Engineering Physics and Mathematics Division

**CALCULATED CROSS SECTIONS FOR
NEUTRON INDUCED REACTIONS ON ^{19}F
AND UNCERTAINTIES OF PARAMETERS**

Z. X. Zhao*, C. Y. Fu, and D. C. Larson

*Chinese Nuclear Data Center, Institute
of Atomic Energy, Beijing, P.R. China

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ABSTRACT

Nuclear model codes were used to calculate cross sections for neutron-induced reactions on ^{19}F for incident energies from 2 to 20 MeV. The model parameters in the codes were adjusted to best reproduce experimental data and are given in this report. The calculated results are compared to measured data and the evaluated values of ENDF/B-V. The covariance matrix for several of the most sensitive model parameters is given based on the scatter of measured data around the theoretical curves and the long-range correlation error of measured data. The results of these calculations form the basis for the new ENDF/B-VI fluorine evaluation.

1. INTRODUCTION

Fluorine is an important material for fusion reactor applications. The use of nuclear models for consistent calculation of neutron and gamma-ray production play an important role in modern evaluation because model calculations can predict the cross sections for reactions and energy regions where no measured data are available, and ensure energy balance.

Guided by measured data, we have performed a comprehensive set of nuclear model calculations for the cross sections, the angular distributions of secondary neutrons and the spectra of all emitted particles and gamma rays for neutron induced reactions on ^{19}F for incident energies from 2 to 20 MeV.

Several nuclear model codes were employed in these calculations. The optical model code GENOA (PE67) was used to determine the optical model parameters. The Distorted Wave Born Approximation code DWUCK (KU72) was used to calculate cross sections and angular distributions of direct-interaction contributions needed as input for the Hauser-Feshbach and pre-compound code TNG (FU88,SH86). The TNG code provided cross sections for the reactions and energy and angular distributions of emitted particles.

The procedures to adjust parameters are discussed in Chapter 2. Chapter 3 includes the model parameters used in these calculations. The calculated results compared to measured data and evaluated values of ENDF/B-V are given in Chapter 4. In Chapter 5, a simple method to estimate the covariance matrix of model parameters and the results for the $n + ^{19}\text{F}$ calculations are given. A short summary is given in Chapter 6.

2. PROCEDURES TO ADJUST PARAMETERS

The calculation included the following reactions: $^{19}\text{F}(n, n'\gamma)^{19}\text{F}$, $^{19}\text{F}(n, 2n)^{18}\text{F}$, $^{19}\text{F}(n, np)^{18}\text{O}$, $^{19}\text{F}(n, n\alpha)^{15}\text{N}$, $^{19}\text{F}(n, p)^{19}\text{O}$, $^{19}\text{F}(n, pn)^{18}\text{O}$, $^{19}\text{F}(n, \alpha)^{16}\text{N}$ and $^{19}\text{F}(n, \alpha n)^{15}\text{N}$. The Q -values of the reactions above are given in Table 1, together with those of the (n, d) and (n, t) reactions.

Table 1. Reaction Q -values

Reaction	Q -values (MeV)
$^{19}\text{F}(n, 2n)^{18}\text{F}$	-10.431
$^{19}\text{F}(n, p)^{19}\text{O}$	-4.036
$^{19}\text{F}(n, d)^{18}\text{O}$	-5.768
$^{19}\text{F}(n, t)^{17}\text{O}$	-7.557
$^{19}\text{F}(n, \alpha)^{16}\text{N}$	-1.523
$^{19}\text{F}(n, np)^{18}\text{O}$	-7.993
$^{19}\text{F}(n, n\alpha)^{15}\text{N}$	-4.013

Much effort was spent on adjusting parameters so that a good simultaneous fit to measured data could be obtained.

To insure consistency of the calculation, a set of Optical Model Parameters (OMP) was obtained through an iteration process. Firstly, using a set of OMP from LA80 as input to DWUCK, the cross sections of the direct interaction were obtained. Then, using the same OMP and the output of DWUCK as input to TNG, the compound elastic scattering cross sections were calculated after adjusting level density parameters to fit most measured reaction data. The level density parameters for ^{19}F , ^{19}O and ^{16}N were adjusted to fit the measured cross sections of (n, n') , (n, p) , (n, α) and $(n, 2n)$ reactions. Finally, with compound elastic scattering cross sections given by TNG, and measured elastic angular distributions, GENOA was used to obtain a new set of OMP as input to DWUCK to begin the next iteration. For angular distributions of elastic scattering from ^{19}F , the measured data at low incident energies of WI58, BI58 and RO61 can not be used to determine the OMP because for these data the contributions from inelastic scattering of the first and second excited levels are very large. Therefore, only angular distributions of BA85 and CL70 at 14 MeV were used to determine OMP. To reduce the number of iterations, we mainly adjusted the depth of the spin-orbit potential in GENOA because the calculations using TNG and DWUCK results were insensitive to this parameter.

3. MODEL PARAMETERS USED

3.1 OPTICAL MODEL PARAMETERS

The optical model potential is defined by

$$V(r) = V_c - V \cdot f_v(r) - i[W \cdot f_w(r) + 4aW_D \frac{d}{dr} f_D(r)] + \left(\frac{h}{m_\pi C}\right)^2 U (\sigma \cdot \ell) \frac{1}{r} \frac{d}{dr} f_u(r) \quad (1)$$

where V_c is the Coulomb potential. The form factor $f_x(r)$ is of the usual Woods-Saxon type with radius $R_x \cdot A^{1/3}$ and diffuseness a_x . m_π is the pion mass. The depths of real well and imaginary surface potential were expressed as

$$V = V_0 + V_1 E_n$$

$$W_D = W_0 + W_1 E_n$$

where E_n is in MeV.

3.1.1 Neutron Optical Model Parameters

The parameters for $n + {}^{19}\text{F}$ were taken from LA80 and adjusted to fit measured angular distribution and cross sections as described in Section 2. For $n + {}^{18}\text{O}$, only the parameters of GR80 from the analysis of the ${}^{18}\text{O}(n, n)$ data are available. Not many parameters are available for $n + {}^{18}\text{F}$ and $n + {}^{15}\text{N}$. The parameters of $n + {}^{18}\text{F}$ were taken as those for $n + {}^{19}\text{F}$. The parameters of $n + {}^{15}\text{N}$ were taken as those of $p + {}^{15}\text{N}$ of FA80. All neutron OMP used in this analysis are given in Table 2.

3.1.2 Charged Particle Optical Model Parameters

The proton OMP for ${}^{19}\text{O}$ obtained from analyzing the data of ${}^{18}\text{O}(d, p){}^{19}\text{O}$ (SE74) were used in this work. The parameters of Fabrici (FA80) for $p + {}^{18}\text{O}$ obtained through analyzing the inelastic scattering angular distribution of ${}^{18}\text{O}(p, p'){}^{18}\text{O}$ were also used in this calculation. The alpha OMP for ${}^{15}\text{N}$ and ${}^{16}\text{N}$ were taken from OE72. All of the charged particle OMP are shown in Table 3.

3.2 LEVEL DENSITY PARAMETERS

The Gilbert-Cameron composite level density formulae as described by Fu (FU76) were used in TNG. The initial level density parameters were obtained based on the information of discrete levels compiled by Ajzenberg-Selove (AJ86, AJ86a,

4 MODEL PARAMETERS USED

AJ87). To fit the measured cross sections for (n, n') , (n, p) , (n, α) and $(n, 2n)$ reactions, the level density parameters for ^{19}F , ^{19}O and ^{16}N were adjusted. The cross sections for tertiary reactions are insensitive to level density parameters of the residual nuclei because the main contributions to the cross sections for these reactions come from discrete levels. The level density parameters used in the calculation are given in Table 4.

Table 2. Neutron optical model parameters

	$n + ^{19}\text{F}$	$n + ^{18}\text{F}$	$n + ^{18}\text{O}$	$n + ^{15}\text{N}$
V_0 , MeV	45.8	46.8	55.7	60.4
V_1	-0.32	-0.32	-0.52	-0.26
W , MeV	0	0	0	0.06E
W_0 , MeV	6.2	6.2	3.3	0.6
W_1	0	0	0.1	0.15
U , MeV	6.3	0	0	0
R_v , fm	1.263	1.263	1.0	1.08
a_v , fm	0.695	0.695	0.645	0.662
R_w , fm				1.46
a_w , fm				0.55
R_D , fm	1.3	1.30	1.28	1.46
a_D , fm	0.481	0.481	0.588	0.55
R_u , fm	1.263			
a_u , fm	0.695			

Table 3. Charged particle optical model parameters

	$p + ^{19}\text{O}$	$p + ^{18}\text{O}$	$\alpha + ^{16}\text{N}$	$\alpha + ^{15}\text{N}$
V_0 , MeV	54.21	46.8	183	183
V_1	-0.32	-0.32	0	0
W , MeV	0	0	10.0	10.0
W_0 , MeV	11.48	6.13	0	0
W_1	-0.25	0	0	0
R_v , fm	1.1	1.10	1.50	1.50
a_v , fm	0.76	0.70	0.57	0.57
R_w , fm			1.50	1.50
a_w , fm			0.60	0.60
R_d , fm	1.36	1.30		
a_d , fm	0.68	0.67		
R_c , fm	1.25	1.21	1.17	1.15

Table 4. Level density parameters
Spin cut-off factor: $C = 0.0888 \times a \times A^{2/3}$

Residual Nuclei	T (MeV)	E_0 (MeV)	a (MeV)	Δ (MeV)	E_c (MeV)	E_x (MeV)
^{19}F	2.06	-0.38	4.00	2.52	5.60	8.00
^{18}F	2.21	-1.38	3.11	0	4.70	4.70
^{19}O	2.00	-0.36	4.00	2.52	3.95	6.00
^{18}O	2.288	0.82	5.00	5.19	6.70	8.00
^{16}N	3.05	2.06	2.04	2.84	8.80	14.00
^{15}N	6.50	-1.01	3.68	0	5.26	8.00

T = nuclear temperature

E_0 = parameter for matching lower energy level density to the higher one.

$a = \pi^2 g/6$ (g = density of uniformly spaced single particle state).

Δ = pairing energy correction.

E_c = continuum cutoff.

E_x = tangency point.

3.3 LEVEL INFORMATION AND BRANCHING RATIOS FOR GAMMA-RAY DECAY

The energy, J^π of the discrete levels and the branching ratios of the gamma-ray decays from the excited levels of the residual nuclei were taken from the compilation of Ajzenberg-Selove (AJ86, AJ86a and AJ87) and are given in Tables 5 to 10.

3.4 DEFORMATION PARAMETERS

The Distorted Wave Born Approximation (DWBA) program DWUCK (KU72) was used to calculate the direct-interaction component of the inelastic scattering cross sections and angular distributions of a number of levels for which deformation parameters were available. Inputs to DWUCK were the neutron optical model parameters in Table 1 and the deformation parameters. There are two sets of deformation parameters (KR73, SW74). Between these two sets, a large discrepancy systematically exists (see Table 11). Krick's parameters (KR73) obtained by analyzing the inelastic scattering of alpha-particles were used in this calculation because good agreement with measured cross sections was obtained. The calculated direct-interaction cross sections of the discrete levels are shown in Fig. 1.

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Table 5. Energy levels and gamma-ray branching ratios for ^{19}F

Initial state			Branching ratios to state N								
N	J^π	E (keV)	1	2	3	4	5	6	7	9	10
1	$1/2^+$	0									
2	$1/2^+$	110	1.0								
3	$5/2^+$	197	1.0								
4	$5/2^-$	1346		0.96	0.04						
5	$3/2^-$	1459	0.21	0.69	0.10						
6	$2/3^+$	1554	0.03	0.05	0.92						
7	$9/2^+$	2780			1.00						
8	$3/2^+$	3907	0.48	0.20	0.14			0.18			
9	$7/2^-$	3999			0.18	0.70	0.12				
10	$9/2^-$	4032				1.00					
11	$7/2^+$	4378			0.80			0.20			
12	$5/2^-$	4549			0.69	0.05	0.08	0.18			
13	$3/2^-$	4558	0.36	0.45	0.09	0.04		0.06			
14	$13/2^+$	4648							1.00		
15	$5/2^-$	4683			0.06	0.63	0.31				
16	$5/2^+$	5106			0.80		0.20				
17	$1/2^+$	5366	0.38	0.42			0.20				
18	$7/2^-$	5430				0.50	0.13			0.30	0.07
19	$7/2^+$	5464			0.04	0.32		0.05	0.59		
20	$3/2^+$	5499		0.25	0.49	0.16	0.10				
21	$5/2^+$	5540	0.08		0.47		0.45				
22	$3/2^-$	5621			0.39	0.61					

Table 6 Energy levels and gamma-ray branching ratios for ^{18}F

Initial state			Branching ratios to state N					
N	J^π	E (keV)	1	2	3	4	5	6
1	1^+	0						
2	3^+	937	1.00					
3	0^+	1042	1.00					
4	0^-	1081	1.00					
5	5^+	1121		1.00				
6	6^+	1701	0.30		0.70			
7	2^-	2101	0.38	0.31		0.31		
8	2^+	2523	0.75	0.21				0.04
9	2^+	3062	0.23	0.77				

Table 7. Energy levels and gamma-ray branching ratios for ^{19}O

Initial state			Branching ratios to state N		
N	J^π	E (keV)	1	2	3
1	$5/2^+$	0			
2	$3/2^+$	96	1.00		
3	$1/2^+$	1472	0.02	0.98	
4	$9/2^+$	2371	1.00		
5	$7/2^+$	2779	1.00		
6	$3/2^+$	3067			1.00
7	$5/2^+$	3155	0.08	0.92	
8	$3/2^+$	3235			
9	$3/2^-$	3945	0.33	0.39	0.28

Table 8. Energy levels and gamma-ray branching ratios for ^{18}O

Initial state			Branching ratios to state N								
N	J^π	E (keV)	1	2	3	4	5	6	7	8	9
1	0^+	0									
2	2^+	1982	1.00								
3	4^+	3555		1.00							
4	0^+	3634		1.00							
5	2^+	3920	0.13	0.87							
6	1^-	4456		0.25	0.03	0.72					
7	3^-	5098		0.75	0.08	0.17					
8	2^+	5260	0.30	0.70							
9	0^+	5336		0.60				0.40			
10	3^+	5378		0.87			0.13				
11	2^-	5530		0.49			0.24	0.27			
12	1^-	6198	0.88			0.03		0.04		0.04	0.01
13	2^-	6351		0.32			0.55	0.13			
14	3^-	6404		0.68	0.07		0.06	0.03	0.10	0.06	
15	0^-	6880						1.00			

Table 9. Energy levels and gamma-ray branching ratios for ^{16}N

Initial state			Branching ratios to state N	
N	J^π	E (keV)	1	2
1	2^-	0		
2	0^-	121	1.00	
3	3^-	297	1.00	
4	1^-	398	0.27	0.73
5	1^+	3355	1.00	

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Table 10. Energy levels and gamma-ray branching ratios for ^{15}N

N	Initial state		Branching ratios to state N			
	J^π	E (keV)	1	2	3	4
1	$1/2^-$	0				
2	$5/2^+$	5270	1.00			
3	$1/2^+$	5299	1.00			
4	$3/2^-$	6324	1.00			
5	$5/2^+$	7155		1.00		
6	$3/2^+$	7301	1.00			
7	$7/2^+$	7567		1.00		
8	$1/2^+$	8313	0.80		0.10	0.10
9	$3/2^+$	8571	0.35	0.65		
10	$1/2^+$	9050	0.90	0.04		0.06

Table 11. Deformation parameters of ^{19}F levels

Energy of level (keV)	J^π	Deformation parameter	
		Krick (KR73)	Swiniarski (SW74)
197	$5/2^+$	0.30	0.55
1346	$5/2^-$	0.242	0.33
1554	$3/2^+$	0.359	0.58
2780	$9/2^+$	0.175	0.22
3907	$3/2^+$	0.081	
4378	$7/2^+$	0.068	
4549	$5/2^+$	0.149	0.20
5106	$5/2^+$	0.126	0.15

3.5 GIANT-DIPOLE RESONANCE PARAMETERS

The gamma-ray transmission coefficient was calculated by the giant-dipole resonance model in TNG. The absorption cross section for giant dipole resonance was assumed to have a Lorentzian shape,

$$\sigma(E_\gamma) = \sigma_m \frac{E_\gamma^2 \Gamma^2}{(E_\gamma^2 - E_m^2)^2 + E_\gamma^2 \Gamma^2} \quad (2)$$

Fig. 1. Calculated direct inelastic scattering.

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where E_γ is the gamma-ray energy. The resonance energy E_m , peak cross section σ_m and full width at half maximum Γ were taken from the empirical formulas (FU62) as follows:

$$\begin{aligned}\sigma_m &= 168NZ/(\pi A\Gamma) \quad (\text{mb}) \\ E_m &= 163(NZ)^{1/2}/A^{4/3} \quad (\text{MeV}) \\ \Gamma &= 5.0 \quad (\text{MeV})\end{aligned}\tag{3}$$

The M1/E1 ratio at $E_\gamma = 7$ MeV was assumed to be 0.1 and the E2/E1 and M2/M1 ratios were assumed to be 0.01 for all gamma-ray energies.

3.6 PARAMETERS FOR PRECOMPOUND EFFECTS

The correlation coefficient for precompound angular distribution was taken as 0.5 from FU88. The scale factor in mean-square matrix element was taken as 4.0.

3.7 (n, d) and (n, t) CROSS SECTIONS AS INPUT TO TNG

In the TNG code, calculation of the (n, d) , (n, t) and $(n, {}^3\text{He})$ reactions are ignored because in general these reactions have small cross sections. These cross sections can be input to TNG as correction factors to reduce proportionally the other TNG calculated cross sections.

By integrating the angular distribution data of Rendic (RE68) and Fazio (FA68), the cross sections for the (n, d) reaction at 14 MeV were obtained as follows:

$$\begin{aligned}\sigma_{nd} \text{ (to g.s. of } {}^{18}\text{O}) &= 12 \text{ mb} \\ \sigma_{nd} \text{ (to 1st s. of } {}^{18}\text{O}) &= 10 \text{ mb}\end{aligned}$$

The cross sections of the (n, d) reaction for other energies were obtained by normalizing the excitation function predicted by Zhao's systematics (ZH88) to 22 mb at 14 MeV and are shown in Fig. 2. For (n, t) reaction, Qaim's spectrum averaged cross section (QA78) and integration of the Rendic angular distribution measurement (RE68) were used to normalize Zhao's systematics (ZH88). The cross sections of the (n, t) reaction obtained are shown in Fig. 3.

Fig. 2. Cross sections of $^{19}\text{F}(n,d)$ reaction.

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Fig. 3. Cross sections of $^{19}\text{F}(n,t)$ reaction.

4. RESULTS AND COMPARISONS

The calculated cross sections, angular distributions, secondary neutron spectra, gamma-ray production cross sections and gamma spectra are compared to the measured data available and the evaluated values of ENDF/B-V.

4.1 (n, p) CROSS SECTION

The comparison of the calculated cross sections to the measured data available is shown in Fig. 4. To obtain good agreement above $E_n = 10$ MeV for both cross sections and gamma-ray production cross sections, a smooth direct interaction cross section of several milli-barns had to be introduced as input to TNG and shown in Fig. 4.

4.2 (n, α) CROSS SECTION

The calculated values are in good agreement with measured data and ENDF/B-V (see Fig. 5).

4.3 $(n, 2n)$ CROSS SECTION

The calculated $(n, 2n)$ excitation function is compared with measured data and ENDF/B-V in Fig. 6. In this calculation, only the reactions which include the emission of first and second particle were considered, therefore, calculated cross sections should be the sum of $(n, 2n)$, $(n, 2np)$ and $(n, 2n\alpha)$. The Q -values for $(n, 2np)$ and $(n, 2n\alpha)$ reactions are -16.038 MeV and -14.846 MeV, respectively so these two reactions should only contribute to a small part of the cross section.

4.4 $(n, np + pn)$ AND $(n, n\alpha + \alpha n)$ CROSS SECTIONS

The $(n, np + pn)$ and $(n, n\alpha + \alpha n)$ here represent the $(n, np) + (n, pn)$ and $(n, n\alpha) + (n, \alpha n)$ reactions, respectively.

No experimental data are available for the $(n, np + pn)$ cross section. In ENDF/B-V, the (n, np) and $(n, n\alpha)$ cross sections were put into MT=91, so the dashed line in Fig. 7 only includes the (n, pn) cross section and similarly, the dashed line in Fig. 8 only includes the $(n, \alpha n)$ cross section. The measured data in Fig. 8 for the $(n, n\alpha + \alpha n)$ cross section was obtained by subtracting the calculated (n, α) cross section from the alpha emission cross section measured by Kneff (KE86) at $E_n = 14.8$ MeV.

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Fig. 4. Cross sections of $^{19}\text{F}(n,p)$ reaction.

Fig. 5. Cross sections of $^{19}\text{F}(n, \alpha)$ reaction.

Fig. 6. Cross sections of $^{19}\text{F}(n, 2n)$ reaction.

Fig. 7. Cross sections of $^{19}\text{F}(n, np + pn)$ reaction. ENDF/B-V includes only the (n, pn) component.

Fig. 8. Cross sections of $^{19}\text{F}(n, n\alpha + \alpha n)$ reaction. ENDF/B-V includes only $(n, \alpha n)$ component.

4.5 INELASTIC CROSS SECTION

For inelastic cross sections, no measured data are available in the energy region $E_n = 2$ to 20 MeV. The comparisons of this calculation with ENDF/B-V for discrete level inelastic cross sections are given in Fig. 9 to Fig. 12 for several levels which have larger cross sections. The calculated discrete level inelastic cross sections were obtained by summing the results of TNG and DWUCK. As seen from Fig. 9 to Fig. 12, these results are consistent with ENDF/B-V. The calculated continuum inelastic cross section is shown in Fig. 13, compared to those of MT=91 in ENDF/B-V. It is not surprising that so large a difference exists between them because MT=91 of ENDF/B-V included not only the $(n, n'\gamma)$ process but also the (n, np) and $(n, n\alpha)$ reaction cross sections.

4.6 ANGULAR DISTRIBUTION OF SECONDARY NEUTRONS

The calculated angular distribution for elastic scattering at 14 MeV by using the OMP in Table 1 and the compound elastic scattering given by TNG is shown in Fig. 14, together with the measured data (BA85, CL70) and ENDF/B-V. The calculation reproduces the measured data very well.

For differential cross sections of inelastic scattering for discrete levels, the measured data of Baba (BA85), Takahashi (TA84), Bonazzola (BO66) and Clarke (CL70) were compared with this calculation. Baba's and Takahashi's data were obtained by integrating their double differential cross section over selected energy regions. Figures 15, 16, and 17 show the sum of differential cross section of the levels with $Q = -1.346$, -1.459 and -1.554 MeV (MT = 53 - 55), $Q = -1.459$ to -4.032 (MT = 54 - 59), and $Q = 2.78$ MeV, respectively. Our calculation is in good agreement with Baba's and Takahashi's measurements.

4.7 SPECTRA OF SECONDARY NEUTRONS

The secondary neutron spectra for $E_n = 14$ MeV in the low outgoing energy region mainly come from the $(n, 2n)$, $(n, np + pn)$ and $(n, n\alpha + \alpha n)$ reactions. Calculated secondary spectra at five angles for $E_n = 14$ MeV in the lab system were obtained by summing the contributions from the reactions above. These spectra are compared to the measured data of Baba (BA85) and Takahashi (TA83) in Figs. 18 to 22. In the calculation, the angular distributions of the second outgoing neutrons were assumed isotropic. A large discrepancy exists between the two sets of measured data. The calculated spectra lie between them.

4.8 GAMMA-RAY PRODUCTION CROSS SECTIONS

The calculated production cross sections for the 110-keV gamma ray from the $(n, n'\gamma)$ reaction are compared to the data of Shi et al. (SH79), Morgan and Dickens (MO75), and Broder et al. (BR69) in Fig. 23. For the 197-keV gamma ray from the $(n, n'\gamma)$ reaction the comparison between the calculation and the measured data of SH79, MO75, BR69, and AR67 are shown in Fig. 24. The calculated production cross sections for the 96-keV gamma ray from the $(n, p\gamma)$ reaction are

Fig. 9. Inelastic scattering cross sections of ^{19}F for 1.346-MeV level.

Fig. 10. Inelastic scattering cross sections of ^{19}F for 1.459-MeV level.

Fig. 11. Inelastic scattering cross sections of ^{19}F for 1.554-MeV level.

Fig. 12. Inelastic scattering cross sections of ^{19}F for 2.780-MeV level.

Fig. 13. Continuum inelastic scattering cross sections of ^{19}F . ENDF/B-V includes (n, np) and $(n, n\alpha)$ cross sections.

Fig. 14. Angular distribution of elastic scattering of ^{19}F at $E_n = 14$ MeV.

Fig. 15. Angular distribution of inelastic scattering of ^{19}F for $Q = -1.346$ to -1.554 MeV at $E_n = 14$ MeV.

Fig. 16. Angular distribution of inelastic scattering of ^{19}F for $Q = -1.459$ to -4.032 MeV at $E_n = 14$ MeV.

Fig. 17. Angular distribution of inelastic scattering of ^{19}F for $Q = -2.78$ MeV at $E_n = 14$ MeV.

Fig. 18. Secondary neutron spectra of ^{13}F at $E_n = 14$ MeV.

Fig. 19. Secondary neutron spectra of ^{10}F at $E_n = 14$ MeV.

Fig. 20. Secondary neutron spectra of ^{19}F at $E_n = 14$ MeV.

Fig. 21. Secondary neutron spectra of ^{10}F at $E_n = 14$ MeV.

Fig. 22. Secondary neutron spectra of ^{10}F at $E_n = 14$ MeV.

Fig. 23. Gamma-ray production cross sections for $E_\gamma = 110$ keV from $^{19}\text{F}(n, n'\gamma)$ reaction.

Fig. 24. Gamma-ray production cross sections for $E_\gamma = 197 \text{ keV}$ from $^{19}\text{F}(n, n'\gamma)$ reaction.

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given in Fig. 25, compared with the measured data of MO75. For the 659-, 937-, 1042-, and 1081-keV gamma rays from the $(n, 2n)$ reaction, the calculation and Corcalciuc's experimental data (CO78) are shown in Fig. 26 to Fig. 29. The gamma-ray production cross sections for 1236 and 1357 keV from the $(n, n'\gamma)$ reaction and 1573, 1653 and 1982 keV from the $(n, np + pn + d)$ reactions are shown in Fig. 30 to Fig. 34, together with the measured data of SH79 and CO78.

4.9 SPECTRA OF GAMMA RAY

The comparisons of this calculation at $E_n = 4.25, 8.5, 13,$ and 18.5 MeV with Dickens's experimental data (DI74) are shown in Figs. 35 to 38. The calculated gamma-ray spectra reproduce the measurements very well.

Fig. 25. Gamma-ray production cross sections for $E_\gamma = 96 \text{ keV}$ from $^{19}\text{F}(n,p)$ reaction.

Fig. 26. Gamma-ray production cross sections for $E_{\gamma} = 659 \text{ keV}$ from $^{19}\text{F}(n,2n)$ reaction.

Fig. 27. Gamma-ray production cross sections for $E_{\gamma} = 937 \text{ keV}$ from $^{10}\text{F}(n, 2n)$ reaction.

Fig. 28. Gamma-ray production cross sections for $E_{\gamma} = 1042$ keV from $^{19}\text{F}(n,2n)$ reaction.

Fig. 29. Gamma-ray production cross sections for $E_{\gamma} = 1081$ keV from $^{19}\text{F}(n, 2n)$ reaction.

Fig. 30. Gamma-ray production cross sections for $E_{\gamma} = 1236 \text{ keV}$ from $^{19}\text{F}(n, n'\gamma)$ reaction.

Fig. 31. Gamma-ray production cross sections for $E_{\gamma} = 1357 \text{ keV}$ from $^{19}\text{F}(n, n'\gamma)$ reaction.

Fig. 32. Gamma-ray production cross sections for $E_{\gamma} = 1573 \text{ keV}$ from $^{19}\text{F}(n, np + pn + d)$ reaction.

Fig. 33. Gamma-ray production cross sections for $E_{\gamma} = 1653 \text{ keV}$ from $^{19}\text{F}(n, np + p + d)$ reaction.

Fig. 34. Gamma-ray production cross sections for $E_{\gamma} = 1982 \text{ keV}$ from $^{19}\text{F}(n, np + pn + d)$ reaction.

Fig. 35. Gamma-ray spectra from $n + {}^{19}\text{F}$.

Fig. 36. Gamma-ray spectra from $n + {}^{19}\text{F}$.

Fig. 37. Gamma-ray spectra from $n + {}^{19}\text{F}$.

Fig. 38. Gamma-ray spectra from $n + {}^{19}\text{F}$.

5. UNCERTAINTIES OF MODEL PARAMETERS

5.1 METHOD

The uncertainties of the model parameters arise from (1) the uncertainties of experimental data used to determine model parameters and (2) drawbacks of the model itself. The first uncertainty can be derived based on the law of error propagation, and the second one can be estimated from the scatter of experimental data around the calculated values (Moment Method). In fact, we only need to know the long-range components of experimental error when the Moment Method is used to estimate the uncertainties of model parameters because the scatter of measured data around calculated values reflect not only the drawbacks of the model used in the analysis, but also the fluctuation of measured data due to statistical error. In the present work, a simple method given in the following was used to determine the covariance matrix of the model parameters

Let

$$Y_k(E_i) = f_k(E_i, \underline{C}) \quad (4)$$

where $Y_k(E_i)$ is a measurable physical quantity such as a cross section; the subscript k denotes a specific type of physical quantity (for example, the (n, p) reaction cross section); E_i represents the argument (for example, incident neutron energy) which is assumed to have no uncertainty, and $f_k(E_i, \underline{C})$ gives the relation between $Y_k(E_i)$ and the model parameter vector $\underline{C}$. In general, many types of measured data (for example, cross section, angular distributions and spectra of different reaction channels) can be used to determine a set of model parameters simultaneously. Assuming that no correlation exists between two different types of data, the covariance matrix, $V_c(M \times M)$ of the M -dimension parameter vector $\underline{C}$ can be written as

$$\begin{aligned} V_c(M \times M) &= \left[\sum_k (F_k(NK \times M))^t V_k^{-1}(NK \times NK) F_k(NK \times M) \right]^{-1} \\ &= \left[\sum_k W_k(M \times M) \right]^{-1} \end{aligned} \quad (5)$$

according to the Least-Squares Method. In the equation above, F_k represents the so-called sensitivity matrix for the k^{th} type of data

$$F_k(i, j) = \frac{\partial f_k(E_i, \underline{C})}{\partial C_j} \quad (6)$$

and $V_k(NK \times NK)$ is the covariance matrix of measured values $\underline{Y}_k = (Y_k(E_1), Y_k(E_2), \dots, Y_k(E_{n_k}))$. The deviations of measurement here is defined as the differences between measured values and the calculated values, that means V_k should include not only the uncertainties of experimental data but also the drawbacks of the model and can be written as

$$V_k = P_k(NK \times NK) R_k(NK \times NK) P_k(NK \times NK) \quad (7)$$

where

$$P_k = \begin{bmatrix} f_k(E_1, \underline{C}) & 0 & \dots & 0 \\ 0 & f_k(E_2, \underline{C}) & \dots & 0 \\ 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & f_k(E_{nk}, \underline{C}) \end{bmatrix} \quad (8)$$

and R_k is the relative covariance matrix

$$R_k(i, j) = \text{Cov}(Y_k(E_i), Y_k(E_j)) / (f_k(E_i, \underline{C}) \cdot f_k(E_j, \underline{C})) \quad (9)$$

If only long-range correlations are important, R_k can be expressed approximately as follows

$$\begin{aligned} R_k(i, i) &= [S_k(E_i) / f_k(E_i, \underline{C})]^2 + D_k^2 \\ R_k(i, j) &= D_k^2, \quad i \neq j \end{aligned} \quad (10)$$

where D_k^2 is the long-range component of the relative uncertainty of the k^{th} data vector Y_k and $S_k(E_i) / f_k(E_i, \underline{C})$ is the short-range component of relative error of $Y_k(E_i)$. In the case of

$$S_k(E_i) / f_k(E_i, \underline{C}) = S_k \quad (\text{constant}) \quad (11)$$

the elements of inverse of matrix R_k can be simply written as

$$\begin{aligned} R_k^{-1}(i, i) &= a_k = 1/S_k^2 - 1/[(NK - 1)S_k^2 + (S_k^2 + D_k^2)S_k^2/D_k^2] \\ R_k^{-1}(i, j) &= b_k = -1/[(NK - 1)S_k^2 + (S_k^2 + D_k^2)S_k^2/D_k^2] \end{aligned} \quad (12)$$

so that

$$\begin{aligned} W_k(i, j) &= (a_k - b_k) \sum_{\ell=1}^{NK} [F_k(\ell, i) F_k(\ell, j) / f_k^2(E_\ell, \underline{C})] \\ &\quad + b_k \left[\sum_{\ell=1}^{NK} F_k(\ell, i) / f(E_\ell, \underline{C}) \right] \cdot \left[\sum_{\ell=1}^{NK} F_k(\ell, j) / f(E_\ell, \underline{C}) \right] \end{aligned} \quad (13)$$

and finally

$$V_c(M \times M) = \left[\sum_k W_k(M \times M) \right]^{-1} \quad (14)$$

The problem is how to determine D_k^2 and S_k^2 . The D_k^2 can be expressed as

$$D_k^2 = D_k^2(\text{exp.}) + D_k^2(\text{th.}) \quad (15)$$

where $D_k^2(exp.)$ denotes the component arisen from measurement and can be obtained by analyzing the experimental conditions; $D_k^2(th.)$ represents those from drawbacks of the model and can be estimated by

$$D_k^2(th.) = \frac{1}{NK - M} \left[\sum_{i=1}^{NK} \frac{Y_k(E_i) - f_k(E_i, \underline{C})}{f_k(E_i, \underline{C})} \right]^2 \quad (16)$$

in the case that the calculated values systematically deviate from the measured one. If the calculated values pass through the k^{th} type of measured data without systematic deviation, the $D_k^2(th.)$ calculated from Eq. (16) will be close to zero. The short-range component S_k^2 can be estimated by

$$S_k^2 = \frac{1}{NK - M} \sum_{i=1}^{NK} \left(\frac{Y_k(E_i) - f_k(E_i, C)}{f_k(E_i, C)} \right)^2 \quad (17)$$

As mentioned above, S_k^2 given by Eq. (17) not only includes random uncertainties in measurement but also reflects the uncertainties from the fact that the model used sometimes can not describe the detailed structure in physical curves very well.

5.2 APPLICATION

Based on the method above, the covariance matrix of a set of the model parameters was obtained. These parameters were used in TNG for calculating cross sections of the reactions induced by neutron on ^{19}F . This study concerned six types of cross sections including those of (n, n') , $(n, 2n)$, (n, p) , (n, α) , $(n, np + pn)$ and $(n, n\alpha + \alpha n)$ reactions and nine of model parameters such as AN, AP, AA (level density parameters for ^{19}F , ^{19}O and ^{16}N), V0, W0 (depths for real and imaginary well), RV, RD (radius of real and imaginary potential), AV, AD (diffuseness of real and imaginary potential).

The partial derivatives of cross sections to parameters as a function of neutron energy were calculated by the difference quotient

$$\begin{aligned} F_k(i, j) &= \frac{\partial f_k(E_i, \underline{C})}{\partial C_j} \\ &= \frac{f_k(E_i, \underline{C}') - f_k(E_i, \underline{C})}{\Delta C_j} \end{aligned} \quad (18)$$

where $\underline{C}' = (C_1, C_2, \dots, C_j + \Delta C_j, \dots, C_m)$ and ΔC_j was taken as $0.01C_j$. The calculated product of partial derivatives and the parameters themselves are shown in Figs. 39 to 44. From these figures, it is found that in general the values of this kind of product for AP, AV and AD are much smaller compared to other parameters. This means that AP, AV and AD have less importance than other parameters in calculating uncertainties of the cross sections. Thus, only six parameters were considered.

Fig. 39. Products of parameters and partial derivatives of total inelastic cross section to parameter.

Fig. 40. Products of parameters and partial derivatives of (n,p) reaction cross section to parameter.

Fig. 41. Products of parameters and partial derivatives of (n, α) reaction cross section to parameter.

Fig. 42. Products of parameters and partial derivatives of $(n, np+pn)$ reaction cross section to parameter.

Fig. 43. Products of parameters and partial derivatives of $(n, n\alpha + an)$ reaction cross section to parameter.

Fig. 44. Products of parameters and partial derivatives of (n, 2n) reaction cross section to parameter.

The measured cross sections for $(n, 2n)$, (n, p) and (n, α) were used to determine V_c . The long-range components of the relative variance, D_k^2 (exp.), were taken from File 33 of ENDF/B-V. The covariance matrix of the six parameters is given in Table 12. The covariance matrix of the cross sections for the $(n, np + pn)$ and $(n, n\alpha + \alpha n)$ reactions were calculated from the covariance matrix in Table 12 and are given in Table 13 and Table 14 and adopted in ENDF/B-VI.

Table 12. Covariance matrix of parameters

Parameter	St. Error, %		Correlation matrix					
AN= 4.00 MeV	8.12	1.00						
AA= 3.68 MeV	4.96	-0.10	1.00					
WO= 6.20 MeV	56.2	-0.67	0.38	1.00				
VO=45.80 MeV	29.9	-0.48	0.03	0.68	1.00			
RV= 1.26 fm	9.39	0.49	-0.20	-0.80	-0.92	1.00		
RD= 1.30 fm	26.5	0.48	-0.25	-0.92	-0.67	0.79	1.00	

Table 13. Covariance matrix of $(n, np + pn)$ cross sections

E_n (MeV)	σ (mb)	St. error (%)	Correlation matrix							
10.0	2.88	15.9	1.00							
11.0	12.32	15.9	0.99	1.00						
12.0	28.26	11.5	0.91	0.91	1.00					
14.0	61.18	10.5	0.66	0.66	0.86	1.00				
16.0	77.07	11.2	0.47	0.47	0.70	0.95	1.00			
18.0	91.15	11.7	0.41	0.41	0.64	0.87	0.97	1.00		
20.0	102.70	11.7	0.41	0.41	0.64	0.87	0.97	0.99	1.00	

Table 14. Covariance matrix of $(n, n\alpha + \alpha n)$ cross sections

E_n (MeV)	σ (mb)	St. error (%)	Correlation matrix									
6.0	26.8	17.2	1.00									
7.0	122.7	17.2	0.99	1.00								
8.0	218.7	13.8	0.71	0.71	1.00							
10.0	412.9	8.29	0.71	0.71	0.58	1.00						
12.0	439.4	8.29	0.71	0.71	0.58	0.99	1.00					
14.1	381.8	11.6	0.70	0.70	0.70	0.88	0.88	1.00				
16.0	333.4	11.6	0.70	0.70	0.70	0.88	0.88	0.99	1.00			
18.0	273.5	14.4	0.59	0.59	0.68	0.78	0.78	0.97	0.97	1.00		
20.0	242.0	14.4	0.59	0.59	0.68	0.78	0.78	0.97	0.97	0.99	1.00	

6. SUMMARY

The nuclear model methods used in calculating the cross sections of neutron-induced reactions on ^{19}F from 2 to 20 MeV have been presented in this report. The calculated results have been compared to the available measured data. The overall quality of the comparison leads to the acceptance of the calculations as evaluated values for ENDF/B-VI and ensures energy balance. A simple method to estimate the covariance matrix of several sensitive model parameters has been discussed and a specific result for $n + ^{19}\text{F}$ calculation looks reasonable.

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