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NUCLEAR MODELS TO 200 MEV FOR HIGH-ENERGY DATA EVALUATIONS

A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee

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ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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- to contribute to sound economic expansion in Member as well as non-member countries in the process of economic development; and
- to contribute to the expansion of world trade on a multilateral, non-discriminatory basis in accordance with international obligations.

The original Member countries of the OECD are Austria, Belgium, Canada, Denmark, France, Germany, Greece, Iceland, Ireland, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The following countries became Members subsequently through accession at the dates indicated hereafter; Japan (28th April 1964), Finland (28th January 1969), Australia (7th June 1971), New Zealand (29th May 1973), Mexico (18th May 1994), the Czech Republic (21st December 1995), Hungary (7th May 1996), Poland (22nd November 1996) and the Republic of Korea (12th December 1996). The Commission of the European Communities takes part in the work of the OECD (Article 13 of the OECD Convention).

NUCLEAR ENERGY AGENCY

The OECD Nuclear Energy Agency (NEA) was established on 1st February 1958 under the name of OEEC European Nuclear Energy Agency. It received its present designation on 20th April 1972, when Japan became its first non-European full Member. NEA membership today consist of all OECD Member countries, except New Zealand and Poland. The Commission of the European Communities takes part in the work of the Agency.

The primary objective of the NEA is to promote co-operation among the governments of its participating countries in furthering the development of nuclear power as a safe, environmentally acceptable and economic energy source.

This is achieved by:

- *encouraging harmonization of national regulatory policies and practices, with particular reference to the safety of nuclear installations, protection of man against ionising radiation and preservation of the environment, radioactive waste management, and nuclear third party liability and insurance;*
- *assessing the contribution of nuclear power to the overall energy supply by keeping under review the technical and economic aspects of nuclear power growth and forecasting demand and supply for the different phases of the nuclear fuel cycle;*
- *developing exchanges of scientific and technical information particularly through participation in common services;*
- *setting up international research and development programmes and joint undertakings.*

In these and related tasks, the NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has concluded a Co-operation Agreement, as well as with other international organisations in the nuclear field.

FOREWORD

A Working Party on International Evaluation Co-operation was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation, and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The working party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The parties to the project are: ENDF (United States), JEF/EFF (NEA Data Bank Member countries), and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries, specifically the Russian BROND and Chinese CENDL projects, are organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

Subgroup 12 of the working party was initiated with the objective to recommend nuclear model codes for the calculation of nuclear data used in different applications. The subgroup was charged with the tasks to co-ordinate the collection of nuclear models, to indicate the range of applicability of each model, to validate model calculations against experiments and to document the findings. Close co-operation was established with the IAEA project to develop a Reference Input Parameter Library (RIPL) for nuclear level densities.

Following the retirement of the original subgroup co-ordinator, G. Reffo, the subgroup limited its activity to the current status of nuclear reaction models used within various codes of importance in intermediate energy nuclear data evaluation work.

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SUMMARY

This report describes the work of the Nuclear Energy Agency's Subgroup 12, which represents a collaborative effort to summarise the current status of nuclear reaction modelling codes and prioritise desired future model improvements. Nuclear reaction modelling codes that use appropriate physics in the energy region up to 200 MeV are the focus of this study, particularly those that have proved useful in nuclear data evaluation work. This study is relevant to developing needs in accelerator-driven technology programs, which require accurate nuclear data to high energies for enhanced radiation transport simulations to guide engineering design.

NUCLEAR MODELS TO 200 MEV FOR HIGH-ENERGY DATA EVALUATIONS

1. Introduction

The work described in this report has been the focus of study of the Nuclear Energy Agency's Subgroup 12, which comprises a group of scientists from countries around the world collaborating under the auspices of the Nuclear Energy Agency's Nuclear Science Committee Working Party on International Evaluation Co-operation (WPEC).

The focus of Subgroup 12 has been: (1) to summarise the status of nuclear reaction modelling codes that can be used in nuclear data evaluation work for incident nucleon energies below 200 MeV; (2) to compile researchers' experience in developing nuclear data libraries with these codes, including the models' strengths and weaknesses; and (3) to prioritise future nuclear reaction theory research that is needed for the production of improved nuclear data evaluations in the energy region up to 200 MeV.

There has been a great deal of activity in recent years in extending nuclear data libraries to higher energies. The bulk of the existing evaluations for incident neutrons extend up to 20 MeV, since this was the important energy range for fission and fusion applications. Recent work has concentrated on extending the neutron evaluations up to higher energies (e.g. the 150 MeV evaluations produced at Los Alamos [1], and in producing proton evaluations to a similar energy. The motivation for this work has been the need for accurate radiation transport simulations in emerging accelerator-driven technologies, for transmutation radioactive waste [2,3], producing tritium [4] and producing energy, as well as in fast neutron and proton radiotherapy studies [5,6].

Numerous laboratories around the world are interested in an improved nuclear modelling capability for producing evaluated data libraries to higher energies. These include laboratories at: Los Alamos, Livermore, Brookhaven, Petten, Tokai, Kyushu, Obninsk, Minsk, Bologna, Bruyères-le-Chatel, Cadarache, Bratislava, and Uppsala. For these reasons it was decided that the

Nuclear Energy Agency could usefully co-ordinate some of these activities. The present work, concentrating on nuclear models, complements the NEA's Subgroup 13 [7], which has focused on details of intermediate energy evaluated data files.

Prior to the development of the new high energy data libraries [1,2,8,9,10], accelerator driven systems, which involve a proton beam with an energy of approximately 1 GeV incident on a spallation target, were simulated using codes that apply intranuclear cascade models. Neutrons below 20 MeV were transported with a data-driven code such as MCNP [11]. Where it was necessary to simulate the transport and interaction of nucleons with energies higher than 20 MeV, codes such as LAHET [12] were used, which apply semiclassical intranuclear cascade methods to simulate the collision physics. However, the physics assumptions made by the INC models do not hold well below 150 MeV as the quantum nature of the scattering, and specific nuclear properties, become important. It is for this reason that it is advantageous to extend the data libraries to higher energies using nuclear reaction models and codes which best reflect the most appropriate nuclear theory in this energy range. The new high energy data libraries can be utilised within the new MCNPX radiation transport code [13], which merges the essential elements in the LAHET and MCNP codes for ease of use. Other projects to develop high-energy evaluations are also currently underway in Europe [2], Japan [8], and Russia [9].

It is useful to note two other projects which have been closely linked to the present work. Firstly, in recent years the NEA has co-ordinated two international code intercomparisons to test the ability of nuclear modelling codes to predict emission spectra [14], and radionuclide yields [15].These intercomparisons have been very useful for quantitatively assessing various nuclear model's strengths and weaknesses. Secondly, the International Atomic Energy Agency has recently completed a project known as the Reference Input Parameter Library (RIPL), which is a compilation of recommended input parameters for nuclear model calculations [16].

The work described here has focused entirely on codes that are used to model specific details of the nonelastic nuclear reaction and break-up processes. Although very important, we have not included optical model codes within the scope of this work.

2. Subgroup 12 activities

Activities completed by Subgroup 12 are summarised below:

1. Meetings were held during international Nuclear Data for Science and Technology conferences at Gatlinburg (1994) and Trieste (1997), and during the 1997 NEA WPEC meeting at Cadarache.

2. Extensive e-mail discussions took place amongst Subgroup 12 participants.

3. A questionnaire was distributed to all participants, soliciting input regarding participants' experience with various nuclear reaction modelling codes, their strengths and weaknesses, and the participants' views on future priorities for nuclear model improvements.

4. The conclusions reached through various discussions, along with the information contained in the completed questionnaires, was compiled in the present report.

3. Results and guide to tables

The nuclear models and codes studied in this report are listed in Tables 1-4. Tables 1 and 2 summarise the nuclear reaction theories and models that are currently used – Table 1 for the equilibrium decay stage of the reaction, and Table 2 for the preequilibrium stage of the reaction. The notation used in these tables is intended to be self-evident to researchers in nuclear reaction theory.

Table 3 summarises the participants' perception of the strengths and weaknesses of the nuclear reaction models within their codes. This summary information is particularly useful for users who wish to determine which is the most appropriate code for their needs. Thus, for instance, the GNASH code [17,18] requires a somewhat complicated input and requires a long CPU running-time for higher energy calculations, but includes extensive details of nuclear structure properties and can therefore be used for predicting isomer production and discrete gamma-ray cross-sections. ALICE [19], on the other hand, cannot predict this information, but it is very easy to run, requires a short CRU running-time, and predicts emission spectra and radionuclide yields relatively accurately. Another example from Table 3 is the MINGUS code [20] that implements the quantum mechanical Feshbach-Kerman-Koonin [21] preequilibrium theory, for enhanced nucleon preequilibrium predictions, but currently does not include preequilibrium cluster emission.

To date, most nuclear data evaluations that extend the evaluated libraries beyond their original upper energy of 20 MeV have been based upon just a few codes: GNASH [17] (for instance, the new LA150 library [1] and the recent Bruyères-Petten evaluations [2]), and ALICE [19] in its various incarnations (for instance, the Obninsk "MENDL" activation libraries [9] and the JAERI high-energy files [8]. These codes are under constant development, as are other codes that will probably play in important role in the future, such as MINGUS [20], QMDRELP [22], PEGAS [23] and EMPIRE-2 [24].

The use of these codes in intermediate energy nuclear data evaluation work, along with future priorities for improved modelling, are described in Table 4.

4. Conclusions: Future research priorities

This report summarises the current status of nuclear reaction models used within various codes of importance in intermediate energy nuclear data evaluation work.

Some common themes stressed by a number of researches for future work of high priority are:

1. There is a need to include more than two multiple preequilibrium ejectiles when the incident energy exceeds approximately 150 MeV. Many participants felt that the model of Blann *et al*. [25,26] is a useful approach for describing these reactions.

2. There is a need for a physics-based preequilibrium cluster emission model with a high predictive capability.

3. There is a need for improved high-energy fission models.

4. There is a need for improved medium energy optical potentials.

5. There is a need to implement some recent developments in level density models, such as those recommended by the IAEA's RIPL project [16], as well as the formalism of Iljinov *et. al*. [27].

6. The Quantum Molecular Dynamics (QMD) theory has been implemented in a very useful code at JAERI [22]. With the ever-increasing speed of computers, this theory will be useful in the future for evaluation work. Priorities for model development include a need to better calculate ground state masses, and thus Q-values, as well as inclusion of precompound cluster emission.

7. The quantum multistep theory of Feshbach, Kerman, and Koonin (FKK) has proved useful [1] as a tool to test the accuracy of simpler models that require less CPU time (and are thus valuable for evaluation calculations on a fine incident energy grid). Additional work is needed to develop this theory to a stage at which it can be routinely used in evaluation work. Participants of Subgroup 12 have organised a workshop at the European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*), Trento, Italy, 26-31 July 1998, to address some of the open problems in this area.

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Particularly thanks go to C. Dunford and P. Oblozinsky who acted as “monitors” of this subgroup.

TABLES

Table 1. Nuclear models used in equilibrium phase of the reaction

Code contributor	Maximum energy	Equilibrium decay	Level density	Trans. co. (inverse x/s)	γ trans. co. (inverse x/s)	Level info.
GNASH M.B. Chadwick P.G. Young	200 MeV	Hauser-Feshbach	Ignatyuk or GC	From OM (scat or ecis code)	KU or BA or W	ENSDF
ALICE M. Blann	400 MeV	Weisskopf-Ewing	Ignatyuk or KR or FG	From OM or sharp cut-off	BA or W	–
ALICE-IPPE Y. Shubin *et al*.	300 MeV	Weisskopf-Ewing	BFG or Ignatyuk or KR	From OM or sharp cut-off	BA or W	–
ALICE-F T. Fukahori	2000 MeV	Weisskopf-Ewing	BFG or KR or FG	Pearlstein OM or sharp cut-off	BA or W	–
EMPIRE-2 M. Herman	50 MeV	Hauser-Feshbach	Ignatyuk, GC, Iljinov or microscopic	From OM (scat code)	KU or W	ENSDF
MINGUS A. Koning	200 MeV	Hauser-Feshbach & Weis. Ew.	Ignatyuk and GC	From OM (ecis code)	BA	–
PEQAG PEGAS E. Betak, P. Oblozinsky	150 MeV	Master-eq. from the exciton model	Williams (Dobes-Betak corrections) or GC	Inv. x/s Chatterjee or, trans. coeff.	Master-eq. (Akkermans-Gruppelaar)	only in DEGAS code version
QMDRELP K. Niita S. Chiba	5 GeV	Weisskopf-Ewing	FG (a=A/8)	Sharp cut-off	–	–

Key to abbreviations used: GC = Gilbert-Cameron model; OM = Optical model; KU = Kopecky-Uhl model; BA = Brink-Axel model; W = Weisskopf model; KR = Kataria-Ramamurthy model; FG = Fermi-gas model; BFG = Backshifted Fermi-gas model; ENSDF = Evaluated Nuclear Structure Data File.

Table 2. Nuclear models used in preequilibrium phase of the reaction

Code contributor	Preequilibrium decay	Partial lev. dens.	Preeq. clusters	Preeq. γ	Number of multiple preeq.
GNASH M.B. Chadwick P.G. Young	Kalbach's exciton model or FKK	Williams mod. by Oblozinsky	Kalbach model	Akkermans- Gruppelaar	2 particles Chadwick model
ALICE M. Blann	Hybrid, GDH or Monte Carlo (HMS model)	Equidist. model of Blann, or microscopic	–	Yes	2 particles (unlimited number in HMS)
ALICE-IPPE Y. Shubin	Hybrid, GDH	Equidist. model of Blann, or	Obninsk cluster model	–	2 particles
ALICE-F T. Fukahori	Hybrid, GDH	Equidist. model of Blann	Iwamoto- Harada-Sato	–	2 particles
EMPIRE-2 M. Herman	NVWY and TUL	Williams, and RPA response fn.	–	Heidelberg MSC model	1 particle
MINGUS A. Koning	FKK	Williams mod. by Oblozinsky, or microscopic calc.	–	–	2 particles Chadwick model
PEQAG PEGAS E. Betak, P. Oblozinsky	Exciton model (spin conserv. versions available)	Williams mod. by Betak-Dobes	–	Akkermans- Gruppelaar	Yes (?)
QMDRELP K. Niita S. Chiba	Quantum Molecular Dynamics	None	–	–	Unlimited number of particles
Lenske codes E. Ramstrom	TUL	RPA response & microscopic	– –	– –	1 particle

Key to abbreviations used: FKK = Feshbach-Kerman-Koonin model; GDH = Geometry-dependent hybrid model; HMS = Hybrid Monte Carlo Simulation; NVWY = Nishioka-Verbaarschot-Weidenmuller-Yoshida model; TUL = Tamura-Udugawa-Lenske model; RPA = Random Phase Approximation.

Table 3. Participation in intercomparisons: Strengths and weakness

Code contributor	Use in code intercomp.	Some strengths of code	Some weaknesses of code
GNASH M.B. Chadwick P.G. Young	Blann's 1994 Michel's 1996 and others	- fairly good predictive capability - discr. γ s & isomers included - recoils spectra included	- somewhat complicated input - preeq. cluster spec. need improving - tendency to underpredict nucleon spectra in 20-40 MeV range
ALICE M. Blann	Blann's 1994 Michel's 1996	- rel. accurate spectra & x/s - simple input, fast - Monte Carlo option available	- no preeq. clusters - no ejectiles A>4
ALICE-IPPE Y. Shubin	Blann's 1994 Michel's 1996	- rel. accurate spectra & x/s - simple input, fast	- no discrete levels so no isomer calculations - angular mom. not conserved
ALICE-F T. Fukahori	Blann's 1994	- fairly good predictive capability especially for isotope prod.	- calculations at reaction thresholds
EMPIRE-2 M. Herman	NVWY and TUL	- modern quantum preeq. - can calc. isomeric x/s - dynamic deform. effects incl. - fast, flexible, simple	- lack of multiple preequilibrium - lack of cluster preequilibrium - no MSD for charge exchange - no provision for direct reactions
MINGUS A. Koning	Blann's 1994 Michel's 1996	- based on ECIS code - ang. dis. from FKK are accurate - overlap of direct & preeq. contrib. - isotope x/s predicted fairly well	- no preeq. clusters, γ s - no multiple HF (only multiple WE) - only 2 multiple preeq. particles - no fission
PEQAG PEGAS E. Betak, P. Oblozinsky	Blann's 1994 Michel's 1996 (and others available)	- one consistent formalism for the complete reaction - simple to use and fast	- no cluster decay - discrete levels and γ s only in the DEGAS code version - uses global parameters (easy, but this limits accuracy)
QMDRELP K. Niita S. Chiba	Michel's 1996	- simple input - sophisticated reaction theory - universal applicability	- long computer time - energy balance sometimes not exact
Lenske codes E. Ramstrom	–	- sophisticated preequilibrium theory - accurate treatment of collectivity	- no multiple preequilbrium - no equilibrium decay included

Key to abbreviations used: Blann's 1994: "International Code Comparison for Intermediate Energies", M. Blann, H. Gruppelaar, P. Nagel and J. Rodens, NEA/OECD (1994); Michel's 1997: "International Codes and Model Intercomparison for Intermediate Energy Activation Yields", R. Michel and P. Nagel, NEA/OECD document NSC/DOC(97)1 (1997); FKK = Feshbach-Kerman-Koonin model; MSD = Multistep direct; MSC = Multistep compound; WE = Weisskopf-Ewing model; HF Hauser-Feshbach model.

Table 4. Use in evaluations and priority future improvements

Code contributor	Use in evaluations	Priority future improvements
GNASH M.B. Chadwick P.G. Young	LANL 100 MeV 1990 libraries LANL 150 MeV 1997 libraries many ENDF evals. <20 MeV LLNL medical libraries	- generalise multiple preeq. for >2 particles - include Blann's Monte Carlo model as preeq. option - utilise new lev. density models, e.g. Iljinov's - include isospin conservation - use forthcoming Madland optical potential
ALICE M. Blann	LLNL medical libraries Used at other labs for evaluation work	- extension of new Monte Carlo model to include heavy ion and photon projectiles, pion ejectiles, recoil spectra, heavy cluster emission - seek a physics-based preeq. cluster model
ALICE-IPPE Y. Shubin	Activation library MENDL-2 evaluation work	- generalise multiple preeq. for >2 particles - develop high-energy fission model - include gamma-ray preequilbrium
ALICE-F T. Fukahori	JENDL high-energy file JENDL photonuclear file	-improve preeq. competition of cluster preeq. - include multistep Hauser-Feshbach decay - include fission calcs. using Fukahori systematics
M. Herman	LANL update of activation library	- include microscopic p-h level densities for MSC - include Blann's Monte Carlo preeq. model as an option - link to the ECIS code - inclusion of cluster preeq. in MSC
MINGUS A. Koning	ECN/NEA libraries to 200 MeV	- include exciton model as a preeq. option - include multiple Hauser-Feshbach decay - include Kalbach's cluster preeq. model - generalise multiple preeq. for >2 particles - include fission - use of dispersive and deformed optical model
PEQAG PEGAS E. Betak, P. Oblozinsky	–	- inclusion of clusters - studying the exciton structure of discrete states
QMDRELP K. Niita S. Chiba	Not yet, but anticipated in the future	- improvements in effective interaction, Lorentz covariance and Pauli potential - extend upper energy limit further

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