VERIFICATION OF THE CROSS-SECTION AND DEPLETION CHAIN PROCESSING MODULE OF DRAGON 3.06

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ABSTRACT

In this paper we present a verification of the module of the lattice code DRAGON 3.06 used for processing microscopic cross-section libraries, including their associated depletion chain. This verification is performed by re-programming the capabilities of DRAGON in another language (MATLAB) and testing them on different problems typical of the CANDU reactor. The verification procedure consists in first programming MATLAB m-files to read the different cross section libraries in ASCII format and to compute the reference cross-sections and depletion chains. The same information is also recovered from the output files of DRAGON (using different m-files) and the resulting cross sections and depletion chain are compared with the reference library, the differences being evaluated and tabulated. The results show that the cross-section calculations and the depletion chains are correctly processed in version 3.06 of DRAGON.

I. INTRODUCTION

This article describes the methodology considered for the verification of the `LIB:` module of DRAGON 3.06. This module is used to process standard microscopic cross section libraries of various format and generate a DRAGON MICROLIB that contains an embedded MACROLIB.[1,2] It also analyzes the depletion chain stored in the library and store it in a compressed format on the same MICROLIB.

Several library formats have been considered here, including:

1. IAEA, a 69 groups WLUP library in the WIMSD4 format.[3]
2. IAEA172, a 172 groups WLUP library in the WIMSD4 format.[3]
3. WIMSLIB, a 69 groups Winfrith based library in the old WIMS-AECL format.[4]
4. E5WLIB, an 89 groups ENDF/B-V based library in the old WIMS-AECL format.[4]
5. E6MLIB, an 89 groups ENDF/B-VI based library in the old WIMS-AECL format.[4]
6. NDAS, the WIMS-IST 89 groups ENDF/B-VI based library in the new NDAS format.[5]

A summary of the contents of these libraries is presented in Table 1. In addition, each isotope has its own set of temperature tabulation for the thermal cross sections (number of temperature tabulations varies from isotope to isotope).[3–5] Some isotopes also have resonance integrals tabulated as a function of temperature and dilution (that varies from isotope to isotope).[3–8]

Here both the contents of the DRAGON MICROLIB and embedded MACROLIB generated for several typical cell problems encountered in CANDU analysis have been analyzed.

Table 1: Contents of the libraries selected for the verification. Here N_I is the total number of isotopes in the library, while $N_{(n,2n)}$ and $N_{s,1}$ respectively represent the number of isotopes with $(n, 2n)$ reactions and anisotropic scattering. N_G^f, N_G^r and N_G^t are respectively the number of fast, resonance and thermal groups in the library.

	N_I	N_G^f	N_G^r	N_G^t	$N_{(n,2n)}$	$N_{s,1}$
IAEA	69	14	13	42	0	3
IAEA172	173	45	47	80	0	3
WIMSLIB	115	14	13	42	> 0	3
E5WLIB	145	24	23	42	> 0	3
E6MLIB	203	24	23	42	> 0	3
NDAS	172	24	23	42	> 0	> 3

Most of the verification is based on a direct comparison between the original information stored in the ASCII file that was used to generate the DRAGON compatible libraries and the information generated using this code.This comparison will be performed using MATLAB m-files[9] since the goal of the verification process is to show that the routines programmed in DRAGON perform as expected. Except for some accumulator variables, DRAGON is mainly programmed in single precision. On the other hand, MATLAB uses double precision. Thus, we can already expect small discrepancies between the results. In this paper, we will first verify the generation of the microscopic cross-sections and then the macroscopic cross-sections. The depletion chain verification will be finally carried out, before we conclude on the improvements introduced during this work.

II. MICROSCOPIC CROSS SECTIONS

The DRAGON MICROLIB contains, for each isotope required to build the MACROLIB (containing the macroscopic cross sections), the multigroup microscopic cross sections interpolated in temperature and dilution. The interpolation algorithm used by DRAGON for the temperature dependent cross sections and the dilution and temperature dependent resonance integrals depend on the specific reference cross section library selected. Here, three library are considered namely: IAEA, E5WLIB and NDAS.

For all these libraries the epithermal cross sections associated with non-resonant isotopes are temperature independent and the information available in the DRAGON MICROLIB is just a direct copy of the contents of the reference library. In this case, the microscopic cross sections $\{\tilde{\sigma}^g\}_m$ read by a MATLAB m-file are compared directly with the information stored on the MICROLIB ($\{\sigma^g\}_m$) and the absolute and relative errors between the contents of the MICROLIB and the original library are computed using

$$\Delta\sigma_{x,m} = \max\left|\tilde{\sigma}^g_{x,m} - \sigma^g_{x,m}\right| \tag{1}$$

$$\bar{\sigma}^g_{x,m} = \frac{(\tilde{\sigma}^g_{x,m} + \sigma^g_{x,m})}{2} \tag{2}$$

$$\delta\sigma_{x,m} = \max\left|\frac{100 \times (\tilde{\sigma}^g_{x,m} - \sigma^g_{x,m})}{\bar{\sigma}^g_{x,m}}\right| \tag{3}$$

for reactions x and

$$\Delta\sigma_{s,l,m} = \max\left|\tilde{\sigma}^{g\to h}_{s,l,m} - \sigma^{g\to h}_{s,l,m}\right| \tag{4}$$

$$\bar{\sigma}^{g\to h}_{s,l,m} = \frac{(\tilde{\sigma}^{g\to h}_{s,l,m} + \sigma^{g\to h}_{s,l,m})}{2} \tag{5}$$

$$\delta\sigma_{s,l,m} = \max\left|\frac{100\times(\tilde{\sigma}^{g\to h}_{s,l,m} - \sigma^{g\to h}_{s,l,m})}{\bar{\sigma}^{g\to h}_{s,l,m}}\right| \tag{6}$$

for the order l contribution to the scattering matrix expanded in terms of spherical harmonics.

For the thermal cross sections associated with non-resonant isotopes a temperature interpolation is required. For the WIMSD4 and WIMS-AECL library format this interpolation is linear in temperature, namely

$$\tilde{\sigma}^{g}_{x,i}(T) = \frac{T-T_2}{T_1-T_2}\sigma^{g}_{x,i}(T_1) - \frac{T-T_1}{T_1-T_2}\sigma^{g}_{x,i}(T_2)$$
$$\tilde{\sigma}^{g\to h}_{s,l,i}(T) = \frac{T-T_2}{T_1-T_2}\sigma^{g\to h}_{s,l,i}(T_1) - \frac{T-T_1}{T_1-T_2}\sigma^{g\to h}_{s,l,i}(T_2)$$

where $\sigma^{g\to h}_{x,i}(T_k)$ and $\sigma^{g\to h}_{s,l,i}(T_k)$ as well as T_k, the temperatures at which the cross sections are tabulated, are extracted directly from the original library in ASCII format. The temperatures T_1 and T_2 are such that $T_1 \le T \le T_2$. In the case where T is above the maximum tabulation temperature or below the minimum tabulation temperature no interpolation takes place and the cross sections at T_2 and T_1 are used respectively.

For isotope with resonance integral tables, the problem is somewhat more complex. In fact, if the isotope is at infinite dilution ($\sigma_e = 10^{10}$), the same process as that used for non-resonant isotopes is considered. In the case where the dilution σ_e is different from 10^{10} the resonance integrals $I_{x,i}(T,\sigma_e)$ associated with isotope i for reaction x must first be interpolated in temperature and dilution before the cross sections are evaluated using

$$\tilde{\sigma}^{g}_{x,i,\text{self-shielded}}(T) = \tilde{\sigma}^{g}_{x,i}(T) + \frac{I^{g}_{x,i}(T,\sigma_e)}{\phi^{g}(T,\sigma_e)} \tag{7}$$

where $\phi^g(T,\sigma_e)$ is the resonant flux computed using[7]

$$\phi^{g}(T,\sigma_e) = 1 - \frac{1}{N_i\sigma_e}\left[I^{g}_{i}(T,\sigma_e) - \sum_h \frac{U^h}{U^g} I^{h\to g}_{s,i}(T,\sigma_e)\right] \tag{8}$$

Here $I^g_i(T,\sigma_e)$ and $I^{h\to g}_{s,i}(T,\sigma_e)$ are respectively the total and scattering resonance integrals, U^h is the lethargy width of group h and N_i the isotopic concentration of isotope i. For libraries in the WIMSD4 and WIMS-AECL format, a linear interpolation in the square root of the temperature is considered. For the dilution, an `AIKINT` interpolation in the square root of the dilution cross section $\sqrt{\sigma_e}$ is used.

For the NDAS library, the temperature interpolation for thermal cross-section (at infinite dilution) is performed with the Ceschino cubic method included in the `ALTERP` subroutine.[10] This method computes a factor f_t for each tabulated abscissa. The interpolated cross-sections are then given by the sum of the tabulated values weighted by the f_t interpolation factors. For the resonance integral, the temperature interpolation is also performed with the the Ceschino method. The dilution interpolation is usually performed with the `ALTERP` subroutine using the $\log_{10}$ value of the tabulated dilutions. One exception is for values of the dilution larger than the last tabulated value (infinite dilution excluded). In this case, a linear interpolation is performed between the highest tabulated dilution and infinite dilution ($\sigma_e = 10^{10}$). The flux required to evaluate the self-shielded cross section using Eq. (7) is also interpolated from the tabulated flux using a procedure similar to that used for the resonance integrals.

The algorithm for verification of MICROLIB generating routines is actually very simple, and corresponds to a few lines to the main MATLAB procedures. All MATLAB m-file use the same pattern:

- Set case options (Isotope, library, temperature/dilution, fissile, P1, several indexes and values).
- Read library and interpolate for selected temperature/dilution. This operation is performed by using a few procedures some being specific to each library and some being identical for all libraries. The information is always put in the same array for all libraries.
- Read DRAGON output files (the MICROLIB). The information is again put in the same array for all libraries. Thus, the error computation is performed by a single m-file which is used for all library and all cases.
- Write output tables automatically (TEX files).

The isotopes without resonance integral tables that were considered are: Hydrogen (`H1`), Deuterium (`D2`) and Oxygen (`O16`). We also selected the following isotopes that have resonance integral tables: ^{235}U (`U235`), ^{238}U (`U238`) and ^{239}Pu (`PU239`). In this case, tests were first performed at infinite dilution before resonance integral contributions were considered. Table 2 shows the results for the total (σ), (n,γ) ($\sigma_{(n,\gamma)}$) and transport correction (σ_{tran}) cross section as well as for the isotropic ($\sigma_{s,0}$) and linearly anisotropic ($\sigma_{s,1}$) scattering matrices for a non fissile isotope. Table 3 provides the same information for a fissile element in addition to the neutron production cross section due to fission ($\nu\sigma_f$). Table 4 shows the results for dilution interpolation. One can observe that the relative error between MATLAB and DRAGON are generally very small (about $10^{-5}\%$) for the various types of cross sections. The small discrepancy is due to the double/single precision nature of the two codes as we pointed out earlier. The only relative errors that fall outside the single precision range for the microscopic cross section verification are the transport correction cross sections and the linearly anisotropic contribution to the scattering matrix for heavy isotopes. However, the absolute errors on these cross sections are small and are either much lower or of the same order as those observed for the isotropic scattering and total cross sections. The impact of these errors on the solution of the transport problem therefore remains within the single precision nature of DRAGON.

Table 2: Maximum errors on temperature interpolated cross sections for D2

	IAEA		E5WLIB		NDAS	
Cross Sections	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)
σ	1.51e-06	25.65	1.35e-06	28.84	1.97e-06	53.99
$\sigma_{(n,\gamma)}$	2.12e-10	15.76	8.33e-11	14.08	6.51e-11	11.94
σ_{tran}	1.68e-06	2068.15	1.87e-06	750.91	2.04e-06	2423.78
$\sigma_{s,0}$	1.25e-06	25.49	1.52e-06	28.00	1.98e-06	53.91
$\sigma_{s,1}$			2.90e-07	26.00	9.09e-07	80.49

Table 3: Maximum errors on temperature interpolated cross sections for U235

	IAEA		E5WLIB		NDAS	
Cross Sections	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)
σ	1.35e-04	11.23	5.00e-04	67.38	7.27e-04	505.27
$\sigma_{(n,\gamma)}$	2.14e-04	120.77	9.61e-04	860.07	1.74e-04	1542.64
σ_{tran}	6.74e-05	>1000	5.89e-04	>1000	3.09e-04	>1000
$\sigma_{s,0}$	1.47e-06	10.20	1.74e-05	118.75	9.34e-05	574.90
$\sigma_{s,1}$			9.02e-08	>1000	5.67e-06	>1000
$\nu\sigma_f$	3.58e-04	9.95	1.48e-03	82.59	1.38e-03	556.81

Table 4: Maximum errors on temperature and dilution interpolated cross sections for U235

		IAEA		E5WLIB		NDAS	
Dilution	Cross Sections	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)
case 1 (*)	$\sigma_{s,0}$	1.20e-06	10.37	6.92e-07	5.42	8.32e-07	6.86
	σ	4.29e-06	8.59	6.31e-06	8.81	1.08e-05	9.49
	$\sigma_{(n,\gamma)}$	7.23e-06	57.11	5.90e-06	26.00	5.63e-06	50.31
	$\nu\sigma_f$	1.11e-05	11.93	8.46e-06	7.79	9.37e-06	8.70
case 2 (*)	$\sigma_{s,0}$	4.35e-07	3.66	8.87e-07	7.21	3.27e-06	27.38
	σ	5.94e-06	8.80	3.87e-05	44.00	1.63e-04	132.81
	$\sigma_{(n,\gamma)}$	4.95e-06	34.36	3.78e-05	93.73	7.16e-05	190.13
	$\nu\sigma_f$	3.61e-06	9.25	9.25e-05	70.56	2.54e-04	156.27
Infinite	$\sigma_{s,0}$	4.35e-07	3.66	4.91e-07	4.42	5.00e-07	4.63
	σ	3.80e-06	5.61	3.26e-06	4.88	8.00e-06	5.38
	$\sigma_{(n,\gamma)}$	3.90e-06	38.71	5.70e-06	64.77	6.64e-06	39.26
	$\nu\sigma_f$	0.00e+00	0.00	3.84e-07	0.30	4.00e-06	5.87

(*) the dilutions differ for each library.

III. MACROSCOPIC CROSS SECTIONS

The verification of the macroscopic cross sections has been performed for all the libraries presented in the introduction.

The procedure to verify the routines associated with the generation of a DRAGON format macroscopic cross sections library (a MACROLIB data structure) is relatively straight forward. We first created MATLAB m-files to read the information stored on the DRAGON MICROLIB data structure generated for a series of problems that are representative of the typical use of DRAGON for CANDU lattice calculations.[9] The information stored on the MICROLIB that is of importance for the verification of the MACROLIB processing routines of DRAGON is the following.

1. The complete set $\{\sigma_I^g\}_m$ of multigroup microscopic cross sections associated with each isotope I required to define a mixture m. The set of cross sections available for each isotope includes minimally the total cross section σ_I^g and the isotropic scattering cross section matrix $\sigma_{I,s,0}^{g\to h}$.
2. The isotopic contents of each mixture $N_{I,m}$.
3. The complete set $\{\Sigma^g\}_m$ of multigroup macroscopic cross sections associated with each mixture m.

This information is then process in the following way. For most vector reactions, including the total, $(n,2n)$ and (n,γ) reactions, we have computed using MATLAB m-files the following multigroup macroscopic cross sections for each mixture m:

$$\tilde{\Sigma}_{x,m}^g = \sum_I N_{I,m}\sigma_{x,I}^g$$

$$\tilde{\Sigma}_{(n,\gamma),m}^g = \sum_I N_{I,m}\sigma_{(n,\gamma),I}^g$$

$$\tilde{\Sigma}_{(n,2n),m}^g = \sum_I N_{I,m}\sigma_{(n,2n),I}^g$$

In addition the vector cross section that is associated with the transport correction is processed using

$$\tilde{\Sigma}_{\text{tranc},m}^g = \sum_I N_{I,m}\sigma_{\text{tranc},I}^g$$

For the various components $l = 0, L-1$ of the expansion to order L of the scattering matrix in terms of spherical harmonics, we have build both the multigroup macroscopic scattering matrix $\tilde{\Sigma}^{g\to h}_{s,l,m}$ and the scattering cross section $\tilde{\Sigma}^{g}_{s,l,m}$ using

$$\tilde{\Sigma}^{g\to h}_{s,l,m} = \sum_I N_{I,m}\sigma^{g\to h}_{s,l,I}$$
$$\tilde{\Sigma}^{g}_{s,l,m} = \sum_h \sum_I N_{I,m}\sigma^{g\to h}_{s,l,I}$$

Finally, the neutron production cross section from fission $\nu\Sigma_f$, the fission cross section and the fission spectrum were processed isotope by isotope using the following procedure:

$$\nu\tilde{\Sigma}^{g}_{f,I,m} = N_{I,m}\nu\sigma^{g}_{f,I}$$
$$\tilde{\Sigma}^{g}_{f,I,m} = N_{I,m}\sigma^{g}_{f,I}$$
$$\tilde{\chi}^{g}_{I,m} = \chi^{g}_{f,I}$$

since these properties are stored independently for each isotope having non vanishing fission cross sections.

This set of macroscopic cross sections $\{\tilde{\Sigma}^g\}_m$ is then compared with the information stored on the MACROLIB ($\{\Sigma^g\}_m$) and the following absolute and relative errors are computed for vector reactions:

$$\Delta\Sigma_{x,m} = \max\left|\tilde{\Sigma}^{g}_{x,m} - \Sigma^{g}_{x,m}\right|$$
$$\bar{\Sigma}^{g}_{x,m} = \frac{(\tilde{\Sigma}^{g}_{x,m} + \Sigma^{g}_{x,m})}{2}$$
$$\delta\Sigma_{x,m} = \max\left|\frac{100\times(\tilde{\Sigma}^{g}_{x,m} - \Sigma^{g}_{x,m})}{\bar{\Sigma}^{g}_{x,m}}\right|$$

where x represents a vector reaction and $\bar{\Sigma}^{g}_{x,m}$ is the average of the cross section provided in the DRAGON MACROLIB and the results of the MATLAB calculation. For the full scattering matrices we used

$$\Delta\Sigma_{s,l,m} = \max\left|\tilde{\Sigma}^{g\to h}_{s,l,m} - \Sigma^{g\to h}_{s,l,m}\right|$$
$$\bar{\Sigma}^{g\to h}_{s,l,m} = \frac{(\tilde{\Sigma}^{g\to h}_{s,l,m} + \Sigma^{g\to h}_{s,l,m})}{2}$$
$$\delta\Sigma_{s,l,m} = \max\left|\frac{100\times(\tilde{\Sigma}^{g\to h}_{s,l,m} - \Sigma^{g\to h}_{s,l,m})}{\bar{\Sigma}^{g\to h}_{s,l,m}}\right|$$

while for the diagonal ($\Sigma^{g\to g}_{s,l,m}$) and total ($\Sigma^{g}_{s,l,m}$) scattering cross section we used respectively

$$\Delta\Sigma^{g\to g}_{s,l,m} = \max\left|\tilde{\Sigma}^{g\to g}_{s,l,m} - \Sigma^{g\to g}_{s,l,m}\right|$$
$$\bar{\Sigma}^{g\to g}_{s,l,m} = \frac{(\tilde{\Sigma}^{g\to g}_{s,l,m} + \Sigma^{g\to g}_{s,l,m})}{2}$$
$$\delta\Sigma^{g\to g}_{s,l,m} = \max\left|\frac{100\times(\tilde{\Sigma}^{g\to g}_{s,l,m} - \Sigma^{g\to g}_{s,l,m})}{\bar{\Sigma}^{g\to g}_{s,l,m}}\right|$$

and

$$\Delta\Sigma^g_{s,l,m} = \max\left|\tilde{\Sigma}^g_{s,l,m} - \Sigma^g_{s,l,m}\right|$$
$$\bar{\Sigma}^g_{s,l,m} = \frac{(\tilde{\Sigma}^g_{s,l,m} + \Sigma^g_{s,l,m})}{2}$$
$$\delta\Sigma^g_{s,l,m} = \max\left|\frac{100 \times (\tilde{\Sigma}^g_{s,l,m} - \Sigma^g_{s,l,m})}{\bar{\Sigma}^g_{s,l,m}}\right|$$

One MATLAB m-file that read the cross sections stored on the DRAGON MICROLIB is created for each library that has been analyzed. Note that each cross section record in the MICROLIB that will be accessed by these m-files is identified by a keyword.[2] Moreover $\Sigma^{g\to h}_{s,0,m}$ and $\Sigma^{g\to h}_{s,1,m}$ are stored in a compressed format and must be extracted using a specialized MATLAB function. In addition, for the verification of $\Sigma^g_{s,0,m}$ and $\Sigma^g_{s,1,m}$, it is necessary to sum over all final groups the microscopic scattering cross section matrices for each isotope using the same MATLAB functions. Finally, the verification for $\Sigma^{g\to g}_{s,0,m}$ and $\Sigma^{g\to g}_{s,1,m}$ was carried out by extracting the diagonal component of the scattering cross section matrices calculated for each mixture. The errors are then computed using a common MATLAB m-file. Different sets of DRAGON input files were considered for each library since the isotope identifier on each library may differ and some library contain only a rather limited number of isotopes. However all the test were selected to be representative of typical CANDU test problems. Some additional verifications were also performed for a limited number of libraries. For example, the test cases for the IAEA-69, WIMSLIB and E5WLIB libraries have been repeated at different temperatures. Similarly, one library (IAEA) has been verified for burned fuel. Perturbations in coolant purity, void fraction and fuel temperature have been performed for E5WLIB. The fact that we have not considered all the libraries for these additional tests is easily justifiable since:

- We are verifying the contents of the MACROLIB assuming the MICROLIB contents is known.
- The `LIB:` routines used to generate the MICROLIB are independent of the explicit cross section library selected.
- Applying at least one verification process for each one of the 6 libraries is in fact only useful to ensure that DRAGON generates a MICROLIB for each library that is valid.

The maximum errors for the different test cases are summarized in Tables 5 to 7. Again relative differences lower that $10^{-4}\%$ are generally observed due to the single precision nature of DRAGON. For the linearly anisotropic scattering cross section where both positive and negative contributions are expected some pathological cases have been found where $\tilde{\Sigma}^{g\to h}_{s,1,m}$ becomes very small, leading to large relative errors $\delta\tilde{\Sigma}^{g\to h}_{s,l,m}$. However, in these cases the associated absolute errors in the cross sections remain small and should have no impact on the transport calculation. The results we obtained for different temperatures, burnup and coolant density show exactly the same behavior as that observed above and are not presented here.

IV. DEPLETION CHAINS

The DRAGON MICROLIB also contains the depletion chains. We have compared them to the original chain available in the libraries. Here three libraries were selected, namely IAEA, E5WLIB and NDAS. The different parameters of those libraries are provided in Table 8. The information required to build a depletion chain is:

1. The names NISOD_i of the isotopes ($i = 1, N_D$) that are present in the depletion chain.
2. The reaction types NREAD_r associated with a given depletion mechanism r is identified by the microscopic cross section name associated with this reaction.
3. The depletion process associated with reaction r for isotope i.
4. The energy (MeV) per reaction $E_{r,i}$ for the depletion process associated with reaction r for isotope i.

Table 5: Maximum errors in $\Sigma^{g\to h}_{s,0,m}$, $\Sigma^{g}_{s,0,m}$ and $\Sigma^{g\to g}_{s,0,m}$ for all mixtures

	$\Sigma^{g\to h}_{s,0,m}$		$\Sigma^{g}_{s,0,m}$		$\Sigma^{g\to g}_{s,0,m}$	
Library	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)
IAEA-69	3.22e-08	20.99	6.69e-08	18.36	3.22e-08	14.12
IAEA-172	5.40e-08	20.27	5.72e-08	18.44	5.40e-08	16.38
WIMSLIB	4.14e-08	16.07	5.43e-08	16.72	4.14e-08	14.78
E5WLIB	4.49e-08	62.16	4.71e-08	16.87	4.49e-08	15.72
E6MLIB	1.95e-07	39.01	4.48e-07	28.02	1.95e-07	32.58
NDAS	4.04e-08	21.96	5.23e-07	71.45	4.04e-08	16.81

Table 6: Maximum errors in $\Sigma^{g\to h}_{s,1,m}$, $\Sigma^{g}_{s,1,m}$ and $\Sigma^{g\to g}_{s,1,m}$ for all mixtures

	$\Sigma^{g\to h}_{s,1,m}$		$\Sigma^{g}_{s,1,m}$		$\Sigma^{g\to g}_{s,1,m}$	
Library	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)
IAEA-69	8.15e-09	61.98	3.71e-08	121.50	8.15e-09	11.62
IAEA-172	3.96e-09	2265.77	4.21e-08	76.29	3.96e-09	11.32
WIMSLIB	4.11e-09	96.43	8.19e-09	10.38	4.11e-09	10.39
E5WLIB	9.34e-09	51191.34	1.20e-08	62.54	9.34e-09	21.89
E6MLIB	4.76e-08	589.57	1.03e-07	34.14	4.76e-08	31.07
NDAS	6.60e-09	319.39	7.62e-08	214.46	6.60e-09	17.65

5. The array λ_i containing the radioactive decay constant λ (10^8 s^{-1}) for isotope i.
6. The parent isotope that generated the isotope i, together with the fractional branching ratio for the production of isotope NISOD_i via a specific reaction from another isotope j, and the yield for the production of the direct fission product m ($m \leq N_P$) by a fission of the fissile isotope l ($l \leq N_F$).

This information, as well as that provided in the ASCII format libraries will be reformatted in the matrices $T_{i,j}$ and $R_{i,j}$ as follows:

1. $T_{j,i}$ contains the type of reaction for the production of isotope $j \leq N_I$ from isotope $i \leq N_I$ and $R_{j,i}$ the yield for this reaction.
2. $T_{N_I+1,i} = 1$ indicates that isotope $i \leq N_I$ decays with a decay constant $R_{N_I+1,i}$ (s^{-1}).
3. $T_{N_I+2,i} = 2$ indicates that isotope $i \leq N_I$ is a fission product.
4. $T_{N_I+3,i} = 3$ indicates that isotope $i \leq N_I$ depletes via a capture reaction.
5. $T_{N_I+4,i} = 4$ indicates that isotope $i \leq N_I$ depletes via an $(n, 2n)$ reaction.
6. $T_{N_I+5,i} = 5$ indicates that isotope $i \leq N_I$ depletes via an $(n, 3n)$ reaction.
7. $T_{N_I+6,i} = 6$ indicates that isotope $i \leq N_I$ is a fissile isotope with energy per fission $R_{N_I+6,i}$ (J).

The verification procedure will again use MATLAB m-files. These perform the following tasks:

1. Read the information stored on the reference `ASCII` library for the IAEA, E5WLIB and NDAS libraries and reformat as described above.

Table 7: Maximum errors in Σ, Σ_{tran}, $\Sigma_{(n,\gamma)}$, $\Sigma_{(n,2n)}$, Σ_f and $\nu\Sigma_f$ for all mixtures

	Σ		Σ_{tran}		$\Sigma_{(n,\gamma)}$	
Library	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)
IAEA-69	3.95e-08	10.41	7.02e-09	9.24	6.58e-09	9.50
IAEA-172	6.68e-08	9.68	8.96e-09	42.97	2.82e-08	84.19
WIMSLIB	1.02e-07	8.20	4.61e-08	85.87	1.12e-07	944.62
E5WLIB	4.44e-08	14.84	8.55e-09	23.30	1.16e-08	14.96
E6MLIB	6.00e-07	32.83	9.76e-08	805.01	2.92e-07	27.38
NDAS	4.37e-07	10.67	8.51e-09	564.05	4.20e-07	11.34
	$\Sigma_{(n,2n)}$		Σ_f		$\nu\Sigma_f$	
Library	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)	Δ (cm^{-1})	δ (10^{-6} %)
IAEA-69	-	-	1.65e-08	8.03	2.32e-08	5.55
IAEA-172	-	-	1.95e-08	10.91	2.11e-08	5.87
WIMSLIB	-	-	7.12e-09	5.29	2.60e-08	4.91
E5WLIB	4.65e-10	8.40	4.65e-09	9.07	2.45e-08	5.62
E6MLIB	8.55e-10	19.67	1.89e-08	8.37	1.43e-08	5.44
NDAS	5.52e-10	6.65	9.39e-09	8.90	1.80e-08	5.47

Table 8: Libraries depletion chain parameters.

number of		IAEA	E5WLIB	NDAS
isotopes	N_I	173	145	172
depleting isotopes	N_D	92	91	103
fissile isotopes	N_F	21	12	5
direct fission products	N_P	61	48	52

2. Read the contents of the depletion chain stored in the MICROLIB and reformat as described above.

3. Compare the records $T_{i,j}$ and $R_{i,j}$ extracted from the MICROLIB and the `ASCII` library and return the average and maximum relative errors in reaction yields, fission energy and decay constant.

4. Generate the relative error tables in a TEX format.

An option in DRAGON is the capability to include or change a depletion chain manually in the input files. This feature is particularly interesting when one needs to look at an element not included in the original library. DRAGON can print the actual depletion chain that is read from a library onto the output files in a format compatible with that used to insert manually decay chain in a DRAGON MICROLIB. To verify this part of the module, we have copied this information into a duplicate of the original input file, replacing the access to the original library by a manual entry of the depletion chain. We ended up with two input files defined for each library type:

1. `Bibl.x2m` that generates the depletion chain on the MICROLIB directly from the cross section library and produces on the output file a list of record that can be used to generate manually a depletion chain.

2. `Biblman.x2m` that generates the depletion chain on the MICROLIB manually using the data produced using the `Bibl.x2m` input file.

Both the automatic (`Bibl.x2m`) and manual (`Biblman.x2m`) MICROLIB can be processed by our MATLAB m-files to compute the errors.

Note that for the E5WLIB and NDAS libraries, some isotopes can decay via two channels with different decay constants. Because of the formatting of the information on the MICROLIB, it is impossible to associate two different decay constants to a single isotope. This problem is resolved in DRAGON using the following procedure:

1. Compute the total decay constant for isotope i using

$$\lambda_i = \sum_j \lambda_{j,i}$$

   This is the information stored in record $R_{N_I+1,i}$.

2. Compute the production rate of isotope j from isotope i by decay using

$$Y_{j,i} = \frac{\lambda_{j,i}}{\lambda_i}$$

   This information is then stored in record $R_{j,i}$.

Tables 9 and 10 show the relative errors for all the libraries with the automatic or manual generation of the decay chains. Discrepancies are actually very small in all cases and are within the range of single/double precision error expected. The manual cases present slightly larger errors because the real values (decay constant, branching ratio ...) in the DRAGON output files have only 6 digits. Thus some precision is lost in the automatic to manual transfer process.

V. CONCLUSIONS

The verification process that we considered for the `LIB:` module of DRAGON is based on the use of MATLAB m-files written in such a way as to duplicate the calculations performed within DRAGON. It indicates that in general the relative errors are within the limits expected from the single precision nature of the code DRAGON. Two exceptions have been noted for the verification of the microscopic and macroscopic cross section namely the linearly anisotropic component of the scattering matrix and transport correction cross section where large relatives errors were observed. However, the impact of these errors on the solution of the transport problem remains within the single precision nature of DRAGON since the absolute errors in these cross sections remain very small.

The depletion chain stored on the DRAGON MICROLIB is identical to the original depletion chain with relative errors in energy per fission, decay constants and production yields that remain within the single precision nature of the code DRAGON. This verification allowed us to correct a compatibility issue in the current version of DRAGON. For isotopes with multiple decay channels, the partial decay constant for each channel had to be replaced by a global decay constant with partial production yield for each decay product. This feature was not required in previous version. Indeed IAEA does not have isotopes with multiple decay constant, and E5WLIB has only one such isotope but with a decay constant several order of magnitude smaller than the other in such a way that it can be neglected. However the NDAS library has an isotope with two decay constants of the same order of magnitude and DRAGON had to be corrected accordingly.

With this verification completed, the code DRAGON can now be used to perform stand-alone transport calculations starting with a microscopic cross section library in the WIMSD4, WIMS-AECL and NDAS format assuming the dilution for each resonant isotope is provided manually. The next steps in our verification process consist in analyzing the self shielding module `SHI:` that computes the dilution for resonance integral interpolation and the burnup module `EVO:` that follows the depletion of the isotopes as a function of time.

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Table 9: Maximum and average relative errors on decay constant, fission energy and production yield for automatic decay chain processing.

	IAEA errors (10^{-6} %)		E5WLIB errors (10^{-6} %)		NDAS errors (10^{-6} %)	
Type	Maximum	Average	Maximum	Average	Maximum	Average
Decay constant	5.72	2.74	7.69	3.00	8.75	3.57
Fission energy	4.70	2.09	5.46	2.49	6.23	2.39
Decay yield	0.00	0.00	2.93	0.66	3.74	0.82
Fission yield	0.00	0.00	5.41	1.55	5.52	2.55
(n, γ) yield	0.00	0.00	0.38	0.05	2.97	0.38
$(n, 2n)$ yield	nd.	nd.	0.00	0.00	0.21	0.09

Table 10: Maximum and average relative errors on decay constant, fission energy and production yield for manual decay chain processing.

	IAEA errors (10^{-6} %)		E5WLIB errors (10^{-6} %)		NDAS errors (10^{-6} %)	
Type	Maximum	Average	Maximum	Average	Maximum	Average
Decay constant	11.06	3.95	9.17	3.65	20.75	4.33
Fission energy	25.21	13.20	23.14	16.95	28.39	17.66
Decay yield	0.00	0.00	8.83	1.97	11.66	2.54
Fission yield	0.00	0.00	11.70	4.34	5.52	2.55
(n, γ) yield	0.00	0.00	0.38	0.05	2.97	0.38
$(n, 2n)$ yield	nd.	nd.	0.00	0.00	0.21	0.09

REFERENCES

[1] G. Marleau, R. Roy, and A. Hébert, *A User Guide for DRAGON 3.06*, Technical Report IGE-174 Rev. 7, École Polytechnique de Montréal (2007).

[2] A. Hébert, G. Marleau, and R. Roy, *A Description of the Data Structures for DRAGON 3.06*, Technical Report IGE-232 Rev. 5, École Polytechnique de Montréal (2007).

[3] WLUP, *Final Stage of the WIMS-D Library Update Project*, `www-nds.iaea.org/wimsd` (2005).

[4] J. V. Donnelly, *WIMS-CRNL, A User's Manual for the Chalk River Version of WIMS*, Technical Report AECL-8955, Atomic Energy of Canada Limited (1986).

[5] D. Altiparmakov, *WIMS-AECL 3.1 Theory Manual*, Technical Report 153-119190-STM-001, Atomic Energy of Canada Limited (2006).

[6] R. J. J. Stamm'ler, and M. J. Abbate, *Methods of Steady-State Reactor Physics in Nuclear Design*, Academic Press, London (1983).

[7] A. Hébert, and G. Marleau, "Generalization of the Stamm'ler Method for the Self-Shielding of Resonant Isotopes in Arbitrary Geometries," *Nucl. Sci. Eng.*, **108**, 230 (1991).

[8] A. Hébert, "Revisiting the Stamm'ler Self-Shielding Method," *25th Annual Canadian Nuclear Society Conference*, Toronto (2004), (Proceedings available on CD-Rom).

[9] MATLAB, *The Language of Technical Computing*, `www.mathworks.com` (2006).

[10] F. Ceschino, "L'intégration approchée des équation différentielles," *Compte rendu de l'Académie des sciences*, **243**, 1478–1479 (1956).