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Assessment of Some Optical Model Potentials in Predicting Neutron Cross Sections

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ABSTRACT

Optical model potential parameters play an important role in the evaluation of nuclear data for applied purposes. The IAEA Coordinated Research Program on "Reference Input Parameter Library for Evaluation of Nuclear Data for Application in Nuclear Technology" aims to release a reference input file of various types of parameters for the evaluation of nuclear cross sections using nuclear model codes. Included in the parameter files are a collection of optical model potentials that are available in the literature to evaluate these cross sections. As part of this research program we assess the applicability of these potentials over a range of target mass and projectile energy.

INTRODUCTION

The International Atomic Energy Agency (IAEA) Nuclear Data Section is sponsoring a Coordinated Research Program (CRP) that is directed at compiling and developing a library of nuclear model parameters that are useful in evaluations of nuclear data.[1,2] The planned product of this CRP is a Reference Input Parameter Library (RIPL) that will contain reliable, state-of-the-art parameterizations for conventional nuclear model codes used in calculations of nuclear data for applications. The motivation for this work is the situation of diminishing resources worldwide for supplying nuclear data, particularly experimental facilities, coupled with the fact that nuclear reaction models have reached a level of considerable reliability which should be preserved. Preparatory meetings were held by the IAEA in Vienna (Working Group Meeting, 4-6 May 1991 and Consultants' Meeting, 13-15 November 1991), and in Sirolo, Italy (Consultants' Meeting, 21-25 June 1993). CRP meetings were held in Cèrvia, Italy, 19-23 Sept. 1994,[1] and in Vienna, Austria, 30 Oct.- 3 Nov. 1995.[2] A third CRP meeting is scheduled for 26-29 May 1997 in Trieste, Italy.

The focus of the RIPL activity is a library of parameterizations for incident radiation at energies up to 30 MeV, primarily incident neutrons, and for outgoing neutrons, protons, alpha particles and gamma rays, although higher energies and incident charged particles and photons are also considered. The areas of emphasis are atomic masses, shell corrections, and deformations; discrete level schemes; average neutron resonances; optical model parameterizations; nuclear level densities (total, partial, fission barriers); gamma-ray strength functions; and continuum angular distributions. The planned output is a complete "starter file" of

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relevant parameters arranged in a processing-oriented format and equipped with a retrieval/processing code. The present report describes initial efforts to assess the validity of a selection of optical model parameterizations that are included in the RIPL library.

The optical model frequently provides the basis for theoretical analyses and/or data evaluations that are used in providing nuclear data for applied purposes. In addition to offering a convenient means for calculation of reaction, shape elastic, and (neutron) total cross sections, optical model potentials are widely used in quantum-mechanical preequilibrium and direct-reaction theory calculations and, most importantly, in supplying particle transmission coefficients for Hauser-Feshbach statistical-theory analyses used in nuclear data evaluations. Consequently, it is important that predictions of such quantities as total, elastic, and especially reaction cross section reasonably reproduce experimental data. In this report we present comparisons to experimental data of neutron total, elastic, and reaction cross sections calculated with a sampling of optical model potentials in the RIPL library.

METHODOLOGY

In this initial assessment we have chosen to investigate several neutron global optical model potentials that are widely used to calculate nuclear data for a representative selection of targets useful in applications. We also include several nuclide-specific potentials in order to investigate the improvement their use facilitates compared to the global potentials. The target nuclei we selected are C, Al, Ca, Fe, Sn, Pb and U, which span a wide mass range and which are all important for applications in nuclear technology. Although the focus of the RIPL starter file of parameters is the incident neutron energy range up to 30 MeV, we have chosen to examine comparative predictions of cross sections over a somewhat wider neutron energy range, E_n = 1 to 150 MeV, in order to also assess the potentials required for higher energy applications such as radioactive ion beam and accelerator-driven transmutation applications.

The global neutron optical potentials we investigate are among the most widely used in large-scale calculations of nuclear data such as, for example, activation data libraries. The global potentials included are the following: (1) Wilmore and Hodgson,[3] (2) Becchetti and Greenlees,[4] (3) Madland,[5] (4) Rapaport et al,[6] (5) Walter and Guss,[7] and (6) Yamamuro.[8] The potentials we study that were derived specially for the specific nuclei in this analysis are those of Dimbylow et al.[9] for C, Petler et al.[10] for Al, Islam et al.[11] for Ca, Arthur and Young[12] for Fe, and Shamu and Young[13] for Pb. In the various studies that resulted in these nuclide-specific potentials, experimental data such as are presented here were included in those analyses.

All optical model calculations presented in this report were performed with the SCAT2 computer program developed by Bersillon.[14] This code has been included in lecture series at the International Centre for Nuclear Physics in Trieste and is widely used by the applied nuclear data community for optical model calculations. For each target nucleus and optical model potential chosen, we calculate the total, elastic and reaction cross sections from 1 to 150 MeV on incident neutron energy grids varying from 1 MeV steps at lower energies to 5 MeV steps at the higher energies. Representative experimental data (described below) were obtained primarily from the online nuclear data service (SCISR compilation) at the National Nuclear Data Center at Brookhaven National Laboratory[15] and from the compilation of Barashenkov.[16]

RESULTS

We present the results of this study in a series of graphical comparisons. For the seven target nuclei that we consider, separate figures are used to illustrate the elastic scattering, reaction, and total cross sections over the entire neutron energy range of 1 to 150 MeV, resulting in a total of 21 figures. Each figure contains curves for all of the global potentials considered, and most of them also contain a calculated curve for an optical potential specific to that nucleus. All figures include comparison with experimental data.[15,16]

Figures 1-3 compare the calculated elastic, reaction, and total cross sections for n + ^{12}C reactions with experimental data. Similarly, Figs. 4-6 show the same comparisons for ^{27}Al, Figs. 7-9 for ^{40}Ca, Figs. 10-12 for ^{56}Fe, Figs. 13-15 for Sn, Figs. 16-18 for ^{208}Pb and Figs. 19-21 for ^{238}U. All experimental data available from the two compilations[15,16] over the energy range covered are included in the figures showing elastic and reaction cross sections, except for the lower energy regions on the graphs. This omission occurs because the optical model calculations only include shape elastic scattering, that is, the compound elastic cross section component is not present. Consequently, we eliminate experimental elastic cross section data from the lower energy regions where we judge compound elastic scattering to be important. Similarly, the experimental data included with the reaction cross section comparisons are actually nonelastic measurements, whereas the optical model reaction cross section calculations include a compound elastic component. Therefore, we also avoid showing nonelastic cross section measurements at lower energies.

In the case of the total neutron cross section, the number of measurements is very large. Consequently, we compare the total cross sections calculations only to a selection of experimental data from the NNDC[15] and the Barashenkov[16] compilations. For the targets C, Al, Ca, and Pb, we limit our comparison to the recent total cross section measurements of Finlay et al.[17] Isotopic experimental data are utilized where available.

CONCLUSIONS

It is difficult to recommend a single global optical model potential based on these comparisons because the results vary over the range of targets included and for the different cross section types. However, some general comments can be made. In every case where local potentials are compared, they give better agreement with the experimental data than do the global potentials. So one firm conclusion is that additional, carefully-chosen nuclide-specific potentials should be included in the RIPL library.

As a general rule, the Wilmore and Hodgson[3] potential appears to consistently give reasonable reaction cross sections up to about 30 MeV, although the elastic (and total) cross sections from this potential become too high above 15 - 20 MeV. The Walter and Guss[7] and the Yamamuro[8] potentials also appear to give reaction cross sections that reasonably agree with the available data. Conversely, the Becchetti and Greenlees[4] potential usually appears to disagree with the experimental data more than the other potentials. The Rapaport potential[6] potential gives reasonable results in most cases. However, the reaction cross section appears to differ more from the experimental data near 14 MeV than does, for example, the Wilmore and Hodgson potential. From these comparisons we conclude that in cases where global potentials must be utilized, it is usually advisable to use the Wilmore-Hodgson potential rather than the Becchetti-Greenlees or Rapaport potentials for incident neutron reactions below 30 MeV, but the Yamamuro and Walter-Guss potentials are also viable options.

The largest differences in the reaction cross sections calculated with the various potentials occur at fairly low energies, which are not tested in these comparisons. To test the low energy reaction and elastic cross section predictions requires carrying out Hauser-Feshbach calculations which were beyond the scope of the present study. Such tests should clearly be carried out.

The Madland[5] potential reproduces the reaction cross section data rather well at energies above about 30 MeV for all the nuclei considered. Similarly, the Madland potential does well for the elastic and total cross sections for the nuclei lighter than Sn. However, for the heavier nuclei the calculated elastic (and total) cross sections differ in shape and magnitude from the experimental data above about 50 MeV, particularly for ^{208}Pb and ^{238}U. Of course, in the case of ^{238}U, a coupled-channels optical model potential in the framework of a rotational model is more appropriate due to the deformed nature of ^{238}U. Finally, it should be pointed out that in developing his global potential, Madland utilized the SNOOPY8 code,[18] which includes both relativistic kinematics and a relativistic treatment of the Schroedinger equation. While our use of SCAT2 without any relativistic corrections is not the primary source of the disagreement with the higher energy elastic and total cross section data for ^{208}Pb and ^{238}U, it does contribute somewhat to the differences with experimental data seen in the comparisons.

In conclusion, we should emphasize that the results presented here are only a beginning of the work needed to fully test the various potentials in the RIPL library. For example, elastic scattering angular distributions should be compared with experimental data, and incident proton reactions should be included in the tests. Additionally, many more target nuclei should be considered, and Hauser-Feshbach calculations are important for the validation of potentials at lower energies.

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FIGURE CAPTIONS

Fig. 1 Measured and calculated elastic scattering cross section of ^{12}C for incident neutrons between 1 and 150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 2 Calculated neutron reaction cross section of ^{12}C compared to measured nonelastic cross sections for E_n = 1-150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 3 Neutron total cross section of ^{12}C for incident neutrons between 1 and 150 MeV. Optical model calculations are compared to the experimental data of Finlay et al.[17]

Fig. 4 Measured and calculated elastic scattering cross section of ^{27}Al for incident neutrons between 1 and 150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 5 Calculated neutron reaction cross section of ^{27}Al compared to measured nonelastic cross sections for E_n = 1-150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 6 Neutron total cross section of ^{27}Al for incident neutrons between 1 and 150 MeV. Optical model calculations are compared to the experimental data of Finlay et al.[17]

Fig. 7 Measured and calculated elastic scattering cross section of Ca for incident neutrons between 1 and 150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 8 Calculated neutron reaction cross section of Ca compared to measured nonelastic cross sections for E_n = 1-150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 9 Neutron total cross section of Ca for incident neutrons between 1 and 150 MeV. Optical model calculations are compared to the experimental data of Finlay et al.[17]

Fig. 10 Measured and calculated elastic scattering cross section of ^{56}Fe for incident neutrons between 1 and 150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 11 Calculated neutron reaction cross section of ^{56}Fe compared to measured nonelastic cross sections for E_n = 1-150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 12 Neutron total cross section of ^{56}Fe for incident neutrons between 1 and 150 MeV. Optical model calculations are compared to measured data from the NNDC[15] and Barashenkov[16] compilations.

Fig. 13 Measured and calculated elastic scattering cross section of Sn for incident neutrons between 1 and 150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 14 Calculated neutron reaction cross section of Sn compared to measured nonelastic cross sections for E_n = 1-150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 15 Neutron total cross section of Sn for incident neutrons between 1 and 150 MeV. Optical model calculations are compared to measured data from the NNDC[15] and Barashenkov[16] compilations.

Fig. 16 Measured and calculated elastic scattering cross section of ^{208}Pb for incident neutrons between 1 and 150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 17 Calculated neutron reaction cross section of ^{208}Pb compared to measured nonelastic cross sections for E_n = 1-150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 18 Neutron total cross section of ^{208}Pb for incident neutrons between 1 and 150 MeV. Optical model calculations are compared to the experimental data of Finlay et al.[17]

Fig. 19 Measured and calculated elastic scattering cross section of ^{238}U for incident neutrons between 1 and 150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 20 Calculated neutron reaction cross section of ^{238}U compared to measured nonelastic cross sections for E_n = 1-150 MeV. Experimental data are from the NNDC[15] and Barashenkov[16] compilations.

Fig. 21 Neutron total cross section of ^{238}U for incident neutrons between 1 and 150 MeV. Optical model calculations are compared to measured data from the NNDC[15] and Barashenkov[16] compilations.