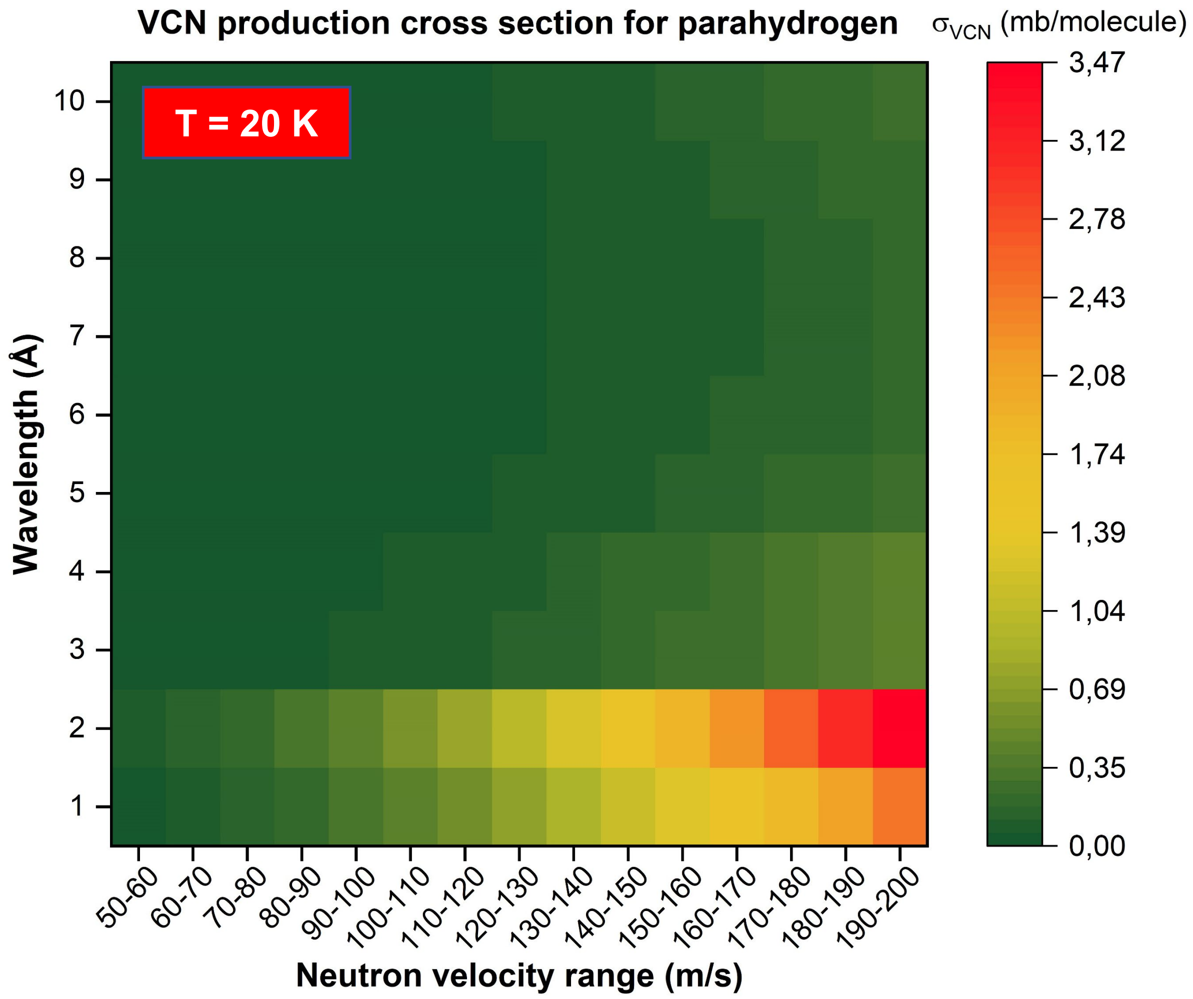




4. Simulation results (6/7)

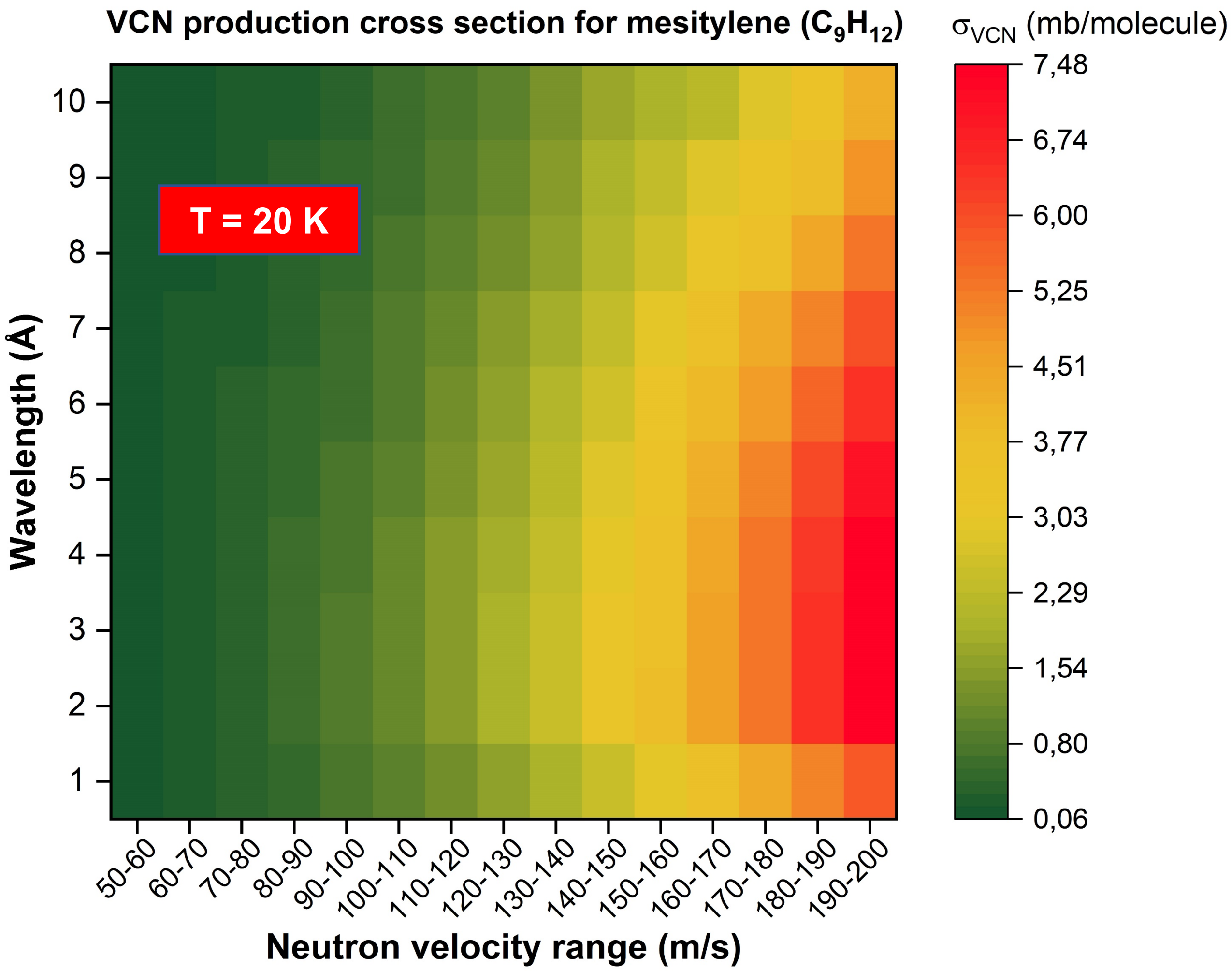
The VCN production cross section for ice and parahydrogen





4. Simulation results (7/7)

The VCN production cross section for mesitylene



5. Conclusion

- Low-energy neutrons have been an extremely productive tool for researches in condensed matter physics, fundamental physics, chemistry, novel materials and life science
- Many projects and research on the development of low-energy neutron sources are being implemented actively in the world
- The production of UCN and VCN for some material was investigated using Monte Carlo code combined with available cross section data
- The existing libraries are insufficient to provide the necessary data for simulations involving the production and transport of UCN
- The need to extend the neutron energy range in the cross section libraries to the UCN energy range for further research regarding UCN
- The investigation contributes to selecting suitable materials for the development of intense low-energy neutron sources and optimizing source design


Thank
you!