Development of calculation tools: Calculation of cross sections for Mn and Cu up to 60 MeV

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Fast-neutron activation cross sections for $^{55}$Mn and $^{63,65}$Cu stable isotopes @ $E_n<60$ MeV
- Global Approach: TALYS-0.64, EMPIRE-2.19
- Local Approach: STAPRE-H

D5: Optical model potential analysis of Deuteron interaction with Fe
D6: Deuteron-induced activation for accelerator materials (Al, Cu, Nb)

Marilena Avrigeanu, Faustin L. Roman, Aura Obreja, Vlad Avrigeanu

Deuteron microscopic double-folding (DF) & phenomenological potentials in analysis of:
- $(d,d)$ angular distributions (DF, SCAT2)
- d total-reaction cross sections @ $E_d<50$ MeV
- activation cross sections (TALYS-0.64, EMPIRE-2.19)
Outline
[ overview presentation at EURATOM-MEdC Association Seminar, 12 March 2007 ]

- Relation to ‘EU Fusion Research Base Survey’,
  [K. Thomsen, 23 Feb 2007, CSA Info Workshop]
  - ‘Neutronics’ – Nuclear Data (ND) bases (p. 7)
  - ‘Nuclear data base status’ (p. 18)

- ND consistent model calculations
- Fast-neutron reaction model analysis  [ TW6  / TTMN-001/ D6 ]
- Deuteron reaction model analysis  [ TW5(6)/ TTMI-004 / D5-6 ]
- Conclusions / Need for further work
- Acknowledgements – EFDA Contract Framework – Actual question marks
There was also a former contribution as part of

EU Fusion Research Data Base Survey

- Acknowledgement of Input
- First attempt of DB classification
- Desired DB properties/qualities
- Examples of existing DB’s p/q
- Summary

Contributors to the Survey

1. IPP-Garching
2. FZ- Juelich
3. FZ- Karlsruhe
4. ÖAW-EURATOM
5. Association ENEA-RFX
6. EURATOM-MEdC
7. EURATOM/UKAEA Fusion Association
8. Institute of Mathematics and Informatics (IMI) of the Bulgarian Academy of Sciences
9. EU PWI Task Force
10. EU ITM Task Force
11. ITPA International Diagnostic Database
12. EFDA CSU-Garching
13. IPP-Greifswald
‘EU Fusion Research Data Base Survey’, K. Thomsen, 23 Feb 2007, CSA Info Workshop:

Neutronics

- The Nuclear Energy Agency (NEA)
- Nuclear Data Services (JEFF, EAF, IEAF)
- European Activation System
- Nuclear Data Center at Japan Atomic Energy Agency
- WWW Servers Related to Nuclear Data
- Table of Isotope Production Cross Sections (ACSELAM)
  S. Tanaka, N. Yamano,
- TALYS software for the simulation of nuclear reactions
Example (4) Nuclear Data Services (JEFF, EAF, IEAF) contd.

3. Data base status
a) Range of data – gaps? – None at present
b) Missing data / variables – None at present

c) Other shortcomings

To facilitate application development from high level languages, advanced interfaces are required from the databases. Such interfaces may be in the form of data access objects for high level languages (like Java or C++) or, preferably, web services. When using multiple data sources inside a single application, it would be very useful to have a common authentication mechanism, in order to reduce the number of passwords required for accessing the data. This can be achieved through generic authentication mechanisms, like PAPI.

Comments on ‘status’ follows…
Nuclear data (ND) **consistent** model calculations

[ E.D. Arthur – P.G. Young, LANL, ’80 ]

YES

i. unitary use of *common model parameters* for different mechanisms

ii. use of *consistent sets* of input parameters - determined by *analyses of various independent* experimental data

iii. unitary account of *whole body* of related experimental data for *isotope chains* and *neighboring elements*

[ activation & particle-emission spectra ]
[ enlarged incident-energy range ]

NO re-normalization or free parameters (*widely-used within ND libraries*)

[ IAEA/NDS RCs (12), Bucharest, 1982-2005 ]
Fast-neutron reaction model analysis (flowchart)

GLOBAL APPROACH

• **EMPIRE-II v.2.19 [ECIS95/SCAT2, DEGAS, MSD-TUL/MSC-H, HF]**
  - neutron/proton spherical optical potential **Koning-Dalaroche (2003)**
  - $\alpha$-particle default optical potential
  - EMPIRE-specific level density, $N_{\text{max}} < 40$
  - DEGAS [$g=A/13\ \text{MeV}^{-1}, K=100\ \text{MeV}^3$]
  - PCROSS

• **TALYS-0.64 (2005-2006), TALYS-0.72 (22.12.2006)**
  [+ Arjan Koning]

LOCAL APPROACH

• **STAPRE-H (v.2006) [SCAT2, GDH, HF] + DWUCK4**
  - p-, $\alpha$- spherical optical potentials
  - BSFG, $E^*<B_n$: $(a,\Delta)$→ $D_0$-, $N_{\text{max}}$-fit
  - $a(E^*),\ E^*\geq B_n$: Junghans/Koning/Chadwick (1998)
  - $I/I_r$: 0.5(g.s.)-0.75(Bn)-1(15 MeV)
  - GDH + $g_{\text{FGM}}(\varepsilon)$, $A_K(p,h),\ f_K(p,h,E,F_1(l,E_i)$
  + $J^\pi_{\text{conservation}}$
  + medium energy $l$-effects

COMPARISON with evaluated ND libraries:

- [ENDF/B-VII.0](http://www.nndc.bnl.gov/exfor1/endf00.htm)
- [JEFF-3.1](http://www.nea.fr/html/dbdata/JEFF)
- [JENDL-3.3](http://wwwndc.tokai.jaeri.go.jp/jendl/j33/j33.htm)
2000-2006  Fast-neutron activation analysis (in Bucharest +):

- all stable $^{50,51}$V isotopes
  
  \[ \text{[Phys. Rev. C 65, 014604 (2001)]} \]

- all stable $^{58,60,61,62,64}$Ni and $^{59}$Co isotopes
  
  \[ \text{[Nucl. Phys. A730, 255 (2004)]} \]

- all stable $^{92,94,95,96,98,100}$Mo isotopes
  
  \[ \text{[Nucl. Phys. A705, 265 (2002)]} \]
  \[ \text{[Phys. Rev. C 71, 044617 (2005)]} \]
  \[ \text{[Nucl. Phys. A764, 246 (2006)]} \]

- all stable $^{180,182,183,184,186}$W isotopes
  
  \[ \text{[Nucl. Phys. A765, 1 (2006)]} \]

- all stable $^{174,176,177,178,179,180}$Hf, $^{181}$Ta isotopes
  
  \[ \text{[PHYSOR-2006, ...]} \]

- all stable $^{55}$Mn, $^{63,65}$Cu isotopes
  
  \[ \text{[Phys. Rev. C 65, 014604 (2001)]} \]

(+ EC/JRC/IRMM-Geel)

(+ EC/JRC/IRMM-Geel)

(+ IRMM, KRI-St.Petersburg)

(+ KRI, UKAEA, TUD-Dresden, NRC-Petten, BNL-Brookhaven)

(+ UKAEA, NRC, BNL)
**2000-2006 WORK SUMMARY** on Mendeleev Table / Table of Isotopes

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Improved validation of the PE model assumptions/formalism

Extension for $E < 60$ MeV / proton-induced reaction data
Consistent parameters setting (sample):
Analysis of neutron total cross sections for $^{55}$Mn and $^{63}$Cu

\begin{figure}
\centering
\includegraphics[width=\textwidth]{diagram.png}
\end{figure}

Vlad Avrigeanu
Euratom-MEdC Association Seminar, 12 March 2007
Consistent parameters setting (sample):
Analysis of neutron-, proton-capture & \((p,n)\) reaction cross sections
Effective of $n/p$ modified OMPs on calculated cross sections ($^{65}\text{Cu}$)
Comparison of the measured, calculated, and evaluated reaction cross sections for the target nucleus $^{55}$Mn.
Comparison of measurements and evaluations of reaction cross sections for the target nuclei $^{63,65}$Cu
Comparison of measurements and global calculations of reaction cross sections for the target nucleus $^{63}$Cu

$^{63}$Cu(n,2n)$^{62}$Cu

$^{63}$Cu(n,p)$^{63}$Ni

$^{63}$Cu(n,α+2d+2n2p)$^{60}$Co

$^{63}$Cu(n,3n)$^{61}$Cu

$^{63}$Cu(n,n'+d)$^{62}$Ni

$^{63}$Cu(n,xd)

$^{63}$Cu(n,α+2d+2n2p)$^{60m}$Co

En (MeV)

E$_{n}$ (MeV)
Comparison of measurements and global calculations of reaction cross sections for the target nucleus $^{65}\text{Cu}$
Deuteron reaction model analysis (2003-2006)

• **NO GLOBAL OPTICAL POTENTIAL (OP) for**  \( d + \text{Nucleus (A<27)} \)
  
  \[ \text{Optical Potential - key ingredient of cross-sections calculations} \]

• **COMPARATIVE ANALYSIS** of global OMPs for  \( d + ^{27}\text{Al}, ^{63,65}\text{Cu}, ^{54,56,58}\text{Fe}, ^{93}\text{Nb} \):
  - Lohr-Haeberli (1974):  \( A \approx 40-209, E=8-13 \text{ MeV} \)
  - Perey-Perey (1963,1976):  \( A \approx 40-208, E=12-25 \text{ MeV} \)
  - Daehnick et al. (1980):  \( A \approx 27-238, E=11.8-90 \text{ MeV} \)
  - Bojowald et al. (1988):  \( ^{27}\text{Al}, ^{89}\text{Y}, ^{120}\text{Sn}, \text{and} ^{208}\text{Pb} \text{ at } E_d=58.7 \text{ and } 85 \text{ MeV} \)

• **None of these global OMP describes data at** \( E<15 \text{ MeV} \)

• **Semi-microscopic OMP by using realistic nucleon-nucleon interaction**
  
  \[ \text{M. Avrigeanu et al., Nucl. Phys. A723,104 (2003); A764, 246(2006)} \]
  
  - Calculations of **microscopic** \( V_R \) optical potential (DF)
  - \( W_D \) and \( V_{SO} \) components: local parameters based on data analysis
  - Data re-analysis with fixed \( W_D \) and \( V_{SO} \) components  \( \rightarrow \) local \( V_R \)

• **Average of the local OMP parameters for**  \( d+ ^{27}\text{Al}, ^{54,56}\text{Fe}, ^{63,65}\text{Cu}, ^{93}\text{Nb} \):
  \( \rightarrow \) cross-sections calculations
Deuteron reaction model analysis (flowchart)

- **SCAT2000** [O. Bersillon]  
  - pure elastic scattering OP analysis

- **DFOLD** [M. Avrigeanu]  
  - double folding method  
    (nucleons, d, $^4$, $^6$, $^8$He + $^4$-$^{124}$A-target nuclei)

- **FRESCO-2003** [I.J. Thompson]  
  - Coupled Reaction Channel (CRC) calculation

- **TALYS-0.64/0.72** [A. Koning et al.] / **EMPIRE-2.19** [M. Herman et al.]  
  - OMP: ECIS-’97 / ECIS’95; SCAT2000  
  - Hauser-Feshbach  
  - EXCITON-2 components / MSD-MSC

**COMPARISON** with evaluated charged-particle ND libraries (E>20 MeV):  
- ACSELAM (E>20 MeV) (Tanaka et al., 1994)
DF / Phenomenological OMP:

d + ^{27}\text{Al}
**DF / Phenomenological OMP: d + $^{54}$Fe**

- **$^{54}$Fe(d,d$_0$)**

  - 10 MeV
    - Goddard - Haeberli (1979)
    - present work
    - BMFP
    - TALYS - default
    - ACSELAM
  - 12 MeV
    - BMFP
  - 13 MeV
    - BMFP
  - 14.5 MeV
    - Hjorth - Lin (1968)

- **d + $^{54}$Fe**

  - 12.3 MeV
    - BMFP
  - 34.4 MeV
    - Newman et al. (1967)
  - 52 MeV
    - Hinterberger et al. (1968)
  - 56 MeV
    - Hatanaka et al. (1980)

- **σ/σ_{Rutherford}**

  - 10 MeV
    - Goddard - Haeberli (1979)
    - present work
    - BMFP
    - TALYS - default
    - ACSELAM
  - 12 MeV
    - BMFP
  - 13 MeV
    - BMFP
  - 14.5 MeV
    - Hjorth - Lin (1968)

- **dσ/dΩ [mb/sr]**

  - 12.3 MeV
    - BMFP
  - 34.4 MeV
    - Newman et al. (1967)
  - 52 MeV
    - Hinterberger et al. (1968)
  - 56 MeV
    - Hatanaka et al. (1980)
DF / Phenomenological OMP: \( d + ^{56,58}Fe \)

- \( ^{56}Fe(d,d_0) \) at 5 MeV
- \( ^{56}Fe(d,d_0) \) at 7 MeV
- \( ^{56}Fe(d,d_0) \) at 12 MeV
- \( ^{58}Fe(d,d_0) \) at 12.3 MeV

- \( \frac{d\sigma}{d\Omega} \) in mb/sr
- \( \sigma_{\text{reaction}} \) in mb

Graphs showing angular distributions and reaction cross-sections for different energies and reactions, comparing experimental data with theoretical predictions.

- Al-Quraishi et al. (2000)
- Burgi et al. (1980)
- Jahr et al. (1961)
- Roche et al. (1974)
- Al-Quraishi et al. (2000)
- De Leo et al. (1996)
- Brown et al. (1973)
- Roche et al. (1974)

The graphs illustrate the comparison between experimental data and theoretical models, including EMPIRE, TALYS, and ACSELAM calculations.
DF / Phenomenological OMP: \(d + {}^{63,65}\text{Cu}\)

\[
\begin{align*}
\sigma_R &\quad \text{Rutherford} \\
\sigma &\quad \text{Total Cross Section} \\
\frac{d\sigma}{d\Omega} &\quad \text{Differential Cross Section}
\end{align*}
\]

- **\(63\)Cu\(d,d_0\)**
  - 12 MeV
  - \(\frac{d\sigma}{d\Omega}\) vs. \(\theta_{\text{c.m.}}\)
  - Present work
  - EMPIRE - default OMP
  - TALYS-default OMP

- **\(65\)Cu\(d,d_0\)**
  - 12 MeV
  - \(\frac{d\sigma}{d\Omega}\) vs. \(\theta_{\text{c.m.}}\)
  - Lee Jr. + (1964)

- **\(34.4\)MeV**
  - \(\sigma/\sigma_R\) vs. \(\theta_{\text{c.m.}}\)
  - Newman+ (1967)

- **\(34.4\)MeV**
  - \(\sigma/\sigma_R\) vs. \(\theta_{\text{c.m.}}\)
  - Neuman+ (1967)

- **14.5 MeV**
  - \(\sigma/\sigma_R\) vs. \(\theta_{\text{c.m.}}\)
  - Hjort+ (1968)

- **12 MeV**
  - \(\frac{d\sigma}{d\Omega}\) vs. \(\theta_{\text{c.m.}}\)
  - Present work
  - EMPIRE - default OMP
  - TALYS-default OMP

- **34.4 MeV**
  - \(\sigma/\sigma_R\) vs. \(E_d\)
  - Bearpark et al. (1965)
  - Neumon+ (1967)
  - Newman+ (1967)

- **34.4 MeV**
  - \(\sigma/\sigma_R\) vs. \(E_d\)
  - Bearpark et al. (1965)
  - Newman+ (1967)
  - Newman+ (1967)

- **12 MeV**
  - \(\frac{d\sigma}{d\Omega}\) vs. \(\theta_{\text{c.m.}}\)
  - Lee Jr. + (1964)

- **14.5 MeV**
  - \(\sigma/\sigma_R\) vs. \(\theta_{\text{c.m.}}\)
  - Newman+ (1967)

- **34.4 MeV**
  - \(\sigma/\sigma_R\) vs. \(\theta_{\text{c.m.}}\)
  - Newman+ (1967)
DF / Phenomenological OMP: $d + \text{natCu}$

\[ \frac{\sigma}{\sigma_{\text{Rutherford}}} \] for $\text{Cu}(d,d_0)$ at 11.8 MeV. 

\[ \frac{d\sigma}{d\Omega} \] at 11.8 MeV with data from Jahr+ (1961).

\[ \frac{d\sigma}{d\Omega} \] at 21.6 MeV with data from Yntema (1959).

\[ \sigma_{\text{reaction}} \] with energy $E_d$ ranging from 0 to 60 MeV.

Comparison of various models and calculations with experimental data.
DF / Phenomenological OMP: $d + ^{93}$Nb

![Graph showing angular distributions and cross-sections for $d + ^{93}$Nb reactions at different energies.](image-url)

- **11.8 MeV**
  - Igo+ (1961)
  - present work
  - EMPIRE - default OMP
  - TALYS - default OMP
  - Hinterberger+ (1968)

- **34.4 MeV**
  - Newman+ (1967)
  - present work
  - EMPIRE - default OMP
  - TALYS - default OMP
  - Jolly+ (1963)

- **52 MeV**
  - present work
  - EMPIRE - default OMP
  - TALYS - default OMP
  - TALYS - default $\sigma_R$
  - ACSELAM
Conclusions

• **Achievements**

  - Unitary description of **all activation** experimental data \((E<60 \text{ MeV})\) by means of **local analyses**: accuracy \(\leq 5\%\)
  - Good results of global calculations (TALYS code): accuracy \(\approx 20-50\%\)
  - Former evaluations (ACSELAM library): accuracy \(\approx 50-100\%\)

• **Further needs**

  - Model validation at **higher energies** \((E>20 \text{ MeV})\) / \(p-, d\)-induced reactions
  - **Microscopic basis** for deuteron optical potential