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WORKSHOP ON NUCLEAR MODEL COMPUTER CODES

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REPORT ON THE INTERNATIONAL NUCLEAR MODEL CODE INTERCOMPARISON COUPLED-CHANNEL MODEL STUDY

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Report on the International Nuclear Model Code Intercomparison
Coupled-Channel Model Study

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... our modest doubt is
... d the beacon of the wise ...
W. Shakespeare

The problem specifications are given in the document NEANDC 128 U and concern the calculation of inelastic cross sections and neutron angular distributions for low energy neutrons exciting the lowest levels of U-238.

1. Comparison of different JUPITOR versions

In general the submitted results, calculated with different versions of JUPITOR, are in good agreement with each other.

The results are identified in Table I. by name of contributor.

- (1) M. Uhl and B. Strohmaier, IRK Vienna, Austria used an extension of the Karlsruhe version, which includes angle integrated cross sections and transmission coefficients /3/.

- (2) S. Igarasi, JAERI, Tokai-mura, Japan used a JUPITOR version containing the following modifications over the original code /7/:

  - it calculates the integrated elastic and inelastic scattering cross sections by Weddle's method (seven points Newton-Cotes method)

  - it gives correct values for 0 and 180 degrees of the differential cross sections (correction of the associated Legendre polynomial routine);

  - one important difference in the calculation of the matching radius: in most versions it is given by

    Rm=rA**(1/3) + 10a (energy independent)

    Igarasi takes as the matching radius the point where the potential tail is smaller than 1.0E-4*E (E is the smallest energy of the outgoing particle). Thus the matching radius is

    Rm=rA**(1/3) + 9.2a + a lg(V/E)

    In fact for the n + U-238 problem the matching radius given by the original formula is too small around energies of 1 keV it is 14.1 fm - in Igarasi's formula it is 20.4 fm. The first value would correspond to an energy of about 20 MeV in Igarasi's version. This accounts for an 18% discrepancy of the shape elastic and 4.6% discrepancy of the reaction cross section at 1 keV when compared with the others.

- (3) E. Sartori, NEA-DB Saclay, France used the ENEA-Bologna version adapted to CDC computers. This version provides numerically angle-integrated cross sections (simple trapezoidal method).

- (4) D. G. Madland, LANL Los Alamos, USA has used the in-house T-2 version, which is Tamura's version prior to any modifications other than corrections of known errors /1/,/2/,/9/.

- (5) A. Prince, BNL Brookhaven, USA used two different versions:
  JPX , a version in which the radial step lengths used to solve the coupled equations must be the same: XMES1=XMES2=0.1 fm ; this modification was introduced in order to speed up the calculations /8/.
  (6) JUPITR, a PDP-10 chain version of the original JUPITOR. In this version XMES1=0.0125 fm and XMES2=0.1 fm for a typical calculation /8/.

- R. P. Kesavan Nair, adapted the original IBM version to CDC. No modifications were introduced other than known errors /13/. The results are not shown in the table as they are practically identical to those of Madland and Sartori.

Table I. and the graphs show that the different contributions are in good agreement for energies of 0.5, 1.0, 2.5 MeV both for elastic, reaction and inelastic cross-sections.

For lower energies the results are more discrepant, due to the different choice of the matching radius.

In general a better agreement is observed for the angular distributions than for the integrated values.

An analysis of the integration methods was carried out and the following was observed:

- No integrated values were given for inelastic and shape elastic cross sections in the original version. The different versions achieve the integration in different ways:
  some integrate the angular distributions numerically by trapezoidal rules or the seven point Newton-Cotes method; surprisingly enough no version carries out an analytical integration by using matrix elements.

- some versions integrate only between the two angle boundaries given in the input. In this specific case some gave integrated values from 2 to 178 degrees. This is the case of the NEA-DB version.

Different integration schemata lead to discrepant results.
The integration over a reduced angular range leads for instance to the fact that the partial cross sections do not sum up exactly to the total cross section. In this specific case the missing fraction varies with energy from 0.05 to 0.2 %.
If the integration is carried out over the full angular interval the discrepancies for the integrated elastic and inelastic cross-section reduce approximately to half.

In order to compare the integration methods all the angular distributions provided on magnetic tape were re-integrated by using the same method. A cubic spline function passing through all the values has been constructed and integrated. This method gives an equivalent precision to the seven point Newton-Cotes formula.

When using the same integration schema the discrepancies reduce even further.

It is recommended that a version of JUPITOR is prepared in which the angle integrated values are computed analytically from the matrix elements.

The exercise specification does not give the atomic masses.
In Table I. the results for exact atomic masses are presented.

A. Prince has provided Table V. in which the sensitivity of atomic masses on the results are studied. These results show clearly that exact masses should be used.

The maximum allowed incoming orbital angular momentum was specified as l(max)=5. The comparison of different coupled channel programs may be difficult in circumstances of coupling to 6+ states.
For physical applications more than 6 partial waves should be used at E=1.0 and 2.5 MeV.

Table II. compares the results for different values of l(max).
The cut-off criterion of JUPITOR is determined only by the maximum allowed incoming orbital angular momentum l(max). If it is set too low, JUPITOR can give inaccurate results, if it is set too high computing time increases and a waste of unnecessary terms in the matrices may be considered.
Table II. shows also the results of ECIS-79 for l(max)=20 as reference.
The ECIS-79 cut-off criterion is not only based on l(max) but also on the importance of the different matrix elements: matrix elements smaller than a given amount are disregarded. This criterion makes sure that unnecessary terms are not taken into account /14/.

2. Comparison of JUPITOR, CCROT/VIB, ECIS-79

The results of the angle-integrated cross sections for JUPITOR, CCROT/VIB and ECIS-79 are shown in Table III.

- The JUPITOR results of M. Uhl and B. Strohmaier are taken as reference values from Table I. /6/.
- CCROT/VIB is a coupled channel program developed at F.E.I. Obninsk, USSR /10/.
- ECIS-79 was developed by Jacques Raynal, CEN Saclay, France /12/, /14/.

Both CCROT/VIB and ECIS-79 compute angle integrated cross-sections analytically from the matrix elements.
Jacques Raynal has provided two solutions: in the first one the program was modified in order to simulate the JUPITOR cut-off criterion and thus make a consistent comparison possible. In the second solution the unmodified code was used with l(max)=20.
Results of CCROT/VIB were provided for two energies; l(max) was set to 4 which is adequate for the two considered energies.
A good agreement can be observed between these codes.

3. Comparison of JUPITOR with ADAPE

This comparison had to be made separatly because integer masses were used.
In Table IV. two JUPITOR results are shown:

- those of the NEA DB JUPITOR version written for a CDC computer
- and those of the JUPITOR version of BARC, India written for a DEC-10 computer. This version does not provide angle integrated elastic and inelastic cross-sections /5/.
- The table shows also the results of ADAPE written for a BESM-6 computer /4/.

The results of JUPITOR and ADAPE differ in that for JUPITOR the non-adiabatic coupled channel model was used while for ADAPE the adiabatic model.
The adiabatic approximation is generally used when the incident energy of the projectile is much higher than the excitation energies of the rotational states. Thus the cross sections calculated at lower energies by making use of this approximation should be less accurate. ADAPE adopts the same radius and diffuseness parameters for the spin orbit potential as given for the real Saxon-Woods potential.
When comparing the angular distributions calculated with JUPITOR and ADAPE increasing deviations are observed for increasing scattering angles /5/.

4. Results of the program CHUCK

The coupled-channel program CHUCK was developed by P. D. Kunz, University of Colorado, USA.
Two solutions derived from two different version were provided. When comparing these results discrepancies were observed which were apparently due to a different interpretation of l(max) (maximum allowed incoming angular momentum or number of partial waves).
These results could not be compared with those of the other coupled channel codes because the channel couplings used did not conform with the problem specification.
The correct coupling was tried out at the NEA DB, but both available versions allow a maximum number of eight coupling equations. While this is an adequate number for low energies it is not sufficient for energies of 1.0 and 2.5 MeV. These results have therefor been omitted from this report.

5. Conclusion

The different coupled-channel programs studied in this comparison exercise show good agreement in the angular distributions for those cases where the same model was used. The discrepancies in the angle-integrated values are due to different integration methods. The use of analytical integrations is recommended.

6. Aknowledgments

The credit of this study goes to the participants, who in addition to generously offering their precious time have also provided many essential suggestions and comments.

7. References

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Figure Captions

JM LANL version of JUPITOR

JI JAERI version of JUPITOR

CCJ NEADB version of JUPITOR

T a b l e I.

Comparison of angle-integrated cross sections computed with different versions of JUPITOR for U-238

Sigma Total (mbarn)

Energy (MeV)	Uhl (1)	Igarasi (2)	Sartori (3)	Madland (4)	Prince-1 (5)	Prince-2 (6)
.001	22794.2	21410.4	22822.1	22822.1	22655.8	22821.2
.01	14622.9	14576.7	14637.6	14637.7	14516.3	14623.3
.1	11112.1	11115.6	11120.0	11119.7	11069.1	11116.7
.5	8710.5	8710.53	8712.93	8711.59	8711.83	8712.03
1.	7002.04	7000.63	7001.58	7000.93	7011.10	7001.24
2.5	7280.36	7279.37	7278.89	7279.69	7273.60	7278.56

Sigma Reaction (mbarn)

Energy (MeV)	Uhl (1)	Igarasi (2)	Sartori (3)	Madland (4)	Prince-1 (5)	Prince-2 (6)
.001	11983.4	12532.2	12001.5	12001.5	11928.0	12016.0
.01	4158.87	4160.48	4164.42	4164.5	4131.00	4164.38
.1	2348.99	2351.99	2350.27	2349.73	2349.11	2352.44
.5	3317.09	3317.85	3316.51	3315.28	3330.90	3318.90
1.	3352.06	3350.75	3349.47	3348.7	3365.97	3351.31
2.5	3727.72	3726.47	3726.22	3725.95	3733.35	3726.67

Sigma (n,n) 0+ Shape-elastic (mbarn)

Energy (MeV)	Uhl (1)	Igarasi (2)	Sartori (3)	Madland (4)	Prince-1 (5)	Prince-2 (6)
.001	10810.8	8878.21	10814.0	10813.9	10727.8	10805.2
.01	10464.1	10416.2	10467.0	10466.7	10385.2	10458.9
.1	8763.16	8763.62	8764.2	8764.2	8719.95	8764.22
.5	5393.41	5392.69	5391.4	5390.3	5380.93	5393.14
1.	3649.98	3649.89	3646.8	3645.3	3646.13	3649.93
2.5	3552.64	3552.88	3540.4	3536.2	3540.25	3551.89

Sigma (n,n') 2+ (mbarn) 0.044 MeV

Energy (MeV)	Uhl (1)	Igarasi (2)	Sartori (3)	Madland (4)	Prince-1 (5)	Prince-2 (6)
.1	36.8251	36.7991	36.884	36.812	36.9862	36.8806
.5	268.746	268.838	268.55	268.49	269.932	268.773
1.	352.348	352.386	351.94	351.89	354.510	352.222
2.5	466.887	466.608	466.44	466.44	467.151	466.499

Sigma (n,n') 4+ (mbarn) 0.148 MeV

Energy (MeV)	Uhl (1)	Igarasi (2)	Sartori (3)	Madland (4)	Prince-1 (5)	Prince-2 (6)
.5	3.56444	3.57505	3.5408	3.5404	3.64621	3.57404
1.	25.7775	25.7942	25.62	25.623	26.3009	25.7749
2.5	86.6879	86.6264	86.455	86.474	87.2484	86.5790

Sigma (n,n') 6+ (mbarn) 0.308 MeV

Energy (MeV)	Uhl (1)	Igarasi (2)	Sartori (3)	Madland (4)	Prince-1 (5)	Prince-2 (6)
.5	.01363	.01363	.01358	.01358	.013624	.013648
1.	1.76725	1.76942	1.761	1.7615	1.76410	1.77032
2.5	19.0185	19.0541	18.988	18.986	19.1340	19.0644

T a b l e II.

Comparison of angle-integrated cross sections computed with JUPITOR for l(max)= 5, 6, 7, 10 and with ECIS-79 l(max)=20

Sigma Total (mbarn)

Energy (MeV)	JUPITOR lmax=5	JUPITOR lmax=7	JUPITOR lmax=8	ECIS-79 lmax=20
1.	7001.58	7071.92	7256.02	7251.68
2.5	7278.89	7449.57	7525.17	7390.99

Sigma Reaction (mbarn)

Energy (MeV)	JUPITOR lmax=5	JUPITOR lmax=7	JUPITOR lmax=8	ECIS-79 lmax=20
1.	3349.47	3422.46	3440.83	3438.91
2.5	3726.22	3781.70	3787.27	3813.90

Sigma (n,n) 0+ Shape-elastic (mbarn)

Energy (MeV)	JUPITOR lmax=5	JUPITOR lmax=7	JUPITOR lmax=8	ECIS-79 lmax=20
1.	3646.8	3649.46	3809.5	3812.77
2.5	3540.4	3667.84	3724.6	3577.09

Sigma (n,n') 2+ (mbarn) 0.044 MeV

Energy (MeV)	JUPITOR lmax=5	JUPITOR lmax=7	JUPITOR lmax=8	ECIS-79 lmax=20
1.	351.94	344.552	354.77	354.869
2.5	466.44	427.906	451.92	418.102

Sigma (n,n') 4+ (mbarn) 0.148 MeV

Energy (MeV)	JUPITOR lmax=5	JUPITOR lmax=7	JUPITOR lmax=8	ECIS-79 lmax=20
1.	25.620	26.5065	25.645	25.4330
2.5	86.455	76.7826	76.474	72.9508

Sigma (n,n') 6+ (mbarn) 0.308 MeV

Energy (MeV)	JUPITOR lmax=5	JUPITOR lmax=7	JUPITOR lmax=8	ECIS-79 lmax=20
1.	1.7610	1.82225	2.2047	2.25810
2.5	18.988	19.8645	19.445	18.8024

Table III.

Comparison of angle-integrated cross sections computed with JUPITOR, ECIS-79, CCROT/CCVIB

Sigma Total (mbarn)

Energy (MeV)	JUPITOR Uhl	CCROT/VIB Manokhin	ECIS-79 Raynal-1	ECIS-79 Raynal-2
.001	22794.2	22781.5	22803.3	22803.3
.01	14622.9		14618.9	14605.3
.1	11112.1	11115.2	11117.2	11117.1
.5	8710.5		8711.72	8905.56
1.	7002.04		7001.03	7251.68
2.5	7280.36		7278.70	7390.99

Sigma Reaction (mbarn)

Energy (MeV)	JUPITOR Uhl	CCROT/VIB Manokhin	ECIS-79 Raynal-1	ECIS-79 Raynal-2
.001	11983.4	11984.1	12007.9	12007.9
.01	4158.87		4161.67	4156.34
.1	2348.99	2348.14	2352.37	2352.36
.5	3317.09		3318.37	3412.77
1.	3352.06		3350.95	3438.91
2.5	3727.72		3726.51	3813.90

Sigma (n,n) 0+ Shape-elastic (mbarn)

Energy (MeV)	JUPITOR Uhl	CCROT/VIB Manokhin	ECIS-79 Raynal-1	ECIS-79 Raynal-2
.001	10810.8	10797.5	10795.5	10795.5
.01	10464.1		10457.2	10449.0
.1	8763.16	8767.04	8764.78	8764.73
.5	5393.41		5393.34	5492.79
1.	3649.98		3650.08	3812.77
2.5	3552.64		3552.19	3577.09

Sigma (n,n') 2+ (mbarn) 0.044 MeV

Energy (MeV)	JUPITOR Uhl	CCROT/VIB Manokhin	ECIS-79 Raynal-1	ECIS-79 Raynal-2
.1	36.8251	36.8080	36.8457	36.8455
.5	268.746		268.840	263.811
1.	352.348		352.351	354.869
2.5	466.887		466.600	418.102

Sigma (n,n') 4+ (mbarn) 0.148 MeV

Energy (MeV)	JUPITOR Uhl	CCROT/VIB Manokhin	ECIS-79 Raynal-1	ECIS-79 Raynal-2
.5	3.56444		3.56989	3.87435
1.	25.7775		25.7625	25.4330
2.5	86.6879		86.5809	72.9508

Sigma (n,n') 6+ (mbarn) 0.308 MeV

Energy (MeV)	JUPITOR Uhl	CCROT/VIB Manokhin	ECIS-79 Raynal-1	ECIS-79 Raynal-2
.5	.01363		.013610	.015770
1.	1.76725		1.76785	2.25810
2.5	19.0185		19.0384	18.8024

Table IV

Comparison of angle integrated cross sections computed with the codes JUPITOR and ADAPE using integer masses.

Sigma Total (mbarn)

Energy (MeV)	JUPITOR NEA DB	JUPITOR BARC	ADAPE BARC
.001	23976.5	23976.5	
.01	15228.6	15228.8	15899.7
.1	11420.8	11420.8	12511.4
.5	8760.94	8759.85	8708.66
1.	6972.00	6971.57	7028.62
2.5	7253.04	7253.92	7441.70

Sigma Reaction (mbarn)

Energy (MeV)	JUPITOR NEA DB	JUPITOR BARC	ADAPE BARC
.001	12788.8	12788.9	
.01	4415.56	4415.74	5238.56
.1	2405.91	2405.74	3649.24
.5	3274.34	3273.31	3299.25
1.	3240.66	3239.96	3330.55
2.5	3654.64	3654.36	3685.36

Sigma (n,n) 0+ Shape-elastic (mbarn)

Energy (MeV)	JUPITOR NEA DB	JUPITOR BARC	ADAPE BARC
.01	10806.		10661.2
.1	9009.1		8862.20
.5	5481.4		5409.41
1.	3726.0		3698.07
2.5	3586.2		3756.34

Sigma (n,n) 2+ (mbarn) 0.044 MeV

Energy (MeV)	JUPITOR NEA DB	JUPITOR BARC	ADAPE BARC
.1	37.682		61.665
.5	261.28		241.59
1.	338.89		306.55
2.5	456.80		408.69

Sigma (n,n) 4+ (mbarn) 0.148 MeV

Energy (MeV)	JUPITOR NEA DB	JUPITOR BARC	ADAPE BARC
.5	2.8763		8.194
1.	21.038		35.778
2.5	79.857		70.179

Sigma (n,n) 6+ (mbarn) 0.308 MeV

Energy (MeV)	JUPITOR NEA DB	JUPITOR BARC	ADAPE BARC
.5	0.01270		0.81
1.	1.6211		1.793
2.5	18.575		16.83

σ_{ToT} (mb)

(MeV)	Case (1)	Case (2)	Case (3)	Case (4)	Case (5)	Case (6)
0.001	22653.3	22654.5	22645.4	23750.6	22655.8	22821.21
0.01	14508.6	14509.2	14511.5	15076.2	14516.3	14623.25
0.10	11068.5	11068.8	11072.9	11363.8	11069.1	11116.66
0.50	8711.69	8711.74	8712.81	8758.77	8711.83	8712.031
1.0	7011.05	7010.99	7011.39	6979.10	7011.10	7001.242
2.5	7273.35	7273.33	7274.09	7247.06	7273.6	7278.561
			σ_{REAC}(mb)			
0.001	11926.6	11927.3	11910.2	12657.7	11928.0	12016.02
0.01	4125.95	4126.17	4120.46	4353.36	4131.0	4164.38
0.10	2349.28	2349.29	2346.58	2397.68	2349.11	2352.44
0.50	3331.20	3331.12	3328.03	3283.61	3330.90	3318.895
1.0	3366.25	3366.11	3363.71	3254.13	3365.97	3351.310
2.5	3733.41	3733.34	3732.77	3662.65	3733.35	3726.671
			σ_{el} (mb)			
0.001	10726.8	10727.2	10735.2	11092.9	10727.8	10805.19
0.01	10382.6	10383.0	10391.0	10722.8	10385.23	10458.87
0.1	8719.25	8719.50	8726.34	8966.14	8719.95	8764.22
0.5	5380.49	5380.62	5384.78	5475.17	5380.93	5393.136
1.0	3644.80	3644.88	3647.68	3724.98	3645.13	3649.932
2.5	3539.94	3539.99	3541.32	3584.40	3540.25	3551.89

$\sigma(2+)$ 0.044MeV

(MeV)	Case (1)	Case (2)	Case (3)	Case (4)	Case (5)	Case (6)
0.001	0.0	0.0	0.0	0.0	0.0	0.0
0.01	0.0	0.0	0.0	0.0	0.0	0.0
0.1	36.9811	36.9814	37.0221	37.6790	36.9862	36.8806
0.5	269.954	269.947	269.656	262.686	269.932	268.773
1.0	354.541	354.525	354.069	341.289	354.510	352.222
2.5	467.147	467.137	467.226	457.793	467.151	466.499
			$\sigma_{nn}(4+)$ 0.148 MeV			
0.001	0.0	0.0	0.0	0.0	0.0	0.0
0.01	0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.0	0.0	0.0	0.0	0.0	0.0
0.5	3.64992	3.64893	3.61174	2.95654	3.64621	3.57404
1.0	26.3180	26.3116	26.1260	21.5896	26.3009	25.7749
2.5	87.2586	87.2514	87.1222	80.6964	87.2484	86.5790
			$\sigma_{nn}(6+)$ 0.308 MeV			
0.001	0.0	0.0	0.0	0.0	0.0	0.0
0.01	0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.0	0.0	0.0	0.0	0.0	0.0
0.5	0.01363	0.01363	0.01359	0.01274	0.013624	0.0136483
1.0	1.76470	1.76457	1.75786	1.62647	1.76410	1.77032
2.5	19.1372	19.1366	19.0728	18.6889	19.1340	19.0644

Case (1) M_n = 1.00867, R_m = 20.4fm

Case (2) M_n = 1.00866, R_m = 20.4fm

Case (3) M_n = 1.00866, R_m = 14.0fm

Case (4) M_n = 1.0, M_{238} = 238.0, R_m = 20.4fm

Case (5) M_n = 1.00866, R_m = 16.0fm } JPX

Case (6) M_n = 1.00866, R_m = 16.0fm } JUPITR

Fig.1 Shape elastic cross section at 2.5 MeV

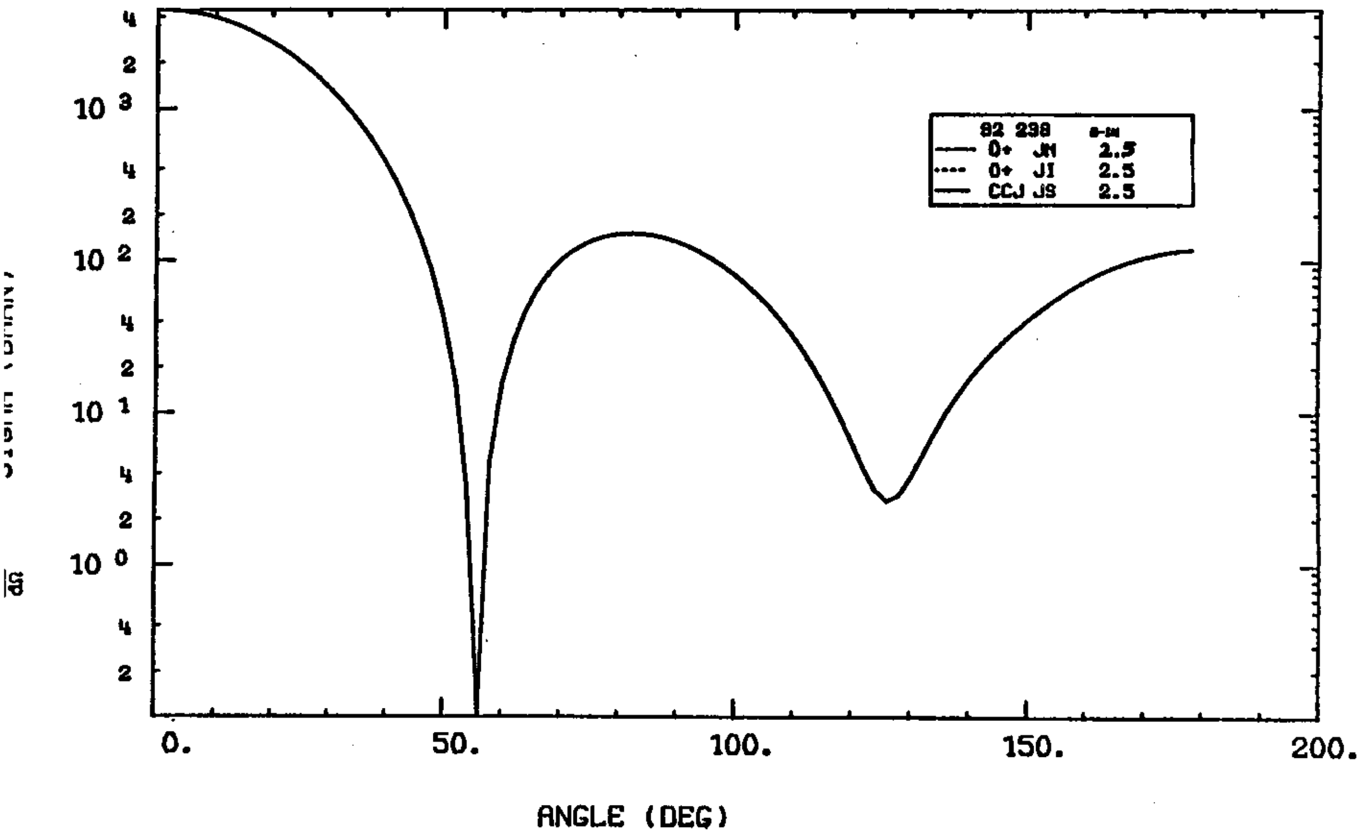


Fig. 2 2+ inelastic cross section at 2.5 MeV

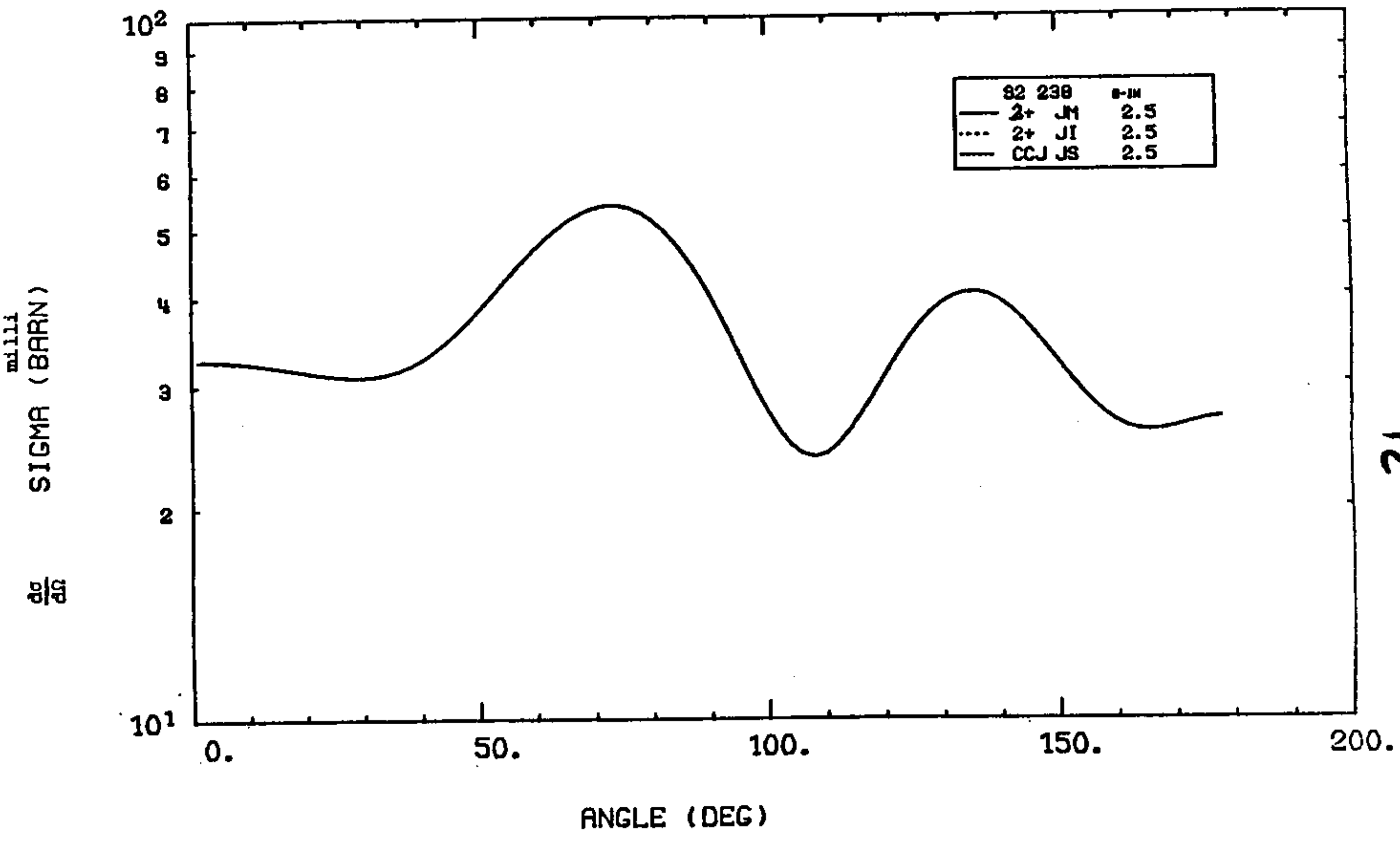


Fig. 3 Shape elastic cross section at 1.0 MeV

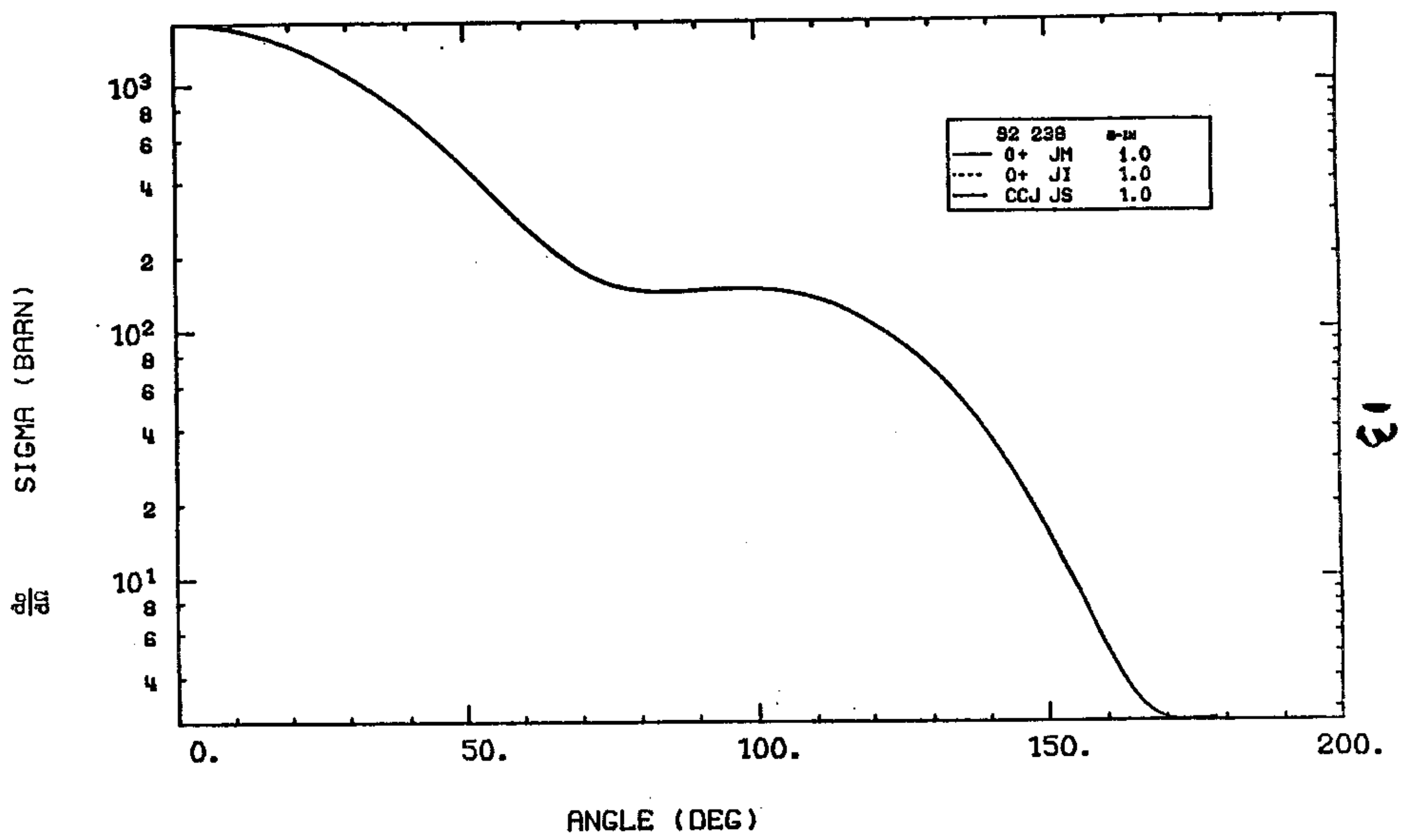
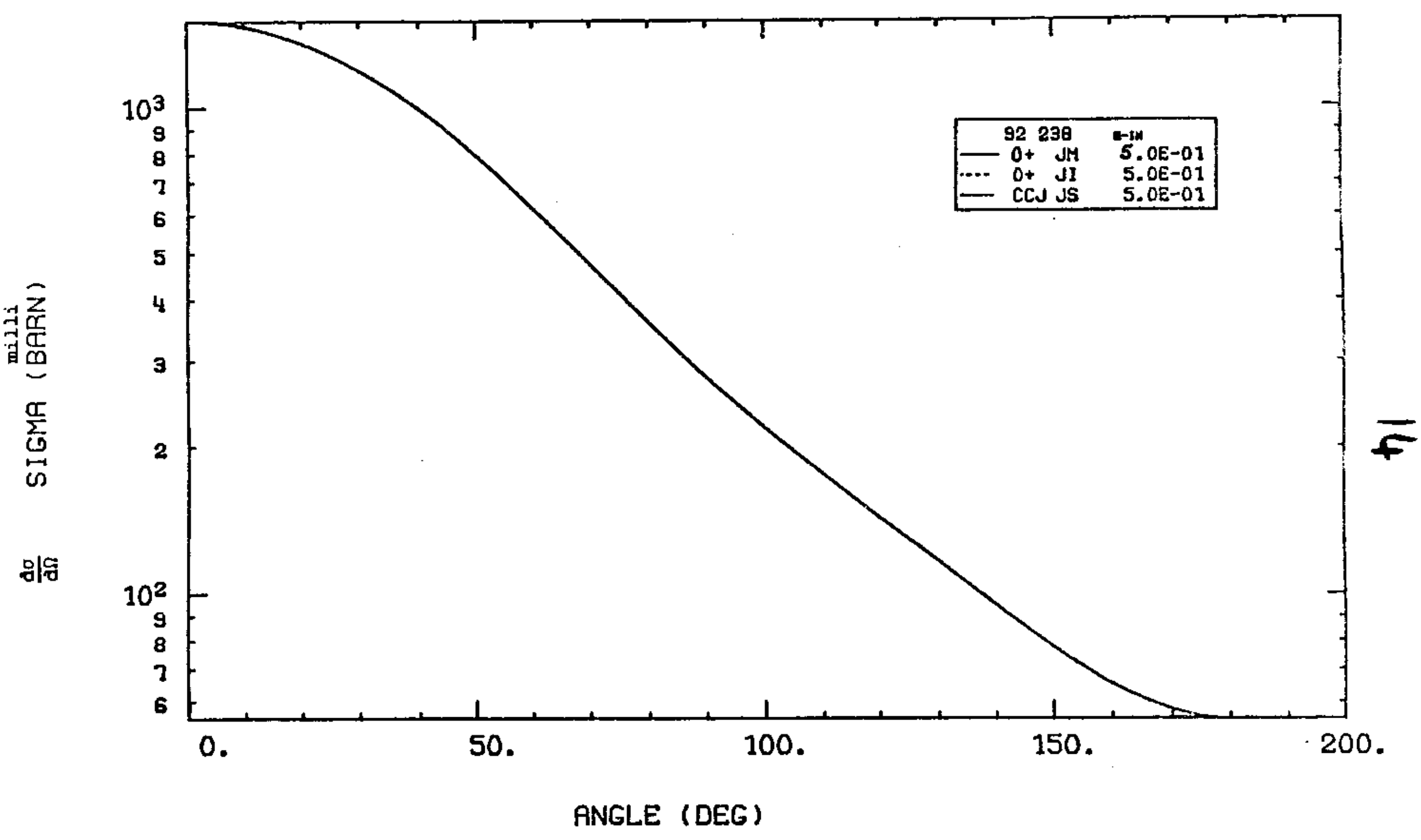


Fig. 4 Shape elastic cross section at 0.5 MeV



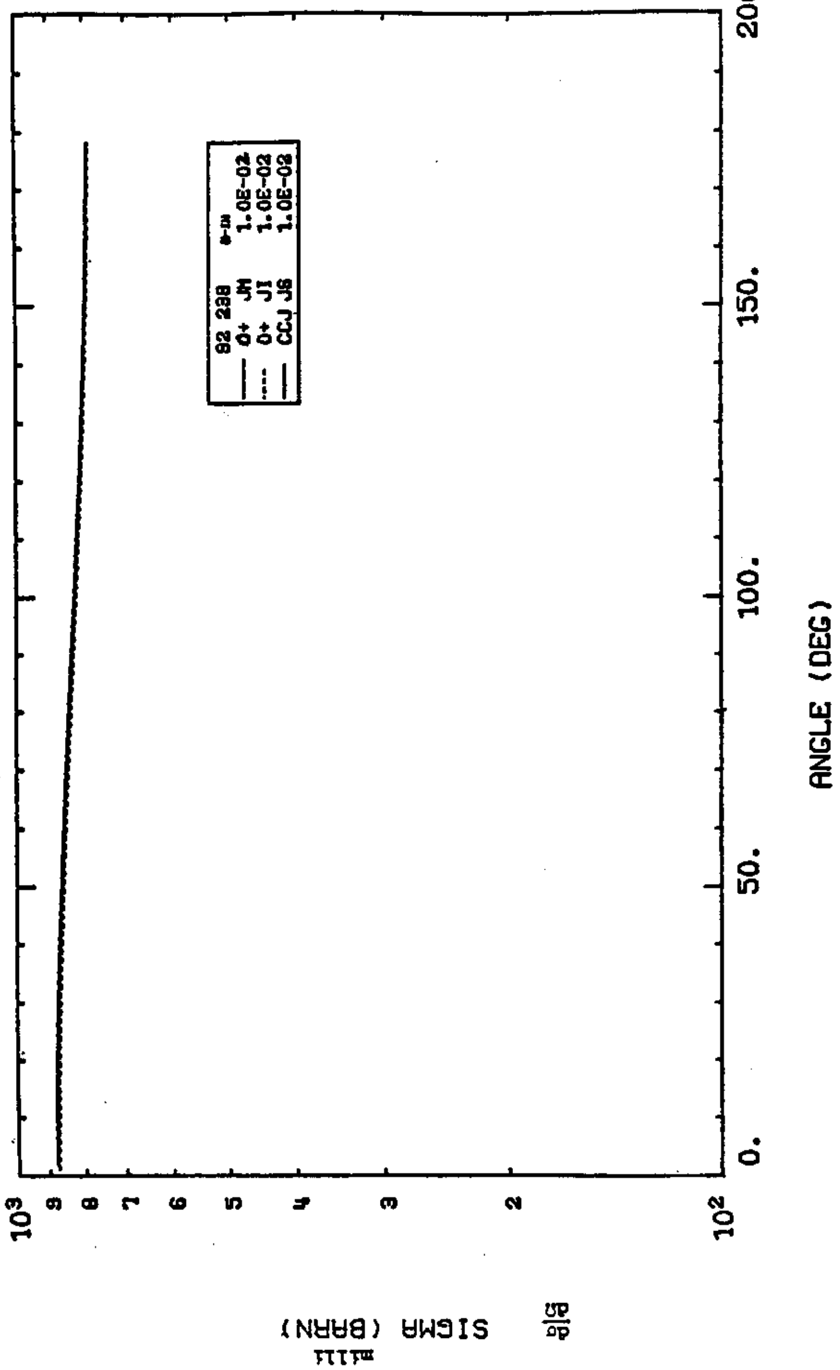


Fig. 5 Shape elastic cross section at 10 keV

INTERNATIONAL NUCLEAR MODEL CODES COMPARISON STUDY

1. Comparison for:

   Coupled channel calculations

   Name of code: ....

2. Physical process:

   n + U-238

   with U-238 states: 0^+(ground st.),2^+(0.044),4^+(0.148),6^+(0.308) energy levels (MeV) and with neutron energies E_n = 0.001,0.01,0.1,0.5,1.0 and 2.5 MeV.

3. Quantities to be compared:

   a. Total cross section.
   b. Integrated cross section for $0^+,2^+,4^+,6^+$.
   c. Reaction cross section
   d. Angular distribution for $0^+,2^+,4^+,6^+$ (from 2^o to 178^o in steps of 2^o).
   e. Scattering coefficients (C-matrix) for each partial wave.
   f. Transmission coefficients (if possible).

4. Model specification:

   Non-adiabatic coupled channel (relevant for JUPITOR).
   Including reorientation (self-coupling).
   Rotational model of deformed target nucleus.
   Woods-Saxon interaction with spin-orbit (optical model).

5. Numerical method:

   Legendre polynomial expansion of the coupled potential (to λ = 4).
   Complex radial form factors.
   Deformation for both real and imaginary potential (neglect it for spin-orbit).

6. Numerical parameters:

   First mesh size: 0.0125 F (relevant for JUPITOR).
   Second mesh size: 0.100 F.
   Matching radius: normally automatically chosen by code (~16 F).
   Number of partial waves: 6

7. Model parameters:

V_R = 46.2 - 0.3 E (Lab) r_r = 1.26 F a_r = 0.63 F

W_S = 3.6 + 0.4 E (Lab) r_i = 1.26 F a_i = 0.52 F

V_{SL} = 6.2 r_s = 1.12 F a_s = 0.47 F

(E in MeV)

$\beta_2 = 0.198,\ \beta_4 = 0.057$

parameters are defined by:

$$V(r) = -V_R f_r - i4a_i W_S \left(-\frac{df_i}{dr}\right) - \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{V_{SL}}{r}\left[-\frac{d}{dr} f_s\right] \vec{\ell}\cdot\vec{\sigma}$$

where

$$f_x = \left[1 + \exp\left(\frac{r-R_x}{a_x}\right)\right]^{-1} \text{ and } R_x = r_x A^{1/3}\left(1 + \sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta)\right)$$

8. Cases to run:

for E_n = 0.001,0.01 and 0.1 MeV include only the 0^+ and 2^+ states
for E_n = 0.5,1.0 and 2.5 MeV include $0^+,2^+,4^+,6^+$

9. Resources:

Computer:

Optimization during compilation:

CPU time needed for the calculation:

10. Comments: