Neutron Moderation
From Quanta to Continuum

Iyad Al-Qasir
Nuclear Data Group

NCSP-TPR meeting
Brookhaven National Laboratory
February 20-22, 2024
Neutron Moderation

- Low Atomic Mass Number
- High scattering cross section
- Low absorption cross section
- High Thermal Conductivity
- High Strength
- Good stability under irradiation
- High oxidation Resistivity

Neutronic

Thermal

Mechanical

Radiation Eff.

Chemical
Neutron Moderation

- Low Atomic Mass Number
- High scattering cross section
- Low absorption cross section

![Graph showing cross sections and collisions for various elements.](image)

![Graph showing number of collisions for different moderators.](image)
Neutron Moderation

- Historically, core moderator and reflector materials consist of relatively simple compounds of a simple material type or simple composition (e.g., H$_2$O, D$_2$O, Be, BeO, Graphite, ZrH$_2$).

- Recently, compact thermal fission reactors are of increased interest due to their potential to lower construction cost, enhance safety, and portability to remote areas.

- They are also considered as a point-source for process industrial heat.

- The compact nature of these cores requires good neutron economy as well as preserving other thermal, mechanical, chemical properties, etc. How do we achieve this?
Multiscale Modeling

- Hierarchical Understanding
- Predictive Capabilities
- Accelerated Development

Quantum Mech.

Microscopic Modeling

Molecular Dynamics

Mesoscale Modeling

Macroscale Modeling

Engineering Design

Macro

Meso

MD

QM

Forcefields, ...
(semi-empirical or 
ab initio)

Atomic, molecular 
structure, ...

DFT, HF, MP2, ...
Electrons, bonds, 
transition states,

Reactions, stabilities, macroscopic 
processes and properties, ...

\[ F = ma \]

\[ F = \dot{H}\Psi = E\Psi \]
Moderators Doping

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Ab (%)</th>
<th>Scatt. XS</th>
<th>Abs. XS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^9$Be</td>
<td>100</td>
<td>7.63</td>
<td>0.0076</td>
</tr>
<tr>
<td>$^{11}$B</td>
<td>80</td>
<td>5.77</td>
<td>0.0055</td>
</tr>
<tr>
<td>$^{15}$N</td>
<td>0.37</td>
<td>5.21</td>
<td>0.000024</td>
</tr>
<tr>
<td>$^{88}$Sr</td>
<td>82.58</td>
<td>6.42</td>
<td>0.058</td>
</tr>
<tr>
<td>Zr</td>
<td>17.28</td>
<td>8.4</td>
<td>0.185</td>
</tr>
</tbody>
</table>

- Low Atomic Mass Number
- High scattering cross section
- Low absorption cross section
Engineering Design/ Two Phase Composite Moderators

- Composite materials are formed by combining two or more materials that have quite different properties, and they do not dissolve or blend into each other.

- The ultimate goal, is to arrive at a bulk material that is structurally and neutronically superior to traditional moderators (graphite, Be, BeO, etc.).

- Could be tailored to properties of interest such as thermal conductivity, strength, or fracture toughness.

Example: Two Phase Composite Moderator

<table>
<thead>
<tr>
<th>Entrained Phase</th>
<th>Matrix Phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scattering</td>
<td>High</td>
</tr>
<tr>
<td>Absorption</td>
<td>Low</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>Fair</td>
</tr>
<tr>
<td>Radiation resistivity</td>
<td>Fair</td>
</tr>
<tr>
<td>Mechanical Stability</td>
<td>Fair</td>
</tr>
<tr>
<td>Examples</td>
<td>Graphite, Be, Be$<em>4^{11}$B, BeO, Be$<em>2$C, YH$</em>{2-x}$, ZrH$</em>{2-x}$</td>
</tr>
</tbody>
</table>

**Be$_2$C**: reacts with moisture to form Be(OH)$_2$. However, as an entrained phase it will not

**YH$_{2-x}$, ZrH$_{2-x}$**: High dense matrix forms barriers that prevents hydrogen leakage

Thank you