Chemical Engineering 412

Introductory Nuclear Engineering

Lecture 3
Atomic & Nuclear Models
Nuclear Energetics
“I wanted to tell you that oft-repeated story because there are many of you who are going to have some very difficult experiences: disappointment, heartbreak, bereavement, defeat. You are going to be tested and tried to prove what you are made of. I just want you to know that if you don’t get what you think you ought to get, remember, “God is the gardener here. He knows what he wants you to be.” Submit yourselves to his will. Be worthy of his blessings, and you will get his blessings.”

Elder Hugh B. Brown
Objectives

• Understand characteristics of nucleus energy states (quantized)
• Know how to approximate nuclear mass using atomic models
• Understand binding energy and mass defect and their implications
• Know how to identify, characterize, and create nuclear interaction equations
• Know how to assess energetics of nuclear interactions
# History of Atomic Theory

<table>
<thead>
<tr>
<th>Date</th>
<th>Discoverer</th>
<th>Essential Contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1896</td>
<td>Becquerel</td>
<td>Radiation emitted from uranium</td>
</tr>
<tr>
<td>1896-1898</td>
<td>Thomson</td>
<td>Electron and the plum pudding model</td>
</tr>
<tr>
<td>1911</td>
<td>Rutherford</td>
<td>Small nucleus contains all charge with electrons orbiting around it</td>
</tr>
<tr>
<td>1913-1915</td>
<td>Bohr</td>
<td>Electron orbits are discrete</td>
</tr>
<tr>
<td>1916+</td>
<td>Sommerfeld</td>
<td>Fine structure occurs from additional discrete numbers with selection rules (attributed to elliptical orbits)</td>
</tr>
<tr>
<td>1925</td>
<td>Schrödinger</td>
<td>Quantum mechanics model of atom – described all details of hydrogen atom and electron energy levels previously empirically deduced</td>
</tr>
<tr>
<td>1932</td>
<td>Chadwick</td>
<td>Neutron discovered</td>
</tr>
</tbody>
</table>
Excited energy states - Electrons

• Bound atomic electrons
  – specific energy levels
  – quantum numbers

• Transitions between energy levels requires:
  – absorption or emission
  – specific wavelengths/energies
  – light (or heat or other energy forms).
Nuclei Also Have Energy Levels

Note the scale change

Atomic Energy Levels (H)  Nuclear Energy Levels (^{12}\text{C})
Nuclear Energy Levels

• Analogous to atomic energy levels
  – Discrete orbital configurations
  – Ground states
  – Excited states (except for smallest nuclei).

• Residual strong force
  – Far stronger
  – Much shorter range (a few nucleons)
  – Higher energy levels
  – Energy changes produce Gamma rays (γ-ray)
Nuclear Energy Levels (cont)

• Energy exchanged
  – innermost electrons (internal conversion)
  – ejection from the atom
  – collapse of an outer electron to the inner orbital with x-ray emission.

• Outer to an inner electronic state:
  – Highly energetic (hence the high-energy x-rays)
  – absorbed by a 2nd electron
  – 2nd electron is ejected – Auger Electron
Liquid Drop Model

- Nucleus is like a liquid drop.
  - Adding more mass (nucleons) does not change the density, just the size.
  - Surface tension and mass compete for droplet stability. In a nucleus, short-range nuclear attractive forces compete with longer range coulombic repulsive forces.
  - Total mass then is
    \[ M = N M_n + Z M_p - \alpha A \]
  - Surface nucleons are not as tightly bound (fewer neighbors)
    \[ M = N M_n + Z M_p - \alpha A + \beta A^{2/3} \]
Liquid Drop Model (contd)

- Coulombic repulsion decreases force, increases mass

\[ M = N M_n + Z M_p - \alpha A + \beta A^{2/3} + \gamma Z^2 / A^{1/3} \]

- Different numbers of neutrons and protons increase mass

\[ M = N M_n + Z M_p - \alpha A + \beta A^{2/3} + \gamma Z^2 / A^{1/3} + \zeta (A - 2Z)^2 / A \]

- Protons and neutrons separately prefer pairs

\[ M = N M_n + Z M_p - \alpha A + \beta A^{2/3} + \gamma Z^2 / A^{1/3} + \zeta (A - 2Z)^2 / A + \delta / \sqrt{A} \]
Nuclear Mass Equation

\[ m = Zm_p + (A - Z)m_n - \frac{E_B}{c^2} \]

\[ E_B = a_v A - a_s A^2 + a_c A^2 - a_a \frac{(A - 2Z)^2}{A} + \frac{a_p [(-1)^Z + (-1)^N]}{2\sqrt{A}} \]

(All units MeV)

<table>
<thead>
<tr>
<th></th>
<th>Lamarch</th>
<th>Least-squares</th>
<th>Wapstra</th>
<th>Rohlf</th>
<th>Text (Shultis)</th>
<th>Bertsch et al.</th>
</tr>
</thead>
<tbody>
<tr>
<td>(M_n)</td>
<td>939.565</td>
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</tr>
<tr>
<td>(M_p)</td>
<td>938.272</td>
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<td>938.272</td>
</tr>
<tr>
<td>(a_v)</td>
<td>15.56</td>
<td>15.80</td>
<td>14.1</td>
<td>15.75</td>
<td>15.835</td>
<td>15.74063</td>
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<tr>
<td>(a_s)</td>
<td>17.23</td>
<td>18.30</td>
<td>13</td>
<td>17.8</td>
<td>18.33</td>
<td>17.61628</td>
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<tr>
<td>(a_c)</td>
<td>0.697</td>
<td>0.714</td>
<td>0.595</td>
<td>0.711</td>
<td>0.714</td>
<td>0.71544</td>
</tr>
<tr>
<td>(a_a)</td>
<td>23.285</td>
<td>23.20</td>
<td>19</td>
<td>23.7</td>
<td>23.20</td>
<td>23.42742</td>
</tr>
<tr>
<td>(a_p)</td>
<td>12</td>
<td>12</td>
<td>33.5</td>
<td>11.18</td>
<td>11.2</td>
<td>12.59898</td>
</tr>
</tbody>
</table>

These semi-empirical models work best for large \(A\).
An Example

Estimate the atomic mass of $^{40}$Ca based on the liquid drop model.

<table>
<thead>
<tr>
<th>Term</th>
<th>Magnitude (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>volume</td>
<td>633.4</td>
</tr>
<tr>
<td>surface</td>
<td>214.389</td>
</tr>
<tr>
<td>Coulombic</td>
<td>83.51</td>
</tr>
<tr>
<td>n-p asymmetry</td>
<td>0</td>
</tr>
<tr>
<td>pairing</td>
<td>-1.77088</td>
</tr>
</tbody>
</table>

Binding energy = $633.4-214.389-83.51-0-(-1.77088)=337.27$

$\text{BE/A} = \frac{337.27}{40}=8.431$

Observed $\text{BE/A} = \frac{342.04}{40}=8.551$

Estimated Atomic Mass = $\frac{(20\times939.565+20\times938.272+20\times0.510999-337.27)}{931.5} \text{ MeV/u} = 39.956 \text{ u}$

$\frac{(20\times939.565+20\times938.789-337.27)}{931.5} \text{ MeV/u} = 39.96759 \text{ u}$

Observed Atomic Mass = 39.9674 u

Atomic Mass based on sum of parts = 40.329 u
Accuracy of Liquid Drop Model

\[ \frac{BE - LDM}{A} \]

Shell Model (Quantum Model)

• Assume each nucleon acts independently of all others.
• All nucleons move in a potential well that is flat inside the nucleus but increases sharply at the edge.
• Much math leads to theoretical prediction of “magic” numbers of nucleons consistent with observations. These are: 2, 8, 20, 28, 50, 82, 126
• Some lists include 14 and sometimes 6 as magic.
• These are analogous to the closed shells of electron orbitals that give rise to noble gases and apply to the neutrons and protons separately. That is, nuclei with a magic number protons or a magic number of neutrons are especially stable, and those with magic numbers of both are doubly magic and exceptionally stable.
Nuclear Stability

- Proton excess leads to decay (coulombic repulsion)
- Neutron excess leads to decay (too large – nuclear force is short-range)
- Odd numbers of either neutrons or protons leads to decay (nucleons like to be paired, especially with like nucleons)
- Certain numbers of nucleons are exceptionally stable
- Neutrons easier to accommodate than protons (coulombic repulsion)

<table>
<thead>
<tr>
<th>Neutrons</th>
<th>Protons</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Even</td>
</tr>
<tr>
<td>Even</td>
<td>159</td>
</tr>
<tr>
<td>Odd</td>
<td>53</td>
</tr>
</tbody>
</table>

266 (255) total stable nuclides
$^4$He is locally stable

max stability is A 60-80 ($^{56}$Fe single most stable)

chart represents binding energy per nucleon

(large nuclei have large total binding energy)
Binding Energy per Nucleon
Mass Excess in MeV
Example

• Calculate the binding energy of an electron in a Hydrogen atom.
Chart of the Nuclides

- Stable
- $\beta^+$
- $\beta^-$
- $\alpha$
- P
- N
- SF
- Unknown
Modern Nucleus Concepts

- Much smaller relative to electron shells than typically depicted (picture at left misleading).
- Includes protons and neutrons, but not as discrete particles. Pairs of protons and neutrons typically share the same physical location (as waves) but have different quantum numbers (spin number differs).
- Slight density variation with increasing distance from center.
- Not necessarily spherical.
- Measurable charge separation in many cases.

[Diagram of a carbon atom with 6 protons, 6 neutrons, and electrons]
A few interesting nucleii

- Halo nuclides – have one or several nucleons orbiting the remaining nucleus. These include
  - 1-neutron – $^{11}$Be & $^{19}$C
  - 2-neutron – $^6$He, $^{11}$Li, $^{17}$B, $^{19}$B and $^{22}$C
  - 4-neutron – $^8$He and $^{14}$Be
  - 1-proton – $^8$B and $^{26}$P
  - 2-proton – $^{17}$Ne and $^{27}$S

- Aspherical nuclides – most heavy nuclides are aspherical, some significantly so.
Nuclear Energetics

- Study of mass/energy changes in nucleus
  - Reactions
    - Binary (2) or ternary (rare) reactions
    - Decays (1 nucleus)
  - Stability
  - Mass Defect
  - Binding Energy/Separation Energy

- Foundational to understanding radioactive decay
Reaction Terminology

• Chemistry
  – Exothermic reactions
    • Generate heat
    • Negative heat of reaction
  – Endothermic reactions
    • Consume heat
    • Positive heat of reaction

• Nuclear chemistry
  – Exothermic = Exoergic
    • Positive Q-values
  – Endothermic = Endoergic
    • negative Q-values

Not “thermal”, because it’s not traditional heat transfer; atomic scale with wave emission and kinetic energy
Mass Defect/Binding Energy

- \( E=mc^2 \) \( \Rightarrow \) \( \Delta E = \Delta mc^2 \)
  - Even for Macroscopic effects, but tiny
    - 10^{-8} \% for formation of \( \text{CO}_2 \) molecule

\( \Delta m = \text{mass defect} \)
  - \( m = \text{nuclear}, \ M = \text{atomic} \) \( \Rightarrow \) How to define \( M? \)
  - \( M(A\text{Z}X) = m(A\text{Z}X) + Zm_e - \frac{BEze}{c^2} \Rightarrow \) How to define \( m? \)
    - \( \Delta m = \frac{BE}{c^2} = Zm_p + (A-Z)m_n - m(A\text{Z}X) \)

- **Binding Energy**
  - \( BE(A\text{Z}X) = [ZM(\frac{1}{1}H) + (A-Z)m_n - M(A\text{Z}X)]c^2 \)

- **Separation Energy**
  - \( Sn(A\text{Z}X) = BE(A\text{Z}X) - BE(A-\frac{1}{2}\text{Z}X) \)
Nuclear Fusion vs. Nuclear Fission

• Nuclear Fusion:
  – \((^2_1H) + (^2_1H) \rightarrow (^4_2He)\)
  – Energy released?
    • 23.85 MeV

• Nuclear Fission
  – \((^{235}_{92}U) \rightarrow (^{117}_{46}Pd) + (^{117}_{50}Sn) + n\)
  – Energy released?
    • ~210 MeV

• Why Fusion?
Reactions

• Nuclear reactions
  – 1, 2, or 3 (rare) particles
  – Sometimes written like Chemical reactions:
    \[ \frac{4}{2}He + \frac{14}{7}N \rightarrow \frac{17}{8}O + \frac{1}{1}H \]

• For single reactions this is common
• For binary nuclear reactions a more compact nomenclature is typical,
  \[ \frac{14}{7}N (\alpha, p) \frac{17}{8}O \]

Lightest nuclides in parentheses

Note: this is the first nuclear reaction detected, by Rutherford
Nuclear Conservation

- Chemical reactions
  - conserve enthalpy, elements, and total mass.

- Nuclear reactions
  - Don’t conserve any of these
  - Do conserve
    - Total energy (mass + kinetic/radiative energy)
    - Nucleons (protons + neutrons)
    - Electrical charge.
  
  - Note *sum* of protons and neutrons (nucleons) is conserved.

- Electrons **NOT** conserved; charge is.