Monte Carlo simulations of a back scatter time-of-flight neutron spectrometer for the purpose of concept testing.

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Abstract

The work focuses on Monte Carlo simulations for finding the optimal back scatter time-of-flight spectrometer design for concept testing at the NESSA facility at Uppsala University. The spectrometer consists of two scintillator detectors, D1 (placed in a neutron beam) and D2 (placed in front of D1), at some distance from each other. A fraction of the neutrons that impinge on D1 back scatter into D2 and information on the neutron energy distribution is acquired using the time-of-flight method. For the given constraints on geometry, resolution and efficiency a best resolution was found to be 6.6% with a corresponding efficiency of $10^{-4}$ which gives a sufficient count rate for a neutron generator producing $10^{11}$ neutrons/s. In order to achieve a minimum of 10 000 counts/h with the same setup a D2 with an area of at least 7 cm$^2$ is required.

1 INTRODUCTION

In order to maintain a maximal fusion power in a tokamak it is important to have information on the fuel ion ratio $n_t/n_d$, where $n_t$ and $n_d$ are the core average tritium and deuterium densities. Neutron spectrometry is a useful tool for estimating the fuel ion ratio in a burning fusion plasma.\[1\] One way of acquiring information on the distribution of neutron energies is by using two detectors, D1 and D2, in a so called time-of-flight (TOF) configuration. Neutrons from the fusion reactions scatter on D1 at some angle, a fraction of these reach D2 and information on the incoming neutron energies is obtained by measuring the TOF between the two detectors.

Implementing a back scatter TOF spectrometer at ITER has been discussed in e.g.\[1, 2, 3\], and currently there are plans to test such a spectrometer concept at Uppsala University using a DT neutron generator producing 14 MeV neutrons at a rate of $10^{11}$ s$^{-1}$ in $4\pi$. The test setup has several constraints: the distance between D1 and D2 can be at most 80 cm due to geometrical limitations around the neutron generator, the full width at half maximum (FWHM) energy resolution should be below 10% and the count rate in D2 should
be such that at least a few thousand events per hour are generated. Furthermore the count rate in D1 should be < 600 kHz in order to minimise the influence of pile-up. The goal of this project is to find the optimal setup of the spectrometer within the given constraints of the test facility.

2 THEORETICAL BACKGROUND

Three neutron producing interactions in a tokamak are:

- thermonuclear DT reaction: fusion reaction of a deuteron and triton in the tokamak plasma which typically produces 14 MeV neutrons.

- thermonuclear DD reaction: fusion reaction of two deuterons in the tokamak plasma which typically produces 2.5 MeV neutrons.

- beam-target DT reaction: fusion reaction between injected neutral deuterium which is ionized in the fusion plasma and tritons which typically produces 14 MeV neutrons.

The fuel ion ratio can be estimated by measuring two of the three neutron emission rates (denoted $R_{DT}$, $R_{DD}$ and $R_{bt}$).

The idea of the time-of-flight technique is to obtain information on the energy distribution by measuring the flight time $t_{tof}$ of a particle between two points with a known distance. In this case the flight time of a neutron between two detectors, D1 and D2, is measured. The non-relativistic kinetic energy of the neutron is given by inserting $v = L/t_{tof}$ into $E = m_n v^2/2$

$$E = \frac{m_n L^2}{2t_{tof}^2}$$

(1)

where $m_n$ is the mass of the neutron and $L$ is the distance between the two detectors. In a TOF spectrometer there are two main viable configurations of D1 and D2, namely the

- forward scattering configuration

- back scattering configuration

In the forward scattering configuration D2 is placed behind (downstream of) D1. A fraction of the neutrons that scatter on D1 in the forward direction are detected by D2. Such a configuration is typically favourable for measuring the 2.5 MeV neutrons produced by the DD reaction, but not the 14 MeV neutrons.\[2\] This is due to the fact that the FWHM energy resolution (defined in equation [7]) degrades as the flight time of the neutron decreases. In
the back scattering configuration D2 is placed in front (upstream) of D1. In order to enable neutrons to back scatter it is necessary to use a deuterated D1. The scattered neutrons transfer most of their kinetic energy to the deuterons in D1 and back scatter into D2 with a kinetic energy given by \[ E_n = \frac{p_n^2}{2m_n} \] where the momentum \( p_n \) of the scattered neutron can be found as a function of the scattering angle \( \theta \) using non relativistic kinematics

\[
p_n = \frac{m_n}{m_d + m_n} \cos \theta p_0 + \sqrt{\left(\frac{m_n}{m_d + m_n}\right)^2 \cos^2 \theta p_0^2 + \frac{m_d - m_n}{m_d + m_n} p_0^2}
\]

(2)

The maximal transfer of kinetic energy to the deuteron occurs when \( \theta = 180^\circ \) and results in a scattered neutron energy of 1.55 MeV. In this report only the back scattering configuration is considered.

### 2.1 Efficiency and resolution

Two features are important to consider when setting up D1 and D2 namely the total efficiency and the FWHM energy resolution. The total efficiency is defined as

\[
\epsilon_{\text{tot}} = P[n(d,n)d] \cdot P[\text{hit D2}] \cdot P[n(p,n)p]
\]

(3)

where \( P[n(d,n)d] = n_d \sigma_{nd} \) is the probability that a neutron scatters elastically on a deuteron in D1. \( \sigma_{nd} \) is the total neutron deuteron elastic scattering cross section at a given neutron energy and \( n_d = \rho_d t_{D1} \) is given by the number density \( \rho_d \) of deuterons in D1 and the thickness \( t_{D1} \) of D1. \( P[n(p,n)p] = n_p \cdot \sigma_{np} \) is given in the same way but for neutrons scattering on protons in D2. The number densities of deuterons/protons in D1/D2 are given by the manufacturer of the scintillators and can be found in tables 3 and 4 in appendix A. \( P[\text{hit D2}] \) is the probability that a neutron scatters in the direction of D2 and is described in section 3.2.

The FWHM energy resolution \( dE/E \) is found by evaluating

\[
\frac{dE}{dv} = \frac{d}{dv} \left( \frac{mv^2}{2} \right) = mv
\]

(4)

giving us

\[
\frac{dE}{E} = \frac{mv}{mv^2/2} \frac{dv}{v} = \frac{2}{v}
\]

(5)

Using the propagation of uncertainties together with \( v = s/t \) where \( s \) is the flight path length.
of the neutron and $t$ is the flight time we find

$$2 \frac{dv}{v} = 2 \sqrt{\left(\frac{\partial v}{\partial t}\right) dt^2 + \left(\frac{\partial v}{\partial s}\right) ds^2} = 2 \sqrt{\frac{dt^2}{t^2} + \frac{ds^2}{s^2}} \approx 2 \frac{ds}{s} \quad (6)$$

The last step in equation (6) is justifiable in our case because the uncertainty in the time measurement $dt$ due to experimental limitations is on the order of a few 100 ps whereas the flight time $t$ is on the order of 20-50 ns. The resolution will thus be dominated by the uncertainty in the flight path $ds$ which stems from the fact that there is no way of determining the exact depth and radial position of the detected neutron in D1 and D2. This uncertainty is proportional to the uncertainty in the time-of-flight. We can thus find the FWHM energy resolution from

$$\frac{dE}{E} = 2 \frac{dt_{tof}}{<t_{tof}>} \quad (7)$$

where $dt_{tof}$ is the FWHM of the neutron TOF spectrum which is found by multiplying the standard deviation of the flight times by a factor $2\sqrt{2\ln2} \approx 2.35$, and $<t_{tof}>$ is the mean value of the flight times. Parameters that affect the resolution and efficiency of the spectrometer are displayed in table 1. Increasing the thickness of D1 and D2 and the area of D2 improves the total efficiency but degrades the resolution since the TOF distribution of the neutrons becomes more spread out which results in an increase in $dt_{tof}$. Similarly, decreasing the distance between the two detectors increases the efficiency and decreases the mean flight time $<t_{tof}>$ as well as $dt_{tof}$. However, $<t_{tof}>$ decreases at a faster rate than $dt_{tof}$ which results in a degraded resolution.

**Table 1:** Parameters of the spectrometer with the values or ranges which were simulated.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>value/range [cm]</th>
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</thead>
<tbody>
<tr>
<td>Radius of D1</td>
<td>$r_{D1}$</td>
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</tr>
<tr>
<td>Thickness of D1</td>
<td>$t_{D1}$</td>
<td>4.5</td>
</tr>
<tr>
<td>Inner radius of D2</td>
<td>$r_{D2, in}$</td>
<td>4.3</td>
</tr>
<tr>
<td>Outer radius of D2</td>
<td>$r_{D2, out}$</td>
<td>[24.3, 44.3]</td>
</tr>
<tr>
<td>Thickness of D2</td>
<td>$t_{D2}$</td>
<td>[0.5, 5]</td>
</tr>
<tr>
<td>Distance between D1 and D2</td>
<td>$L$</td>
<td>[40, 80]</td>
</tr>
</tbody>
</table>
2.2 Kinematics and counting rate

The probability to scatter into some solid angle is given by

\[ P_\theta = n_d \sigma_\theta \]  \hspace{1cm} (8)

where \( \sigma_\theta \) is obtained by integrating the differential cross section \( d\sigma/d\Omega \) over some angle

\[ \sigma_\theta = \frac{2\pi}{\theta_2 - \theta_1} \int_{\theta_1}^{\theta_2} \int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin(\theta) \sin(\phi) d\phi \]  \hspace{1cm} (9)

Evaluating this for a certain number of angle intervals one finds the scattering probability distribution shown in figure 1.

**Figure 1:** Probability distribution of the scattering angle of 14 MeV monoenergetic neutrons on deuterons. The figure shows the probability to scatter into a bin of width \( \pi/100 \) where the points corresponds to the bin center.
Once the scattering angle is chosen the energy of the scattered neutron can be determined. A 14 MeV neutron has

$$\frac{v}{c} = \sqrt{\frac{(E_k + m_n)^2 - m_n^2}{(E_k + m_n)^2}} \approx 0.17$$

(10)

where $v$ is the velocity of the neutron, $c$ is the speed of light in vacuum, $E_k = 14$ MeV is the kinetic energy of the neutron and $m_n$ is the neutron mass. This gives

$$\gamma = \frac{1}{\sqrt{1 - \left(\frac{v}{c}\right)^2}} \approx 1.015$$

(11)

giving an error less than 2% so it is sufficient to use non relativistic kinematics to determine the energy of the scattered neutron.

3 SETUP OF SIMULATION

In this section the setup of the simulation is described. In section 3.1 the geometry of the setup is discussed and in section 3.2 the simulation algorithm is described.

3.1 Geometry

The geometry of the experimental area can be seen in figure 2. A DT neutron generator producing 14 MeV neutrons at a rate of $10^{11}$ s$^{-1}$ is placed with it's center 20 cm from a shielding wall which is 60 cm thick. To simplify simulations the neutron source is point like and produces monoenergetic neutrons. There is a circular hole in the wall which collimates the neutron beam with a radius equal to the radius of D1. The spectrometer is placed on the other side of the shielding wall with D2 placed against the wall.

An example of the geometry of the simulated spectrometer can be seen in figure 3. D1 is a cylinder shaped deuterated liquid scintillator with a radius $r_{D1} = 2.3$ cm and thickness $t_{D1} = 4.5$ cm. The D1 dimensions are chosen such that the radius encompasses the neutron beam and the count rate in D1 is not larger than 600 kHz (as is calculated in section 5) in order to minimise the influence of pile-up. D2 is an annulus shaped plastic scintillator with an inner radius $r_{D2, in} = 4.3$ cm. The outer radius of D2, thickness of D2 and distance between the detectors are varied between $r_{D2, out} = [24.3, 44.3]$ cm, $t_{D2} = [0.5, 5]$ cm and $L = [40, 80]$ cm. The specifications of the two scintillators can be found in the appendix and the geometrical parameters of the setup are displayed in table 1.
Figure 2: Geometry of the experimental hall. A DT neutron generator (denoted by an x) is placed with its center 20 cm from a 60 cm shielding wall (hatched rectangle) with a collimating hole of radius 2.3 cm. D2 with an inner radius of 4.3 cm is placed on the other side of the wall. D1 with a radius of 2.3 cm and a thickness 4.5 cm is placed at some distance from D2. The figure is not according to scale.

Figure 3: Geometry of the simulated spectrometer. D1 (orange ring) is a deuterated scintillator detector, D2 (green annulus) is a fast plastic scintillator detector. 20 back scatter events are displayed (red lines). The figure is not according to scale.
3.2 Simulation algorithm

A cartesian coordinate system is defined with the z-axis pointing from the center of D1 towards D2. Neutrons incident perpendicularly on the front of D1 generate scattering events uniformly distributed in the volume of D1. The scattering angle $\varphi_{nd}$, defined as the angle between the neutron beam and the scattered neutron (the polar angle is thus $\phi = \pi - \varphi_{nd}$), is chosen corresponding to the 14 MeV differential scattering cross section on deuterons as explained in section 2.2. The differential cross sections were taken from the JEFF-3.2 library. In order to speed up the code only the useful part of the probability distribution is sampled. Only angles within an interval $[\theta_{\min}, \theta_{\max}]$ large enough to cover all connecting points between D1 and D2, are considered. When the angle bin has been chosen, the final scattering angle is randomly selected within the bin. The azimuthal angle is chosen uniformly between $[0, 2\pi]$. A depth in D2 is randomly selected from a uniform distribution. If the point where the neutron ends up is within the radius of D2 it is registered as a hit and the neutron TOF is recorded.

D2 is divided into segments, each with a width of 5 cm with the number of segments depending on the outer radius. The total efficiency of the setup is found by summing up the efficiency for each segment using equation 3. Since only a part of the scattering probability is used an efficiency factor $\kappa$ must be introduced to determine the probability to hit D2 according to

$$P\text{[hit D2]} = \kappa \sum_i P_i \text{[hit D2]}$$

where $P_i \text{[hit D2]}$ is the ratio of the number of particles that hit segment $i$ and the total number of particles that reach D2 and $\kappa$ is the probability to scatter into the angles limited by $\theta_{\min}$ and $\theta_{\max}$.

The FWHM energy resolution is determined by centering each segments TOF distribution around zero (see figure 4), summing them up and dividing the FWHM by the mean flight time according to equation 7. The FWHM is determined as explained in section 2.1.

The algorithm described above is repeated for many different spectrometer setups where each setup has a different $L$, $r_{D2,\text{out}}$ or $t_{D2}$ as explained in section 3.1. The energy resolution and efficiency for each spectrometer setup is saved and run through a code which performs a multiobjective optimisation (commonly known as Pareto optimisation). The Pareto optimisation code divides the resolution into a number of intervals and finds the maximal efficiency for each interval. For each maximal efficiency the parameters of the spectrometer
is determined as seen in figure 6.

4 RESULTS

6300 different spectrometer designs with different parameters were simulated, for each setup 20 000 events were generated. The efficiency and resolution for each setup can be seen in figure 5.

Figure 4: Example of TOF distributions of four segments in D2 centered around zero (left panel) and the sum of all distributions (right panel).

Figure 5: Total efficiency and FWHM energy resolution of 6300 different spectrometer setups. Each dot represents a spectrometer setup with a certain \( t_{D2}, L \) and \( r_{D2, \text{out}} \). The Pareto front marked with a red line corresponds to the spectrometer setups with the highest efficiency for a given resolution.
The points with highest efficiency for a number of different resolutions are shown as numerated squares in panel A in figure 6. The numerated squares and the blue circle in B and C can be used to find the resolution and efficiency for the given setup. The three panels in figure 6 are interrelated, this becomes simple to see if one imagines a three dimensional matrix with the thickness, distance and radius on the different axes with a resolution and efficiency coupled to each element in the matrix. Panel A is then showing the resolution and efficiency of each element, panel B and C are showing the distance axis plotted against the axis with thickness and radius respectively. The blue circle shows the best resolution achieved, $\frac{dE}{E} = 6.6\%$ with an efficiency of $\epsilon_{\text{tot}} = 1.0 \cdot 10^{-4}$. This corresponds to a setup where the distance between the detectors is $L = 80$ cm, the thickness of $D_2$ is $t_{D_2} = 0.5$ cm and the outer radius of $D_2$ is $r_{D_2, \text{out}} = 34.3$ cm. The first three points and the minimal resolution in figure 6 are summarized in table 2.

**Figure 6:** The left panel A shows the efficiency and FWHM resolution for each spectrometer. The numerated squares correspond to the highest efficiency for a certain resolution. The blue circle corresponds to the smallest resolution. The shaded area contains the points for which the resolution is below 10%. The middle panel B displays the distances between $D_1$ and $D_2$ and thickness of $D_2$ of the different spectrometer designs. The right panel C shows the same distances as in B but with the outer radii of $D_2$. 

Figure 6: The left panel A shows the efficiency and FWHM resolution for each spectrometer. The numerated squares correspond to the highest efficiency for a certain resolution. The blue circle corresponds to the smallest resolution. The shaded area contains the points for which the resolution is below 10%. The middle panel B displays the distances between $D_1$ and $D_2$ and thickness of $D_2$ of the different spectrometer designs. The right panel C shows the same distances as in B but with the outer radii of $D_2$. 

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Table 2: Summary of the minimal resolution and first three enumerated points in figure 6

<table>
<thead>
<tr>
<th>Resolution Efficiency ($10^{-4}$)</th>
<th>L [cm]</th>
<th>r_{D2, out} [cm]</th>
<th>t_{D2} [cm]</th>
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</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>6.6%</td>
<td>1.0</td>
<td>80.0</td>
</tr>
<tr>
<td>Point 1</td>
<td>7.0%</td>
<td>3.1</td>
<td>80.0</td>
</tr>
<tr>
<td>Point 2</td>
<td>8.5%</td>
<td>7.0</td>
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<tr>
<td>Point 3</td>
<td>10.4%</td>
<td>10.3</td>
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5 Discussion & Conclusions

Monte Carlo simulations of back TOF neutron spectrometer setups have been performed given a set of geometrical constraints and requirements of count rates, FWHM energy resolution and efficiency. By varying parameters of the setup, including the distance between D1 and D2 and the outer radius and thickness of D2, the efficiency was maximised for a given resolution. As expected the best resolution is found at large distances. The resolution degrades while the efficiency improves as distance decreases and thickness increases which is apparent in the left and center panels of figure 6. Large D2 radii are as expected favoured for a maximal efficiency. Regarding the efficiency requirement of producing at least 10 000 counts per hour in D2 a quick calculation shows that this will most likely not be an issue. Given a neutron source with an intensity of $S = 10^{11} \text{s}^{-1}$ and a setup corresponding to the minimal resolution, a neutron intensity at D1 is given by

$$I = A_{D1} \frac{S}{4 \pi D^2} = 5.1 \times 10^6 \text{ neutrons/s}$$

(13)

where $D = 160.5 \text{ cm}$ is the distance from the center of the neutron source to the center of D1 and $A_{D1} = \pi r_{D1}^2 = 16.6 \text{ cm}^2$ is the area of D1. This gives a count rate in D1 of 595 kHz. With a total efficiency of $1.0 \cdot 10^{-4}$ the count rate at D2 is around 500 Hz. However, given edge effects and secondary scattering the total efficiency is likely to be smaller than the stated. The smallest required total efficiency of the same setup for a count rate of 10 000 counts/h (10 000/3600 Hz) can be found by

$$\epsilon_{\text{req}} = \frac{10000/3600}{I} = 5.4 \cdot 10^{-7}$$

(14)

which gives the possibility to further degrade the efficiency and size of D2 in favour of resolution. By scaling down the radius of D2 in the example above (5 mm thick D2 at 80 cm distance from D1) to achieve a count rate of 10 000 counts/h one finds that the area of D2 needs to be at least 7 cm$^2$. The points numerated 1-6 in figure 6 suggests that the best
way to increase resolution is to increase the distance between the detectors and decrease the thickness of D2. We have however already hit our geometrical constraints concerning the distance and thickness. Varying the radius does not have a very large impact on the resolution. The explanation for this has to do with the segmentation of D2 and the way the FWHM is determined. As can be seen in the left panel of figure[4] each segment of D2 has a TOF distribution with a total width of around 4 ns no matter how far out the segment is from the center. This means that increasing the radius of D2 does not necessarily broaden the spectrum seen in the figure. However, the average flight time increases slightly which would imply a small decrease in $dE/E$.

The thickness of D1 has an impact on both the resolution and efficiency of the spectrometer. Increasing the thickness improves the efficiency to a certain degree but also increases the probability of secondary scattering events to occur which has a negative impact on the resolution. As part of a future work it could be relevant to vary the thickness of D1 as well as other parameters.

The spectrometer design fulfills the resolution requirements of $< 10\%$. The best resolution was found to be 6.6% with a corresponding efficiency of $10^{-4}$. The efficiency of the spectrometer design is sufficient to perform a test at the NESSA facility within a reasonable amount of time.

REFERENCES


A Scintillator properties

The specifications of the scintillator detectors used for the simulations are shown in figure 3 and 4.


<table>
<thead>
<tr>
<th>PROPERTIES</th>
<th>EJ-315</th>
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<tbody>
<tr>
<td>Light Output (% Anthracene)</td>
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<tr>
<td>Scintillation Efficiency (photons/1 MeV e-)</td>
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<td>Refractive Index</td>
<td>1.498</td>
</tr>
<tr>
<td>Flash Point (°C)</td>
<td>-11</td>
</tr>
<tr>
<td>Boiling Point (°C at 1 atm)</td>
<td>79</td>
</tr>
<tr>
<td>D Atoms per cm³ (×10^{22})</td>
<td>4.06</td>
</tr>
<tr>
<td>H Atoms per cm³ (×10^{22})</td>
<td>0.0287</td>
</tr>
<tr>
<td>C Atoms per cm³ (×10^{22})</td>
<td>4.10</td>
</tr>
<tr>
<td>Electrons per cm³ (×10^{25})</td>
<td>2.87</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Properties</th>
<th>EJ-228</th>
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<tbody>
<tr>
<td>Light Output (% Anthracene)</td>
<td>67</td>
</tr>
<tr>
<td>Scintillation Efficiency (photons/1 MeV e⁻)</td>
<td>10,200</td>
</tr>
<tr>
<td>Wavelength of Maximum Emission (nm)</td>
<td>391</td>
</tr>
<tr>
<td>Light Attenuation Length (cm)</td>
<td>-</td>
</tr>
<tr>
<td>Rise Time (ns)</td>
<td>0.5</td>
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<tr>
<td>Decay Time (ns)</td>
<td>1.4</td>
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<tr>
<td>Pulse Width, FWHM (ns)</td>
<td>1.2</td>
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<tr>
<td>H Atoms per cm³ (×10²²)</td>
<td>5.15</td>
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<tr>
<td>C Atoms per cm³ (×10²²)</td>
<td>4.69</td>
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<tr>
<td>Electrons per cm³ (×10²²)</td>
<td>3.33</td>
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<tr>
<td>Density (g/cm³)</td>
<td>1.023</td>
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<table>
<thead>
<tr>
<th>Polymer Base</th>
<th>Polyvinyltoluene</th>
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<tbody>
<tr>
<td>Refractive Index</td>
<td>1.58</td>
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<tr>
<td>Softening Point</td>
<td>75°C</td>
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<tr>
<td>Vapor Pressure</td>
<td>Vacuum-compatible</td>
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<tr>
<td>Coefficient of Linear Expansion</td>
<td>7.8 × 10⁻⁵ below 67°C</td>
</tr>
<tr>
<td>Temperature Range</td>
<td>-20°C to 60°C</td>
</tr>
<tr>
<td>Light Output (L.O.) vs. Temperature</td>
<td>At 60°C, L.O. = 95% of that at 20°C No change from -60°C to 20°C</td>
</tr>
</tbody>
</table>