The Methodology of Nuclear Data Evaluation & the Next Version of CENDL

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1. Introduction of China Nuclear Data Activities
2. The Methodology of Nuclear Data Evaluation
3. Recent Progress of China Nuclear Data Project
4. New Version of CENDL
5. New Generation of Nuclear Data and Library?
1. Introduction of China Nuclear Data Activities

✓ The goal of China nuclear data activities is supplying the nuclear data to feed the needs of the nuclear peaceful applications.

✓ The activities consists of nuclear data measurement and related study, evaluation and model study, data library establish and management and nuclear data benchmark testing and validation.

✓ The mainly activities are being carried out by China Nuclear Data Center(CNDC), China Institute of Atomic Energy(CIAE) and China Nuclear Data Coordination Network(CNDCN) and more than 10 institutions and universities are involved CNDCN.
1.1 Chinese Nuclear Data Activity Structure
1.2 General Information of CNDC

**CNDC View**
- China Nuclear Data Center (CNDC) was established in 1975.
- CNDC joined the nuclear data activities of IAEA as the national nuclear data center of China since 1984.

**Main task**
- The nuclear data evaluations, libraries and relevant technique researches
- The exchange of nuclear data activities with IAEA, foreign nuclear data centers and agencies
- The management of domestic nuclear data activities
- The services for domestic and foreign nuclear data users.

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The Chief Nuclear Data Evaluations in CNDC

- Neutron Reaction Data
- Activation Data
- Fission Yield Product
- Covariance Uncertain Data
- Decay Data and Structure
- Integral validation
1.2 Inf of the Facilities:

✓ The facilities were used for the nuclear data measurements and studies including the HI-13 tandem accelerator, 600kV-Cockcroft-Walton accelerator and 5SDH-2 tandem accelerator at CIAE and 4.5-MV Van de Graaff accelerator at Peking university and 300kV-Cockcroft-Walton accelerator at Lanzhou university.

✓ The China experimental fast reactor (CEFR,) was reached the critical on 21 June 2010, and China advanced research reactor (CARR) has been reached the critical on 13, May 2010 at CIAE and will be used for nuclear data related research.

✓ The China Spallation Neutron Source and some other facilities are under constructing in China.
CARR@CIAE (60MW, neutron flux: $8 \times 10^{14} \text{n/cm}^2 \cdot \text{s}$)
CEFR@CIAE (65 MW)
The China Spallation Neutron Source.

Schematic layout of the back-streaming neutron endstation at China Spallation Neutron Source (under construction)
The facilities in China Nuclear Data Key Lab.
2. The Methodology of Nuclear Data Evaluation

- Need Analysis
- Benchmark Test (5)
- S/U Analysis
- User Need
- User Application
- Data Processing (4)
- Application File
- Model Cal. & Eval. (2)
- Benchmark Exp.
- Lab. and Check (3)
- Data Adjustment
- Exp. Measurement (1)

CENDL-3
ENDF
2.1 The Nuclear Data in Th/U Fuel Cycle

- The new generation of nuclear energy system (International Generation-IV) was established in 2000. Six most promising technologies were selected, including three thermal reactors and three fast reactors;

- Comparing to the current employed reactors, several prominent features are existed, such as highly economic; enhanced safety; minimal waste; proliferation resistant;

- Thorium is believed to be the potential nuclear energy material, and important in the Gen IV reactor design:
  1. Thorium is more abundant on Earth than Uranium;
  2. Th-U fuel cycle does not irradiate $^{238}$U and therefore does not produce transuranic materials like Pu, Am, Cm, etc; thus, Th-U waste will be less toxic;
  3. Thorium cycles exclusively allow thermal breeder reactors;
  4. Thorium can (practically) breed without making weapons material.
- Th, Pa and U are involved in the Th/U fuel cycle
- 12 chief elements (Colored in the Figure) related to the transfer from $^{232}$Th - $^{233}$U
- 4 elements around the chief chain
- Different decay modes, $(n,2n)$, $(n,f)$, $(n,\gamma)$ reactions
Nuclear data required in the study of neutron physics

The complete neutron reactions data, fission yield production, nuclear structure and decay data related to the elements of Th, U and Pa (not included in U/Pu fuel cycle) are necessary in the Th/U fuel cycle study.
2.1 Theoretical Model Codes for Nuclear Reaction

The model theory in low energy region (En ≤ 20 MeV)

- **Resonance region:**
  - R Matrix

- **Dirac Reaction:**
  - Phenomenological optical model potentials (OMPs) for near-spherical nuclides;
  - OMP with Couple channel;
  - Distorted wave function Born approximation

- **Compound Nuclei:**
  - Evaporation model;
  - Hauser-Feshbach model

- **Pre-equilibrium emission:**
  - Exciton model;
  - Kalbach systematics
Model Codes for Nuclear Data

1. SAMMY: Nancy M. Larson, ORNL, 1980-
2. ALICE: Blann, LLNL, 1974-
3. GNASH: Young, Arthur and Chadwick, LANL, 1977-
4. TNG: Fu, ORNL, 1980-
5. STAPRE: Uhl, Univ. Vienna, 1980-
6. UNF: Zhang Jingshang, CNDC, 1985-
7. EMPIRE: Herman, ENEA, IAEA, BNL, 1982-
8. EXIFON: Kalka, Univ. Dresden, 1989
9. TALYS: Koning, Hilaire, Duijvestijn, NRG/CEA, 1998-
10. CCONE: O. Iwamoto, JAEA/NDC, 2007-

... ...
(n,p) cross sections for all natural isotopes between Li and Bi

TALYS系统计算从Li到Bi所有天然核素的 (n, p) 反应截面的结果
\( n^{+10}\text{B} \) 双微分截面LUNF计算结果和实验数据比较

\( n^{+12}\text{C} \) 双微分截面LUNF计算结果和实验数据比较
3. Recent Progress of China Nuclear Data Project

3-1 CENDL project

China Evaluated Nuclear Data Library (CENDL) is a general purpose evaluated nuclear data file. The updated vision CENDL-3.1 was released in 2009 and provided for all users by ENDF format.

According to the back feed from the benchmark testing and users, some data files of CENDL-3.1 were re-evaluated in recently two years. These nuclei including the actinides $^{241}$Am, $^{234,235}$U, $^{237}$Np, $^{233}$Th and some structural materials $^{54}$Fe, $^{97}$Mo, $^{186}$W(p,n), (p,2n) $^{208,207,206,204}$Pb et al.
(a) Comparison with original measured data

(b) Comparison with corrected measurements

Fig. Comparison of evaluated data with measured data for $^{237}$Np(n, 2n) reaction
The comparison of evaluated $^{241}$Am(n,2n) with other data
The comparison of CENDL-31-REV, CENDL-31, ENDF/B-VII for $^{233}$U(n, f) reaction.
3-2 Related Methodology Studies
R-Matrix Used for Light Nuclei CS Evaluation

**APRML** is a nuclear reaction code for calculating and fitting light nuclei cross sections, developed at CNDC and Nankai University. It is based on R-matrix theory and compiled with FORTRAN language. It can be used for calculating light nuclei cross section and angular distribution. APRML was compiled and adjusted less than a year, many mistakes and bugs have been fixed. The code has been compiled and some functions are under debugging and testing.

The comparisons of the preliminary calculation and experimental data of total CS for n+\(^6\)Li
Neutron C.S. Covariance Evaluation

A covariance evaluation system, COVAC, is being developed for structure and fission nuclides. In this system, experimental data including their errors were firstly pre-analyzed and handled.

In this framework, the high fidelity covariance file can be obtained with combining the theoretical and experimental uncertainties and correlations.
The correlation coefficient matrix of the recommended cross sections of $^{48}\text{Ti}(n, \text{tot})$ & $(n, p)$ & $(n, a)$

The correlation coefficient matrix of the experimental cross sections of $^{40}\text{Ca}(n, \text{tot})$
Fission yield products-semi-empirical model

The model was based upon the basic idea of Brosa model, the fission system energy included the macro energy and the shell effects at \( N \sim 82 \) and \( N \sim 88 \), could be expressed in eq. [1] approximately and shown in the figure below:

\[
E(E_0^*, N) \approx E_{\text{mac}}(N) + \sum_{i=1,2} \delta U_{\text{sh},i}(N) \exp(-\gamma \varepsilon) \tag{1}
\]

\( N_{\text{SL}} \) (neutron number): the center of Super Long fission

\( N_{\text{sh}1,2} \): the shell positions, also the centers of the Standard I and II fissions.

Shell effects at \( N \sim 82 \) and 88

\( E_0^* \): Excitation energy of the compound.

Factor: Shell effect weaken with temperature

(\( \varepsilon \): stands for the syst. energy without temp. correction)
Para. set 1: fitted from all concerned measured yield data;
Para. set 2: fitted from measured yield energy-dependence data.
The yield step-increased in the Valley and Wings area of mass A, decreased in the Peaks area, and vibrated near the joints (A=88, 103, 133, 149.8)
Prompt Neutron Multiplicity Distribution for $^{235}$U(n,f) at Incident Energies Up to 20 MeV

The total excitation energy partitions between the complementary light and heavy fission fragments for the n+$^{235}$U fission reaction are given at incident energies up to 20 MeV. The average neutron kinetic energy $\langle \varepsilon \rangle(A)$ and the total average energies removed by $\gamma$ rays $E_\gamma(A)$ as a function of fission fragment (FF) mass at different incident neutron energies are presented. The prompt neutron multiplicity distribution $\nu(A)$ for n+$^{235}$U fission at different incident neutron energies are calculated. The results are checked with the total average prompt neutron multiplicities and compared with the experimental and evaluated data. These results can be used for the prompt fission neutron multiplicity and spectrum evaluation, and the calculated $\nu(A)$ distribution provides the data to deduce the post-neutron emission mass yields from the already known pre-neutron emission mass yields. The former is very important for the application.
Fig. 11 FF pair multiplicity of the $^{235}$U(n,f) reaction at thermal neutron energy (a) and higher neutron energies (b)
Nuclear Data S/U Method Study

The Function of Present S/U Method

- one-dimensional S/U analysis code SENS1D
- benchmark facilities, such as Godiva, Jezebel and Flattop, with or without reflecting material

The Module Design of SENS1D System

START

SETUP

SCALE DRIVE

CONTROL

INPUT

LOADSCALE

LOADAMPX

LOADCOV

CORE

SENS

COMBINE

ERROR

OUTPUT

SAVE

PLOT

END

--

MC Perturbation

Determined Method

MC Dirac Perturbation

Leakage Spec., $k_{eff}$ of Fast assemblies

Sensitivity Calc.

Conjugate (Gen. Perturbation)

TotalMC

Determined Conjugation

$k_{eff}$ of Fast assemblies
Sensitivity of $^{239}\text{Pu}$

Preliminary $k_{\text{eff}}$ sensitivity coefficient of $^{239}\text{Pu}$ (absolute value) calculated by SENS1D

- SENS1D can now calculate the explicit sensitivity coefficient of $k_{\text{eff}}$ to several input CS data, including $(n, f)$, $(n, \text{non})$, $(n, \text{el})$ and total = $(n, f)+(n, \text{non})+(n, \text{el})$,

- Combine the multi-group covariance data to calculate the uncertainty of $k_{\text{eff}}$ due to the above input CS data.

- SENS1D can be used for the S/U analysis of one-dimension benchmark facilities, such as Godiva, Jezebel and Flattop, with or without reflecting material.
The System of Benchmark Testing and Validation in CNDC

ENDITS

Radioactive Shielding Benchmark testing

Fusion radiation shielding benchmark experiments
Fission radiation shielding benchmark experiments
U, Pu metal fast spectrum assemblies
U, Pu metal intermediate spectrum assemblies
HEU & LEU solution thermal spectrum assemblies
LEU fuel rod thermal spectrum assemblies
Pu solution thermal spectrum assemblies
U233, Th232 critical assemblies

Critical benchmark testing (ICSBEP)

Benchmark testing of fission products
Benchmark testing of specific elements
Integral Exp. of Capture C.S.
The Systematics of (n,2n) Reaction Excitation Function

Based on the constant temperature evaporation model taking the competition of (n,3n) reaction and the contribution of preequilibrium emission into account, the systematics formulae of (n,2n) reaction excitation function have been established.

There are two systematics parameters $T$ and $\sigma_{n,M}$ can be adjusted in the formulae. For getting the two parameters, the new evaluated data of (n,2n) reactions were adopted and fitted by means of the nonlinear least squares method. The fitted results agree fairly well with the measured data at $45 \leq A \leq 210$ below 30 MeV. Based on a body of new measurements, the reliability to predict (n,2n) reaction excitation function is improved.
Fig. Excitation function of the (n,2n) reaction for $^{181}\text{Ta}$. 
Other Innovative Methodology Study

- **Microscopic global OMP study based on relativistic Dirac Bruckner Hartree-Fock**

**PHYSICAL REVIEW C 85, 034613 (2012)**

**Relativistic nucleon optical potentials with isospin dependence in a Dirac-Brueckner-Hartree-Fock approach**

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*(Received 19 December 2011; published 26 March 2012)*

The relativistic optical model potential (OMP) for nucleon-nucleus scattering is investigated in the framework of the Dirac-Brueckner-Hartree-Fock (DBHF) approach using the Bonn-B one-boson-exchange potential for the bare nucleon-nucleon interaction. Both real and imaginary parts of isospin-dependent nucleon self-energies in the nuclear medium are derived from the DBHF approach based on the projection techniques within the subtracted $T$-matrix representation. The Dirac potentials as well as the corresponding Schrödinger equivalent potentials are evaluated. An improved local density approximation is employed in this analysis, where a range parameter is included to account for a finite-range correction of the nucleon-nucleon interaction. As an example the total

**The reaction study for unstable nuclei based on very fundamental theory.**
Systematic study of covariance of (n,tot) CS based on the relativistic Dirac Bruckner Hartree-Fock microscopic global OMP

\[ \Delta \tilde{C} = (F_1^T V_{\text{exp}}^{-1} F_1)^{-1} F_1^T V_{\text{exp}}^{-1} (Y_{\text{exp}} - Y_{\text{理论}}) \]

\[ \tilde{V}_C = (F_1^T V_{\text{exp}}^{-1} F_1)^{-1} \]

\[ \tilde{Y}_{推荐} = F_2 \Delta \tilde{C} + Y_{\text{理论}} \]

\[ \tilde{V}_{推荐} = a^2 N (F_2 \tilde{V}_C F_2^T) \]

This covariance is evaluated after LS calculation.
## 4. New Version of CENDL

### The Latest Versions of the well-known Lib.

<table>
<thead>
<tr>
<th>Name</th>
<th>ENDF/B-VII.1</th>
<th>JENDL-4.0</th>
<th>JEFF-3.1</th>
<th>CENDL-3.1</th>
<th>ROSFOND2.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Country</td>
<td>USA</td>
<td>Japan</td>
<td>Europe</td>
<td>China</td>
<td>Russian</td>
</tr>
<tr>
<td>Num. Nuclide</td>
<td>423</td>
<td>406</td>
<td>381</td>
<td>240</td>
<td>686</td>
</tr>
<tr>
<td>Range of Nuclide</td>
<td>1-H-1—100-Fm-255</td>
<td>1-H-1—100-Fm-255</td>
<td>1-H-1—100-Fm-255</td>
<td>1-H-1—98-Cf-249</td>
<td>1-H-1—96-Cm-244</td>
</tr>
</tbody>
</table>
Next CENDL will be:

The CENDL-3.2 is general purpose evaluated nuclear data file which consists of the neutron reaction sub-library, the activation sub-library, decay data sub-library and fission yield sub-library. CENDL-3.2 can be used for the nuclear engineering, nuclear medicine and nuclear science etc. fields.

The CENDL-3.2 is based on the previous version of CENDL and other special purpose libraries established by China Nuclear Data Center (CNDC), the updated experimental information and new nuclear data evaluation methodologies.
The nuclei region of the new neutron reaction sub-library will be extend comparison with the CENDL-3.1 and the materials number will up to 300, which can be covered almost needs for the nuclear engineering, nuclear power and related fields.

The high fidelity covariance files for some important structural materials, actinide and low fidelity covariance files for other nuclei will be included in the sub-library. All the covariance files will be evaluated through a covariance evaluation system COVAC developed by CNDC.
The benchmark testing and validation for the CENDL-3.2 will be performed through the updated Evaluated Nuclear Data Integra Test System (ENDIST) established at CNDC.

Activation sub-library will contain the most important excitation functions for more than 600 nuclei which can be used for nuclear reactor design, operation and nuclear safety etc. Some of the evaluated data will be obtained based on the updated measurements and mode calculations.
Decay data sub-library contains the updated decay information for more than 2000 nuclei, and more than 200 new evaluations will be carried out by Chinese evaluators, other the data come from the new results of the NSDD.

Fission product yield sub-library will provide the evaluated fission yields by various methods for the neutron introduced fissions for the U, Pu and Th etc.
5. New Generation of Nuclear Data and Library?

The problem is becoming serious because the increase of nuclear data need and the familiar experts are missing.

More nuclear data requirements including the region of nuclei, energy, accurate and the application of the nuclear data etc are proposed according the nuclear technology applications extending.

Can the existed/developing nuclear data libraries support the increasing need of nuclear applications?

Can the conventional way and technology of nuclear data produce satisfy the new nuclear data users?

What is the next generation of nuclear data for future?
Thank you for your attention! Comments and suggestion welcome!
1. The Nuclear Data in Th/U Fuel Cycle

Six most promising technologies selected in Gen VI:

Three thermal reactors:
Very high-temperature gas-cooled reactor (VHTR); Molten salt reactor (MSR);
Super-critical water-cooled reactor (SCWR);

Three fast reactors:
Gas-cooled fast reactor (GFR);
Sodium-cooled fast reactor (SFR);
Lead-cooled fast reactor (LFR);

Prominent features of Gen. VI reactors:
Highly economic; Enhanced safety; Minimal waste; Proliferation resistant