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Development of Thermal Scattering Law for Hydrogen Fluoride for Criticality Safety Applications

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ABSTRACT

Precise estimation of thermalization of neutrons in moderators relies on high-fidelity thermal scattering cross-sections, often termed as thermal scattering law (TSL). TSL libraries for several moderator materials like light water, heavy water, polyethylene, etc., are available in standard cross-section data libraries in ENDF format. However, cross-section data for moderators like Hydrogen Fluoride (HF) is still missing in libraries like ENDF/B-VIII.0, JEFF-3.3, and others. Some discrepancies between modeling and experimental data were observed for benchmarks involving HF as a moderator. This difference is believed to be partly linked to the lack of TSL data for HF. Development of new TSL data for HF may help improve criticality safety calculations. This paper presents the newly developed TSL data for HF based on molecular dynamics (MD) simulations. A bibliographical study of the available experimental and atomistic simulation data suitable for our application was carried out. MD simulations using the GROMACS code have been performed to generate phonon spectrum for a series of temperatures required for criticality safety applications. The phonon spectrum at different temperatures is then used by the LEAPR module of the NJOY code to generate TSL for H bound in HF and F bound in HF. The HEU-SOL-THERM-039 benchmark available in the ICSBEP database and a hypothetical critical benchmark using the CRISTAL V2 package is used to verify and validate the newly generated TSL and evaluate its impact on k_{eff} results for criticality-safety studies. Significant improvement in the C/E of the neutron multiplication factor is observed for the benchmarks using the newly generated TSL data.

Key Words: hydrogen fluoride, thermal scattering law, molecular dynamics, criticality safety

1 INTRODUCTION

Fast energy neutrons generated in nuclear systems undergo scattering with the moderators and are slowed down to thermal energies. During the thermalization process, when the neutron energies are comparable to the bound energies of the scattering atom/molecule, there is an exchange of energy and momentum between the neutron and the scattering medium. This effect is governed by the $S(\alpha, \beta)$, often referred to as the thermal scattering law (TSL), and the cross-sections are termed as thermal scattering

cross-sections. The $S(\alpha, \beta)$ drives the estimation of double differential cross sections for a neutron with incident energy E , scattering in a moderator material at temperature T to a final energy E' , and scattering cosine μ , following Eq. 1 and 2 [1].

$$\frac{d^2\sigma}{d\mu dE'}(E \rightarrow E', \mu) = \frac{\sigma_b}{4\pi K_B T} \sqrt{\frac{E'}{E}} S(\alpha, \beta) \quad (1)$$

$$\alpha = \frac{E' + E - 2\mu\sqrt{EE'}}{AK_B T} \quad \text{and} \quad \beta = \frac{E' - E}{K_B T} \quad (2)$$

where σ_b represents the bound scattering cross-section of the material, α the change in momentum, and β the change in energy.

TSL data for several moderator materials, for instance, light water, heavy water, polyethylene are available in standard cross-section data libraries like ENDF/B-VIII.0, JEFF-3.3, and others. However, TSL for moderators like Hydrogen Fluoride (HF) is still missing. Initial work carried out at IRSN suggests that the inclusion of thermal scattering cross-section of HF can help improve criticality safety calculations with benchmarks involving HF as a moderator. Additionally, Fluorine isotope (^{19}F) is an important nuclide, and there are issues with its cross-sections that may be solved with the knowledge of thermal scattering cross-section data of HF.

A commonly used tool by the reactor physics community for generating TSL data is the LEAPR module of the NJOY code [2]. The energy exchange process between the neutron and the scattering atom leads to the excitation/deexcitation of vibrational and rotational modes of the moderator material, which is represented by the phonon spectrum. LEAPR calculates the thermal scattering cross-section data, using the phonon spectrum of moderator materials as a primary input. Hence, a precise estimation of the phonon spectrum of HF at the required temperatures is essential to generate accurate TSL data for HF. In general, one can use the experimental phonon spectrum of moderators to generate TSL data, although effects like experimental resolution and multiple phonon scattering events should be correctly accounted for. In the absence of precise experimental data, atomistic simulations are carried out to obtain the phonon spectrum at required temperatures. For moderators like HF, the available experimental data is scarce and this work leverages over the classical molecular dynamics (MD) simulations to generate the phonon spectrum at temperatures and pressures required for criticality safety applications.

2 HYDROGEN FLUORIDE (HF)

Hydrogen fluoride (HF) has a wide application in several industries like pharmaceutical, petrochemical, polymers and is used as a refrigerant. In the nuclear industry, HF is involved in many processes of the front end of the nuclear fuel cycle: production of UF_4 , enrichment of U, fabrication of UO_2 and, UF_6 transportation. In particular, HF is an impurity of UF_6 and is a product of the chemical reaction between UF_6 and water. In criticality safety assessment of UF_6 systems, as water quantities used are close to zero, HF must be considered as a moderator, which slows down the fission neutrons. The operating range of systems using HF is between -60°C and $+130^\circ\text{C}$. HF is a diatomic molecule with a boiling point of 292.15 K, which is much higher, unlike other hydrogen halides due to formation of strong hydrogen bonds [3]. Properties of hydrogen halides are deeply influenced by the degree and strength of hydrogen bonds between the nearest neighboring molecules. There is vast information in the literature about the formation of hydrogen bonds in the halides based on theoretical studies and experimental data [3-8]. Studies on solid HF show that the molecules are organized in parallel zig-zag chains. Some evidence indicates the presence of polymeric aggregates. From the vapor dependence in the infrared absorption bands, the existence of two, four, and six molecules has been observed. The structure of solid HF is in the form of long zig-zag chains of HF molecules and a similar arrangement in liquid state but with shorter chains of around five or six HF molecules. This continues even in the gaseous phases, where increasing values of specific heat and gas

density are consistent with the formation of chains or rings of between four and eight molecules. Covalent bonds link the H and F atoms of HF molecules, and molecules in chains are bonded by hydrogen bonds which provide structural strength. Considering the experimental evidence, the most probable state of HF would be a mix of structures of rings and chains. The molecular structure, arrangement of different atoms in the molecule, hydrogen bonds, etc., are some of the key factors that define the phonon spectrum of a material. Despite being the most strongly associated liquid in the group of hydrogen halides, little is known about liquid HF. This scarcity has hindered the development of adequate empirical potentials for the simulation of HF.

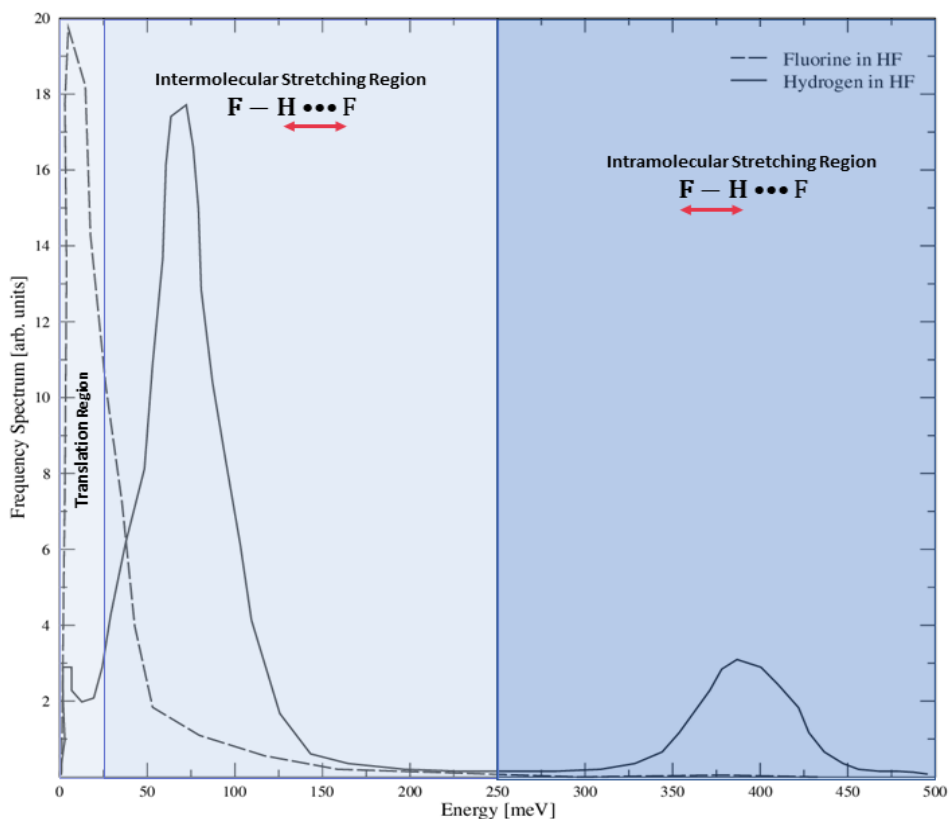


Figure 1: A sketch of the phonon spectrum of both H bound in HF and F bound in HF.

As mentioned in the previous section, accurate information of the phonon spectrum of liquid HF would drive the generation of the TSL for HF. Figure 1 represents a sketch of the phonon spectrum of liquid HF for both H bound in HF and F bound in HF [3]. Different interaction regions of F and H spectrum can be seen, i.e., the translation region, the intermolecular stretching region, and the intramolecular stretching region. The H spectrum extends up to high energies, whereas the F spectrum is only limited to low energies due to significant difference in the atomic mass of F and H atoms.

It is well known that the phonon spectrum of liquids with significant thermal expansion changes with temperature. HF being volatile at room temperature, is often pressurized to maintain it in liquid state. It is thus necessary to have good information on the temperature dependence of the phonon spectrum of liquid HF. A bibliography study of the available data on HF is thus essential to obtain more information on the behavior of HF, in particular, the phonon spectrum. This study will also serve as a guiding tool to carry out new MD simulations of HF learning from the literature.

3 BIBLIOGRAPHIC STUDY OF THE AVAILABLE DATA OF HF

There is some information about HF in the literature based on theoretical studies and experimental data. The bibliography data on the experimental side is available for X-Ray, Raman, Infrared and time-of-flight experiments and on the theoretical side based on ab initio and MD simulations. Significant information about the phonon spectrum of liquid hydrogen fluoride is still limited in the literature, both for experiment and simulation data. However, a bibliography study of the properties of HF will help validate any new MD simulation at different temperatures and pressures.

3.1 Analysis of the Available Experimental Data

Various experiments to analyze the properties of hydrogen fluoride have been studied. Neutron scattering experiments representing the intermolecular stretching were carried out by Boutin et al [4]. Raman and infrared spectroscopy data to study the intramolecular stretching region were carried out by Sheft et al [9] and Desbat et al [10].

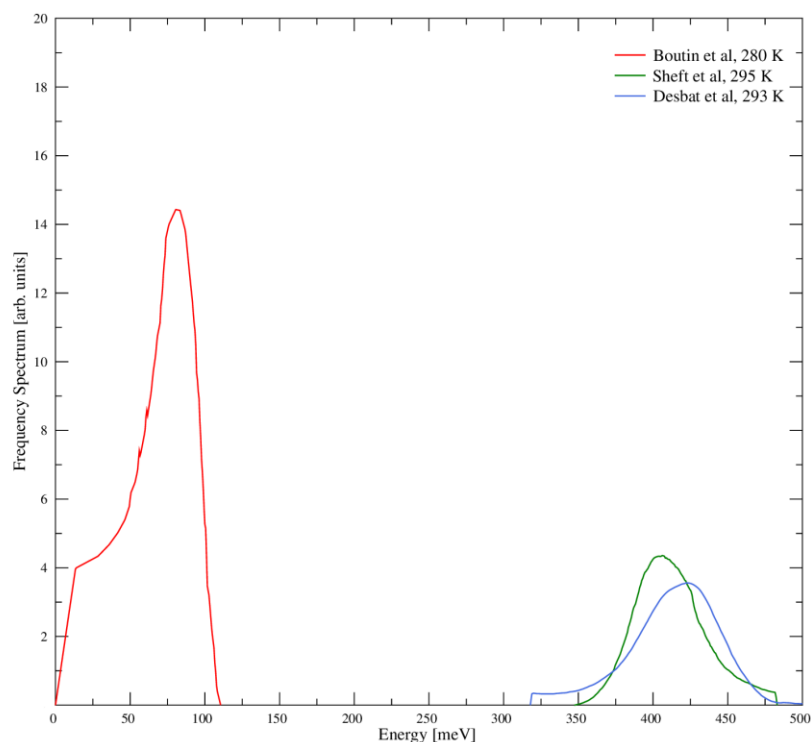


Figure 2: Phonon spectrum of HF based on experimental data.

Frequency spectra obtained from the experimental bibliographic study shows that hydrogen fluoride has two principal regions: the intermolecular stretching region which appears as a broad band between 50 meV and 124 meV [4,9]. This region has a peak around 70 meV. The secondary region corresponds to intramolecular stretching. This region is located between 372 meV and 446 meV [9] and has a peak around 410 - 420 meV. No experimental data covering the entire energy region of the phonon spectrum exists. As shown in Fig. 2, the Boutin et al. data covers the intermolecular stretching region and the two experiments by Sheft and Desbat cover the intramolecular region. Knowledge acquired with this experimental data analysis also serves as a guide to obtain the overall weights and energies of the different regions essential to prepare the necessary inputs for the generation of TSLs.

3.2 Analysis of the Available Simulation Data

Phonon spectra obtained from the simulation data provides the flexibility of getting information on not only the molecule but also for individual atoms as well, i.e., H in HF and F in HF. Four simulation data were studied in this present work. The first one was carried out by Klein et al [6] that is based on MD simulation of HF. The other three data studied are Rothlisberger et al [3], Jedlovsky et al [8], and Sergei et al [5] which are based on ab initio molecular dynamics simulations. A comparison of the phonon spectrum obtained from these simulations is presented in Fig. 3.

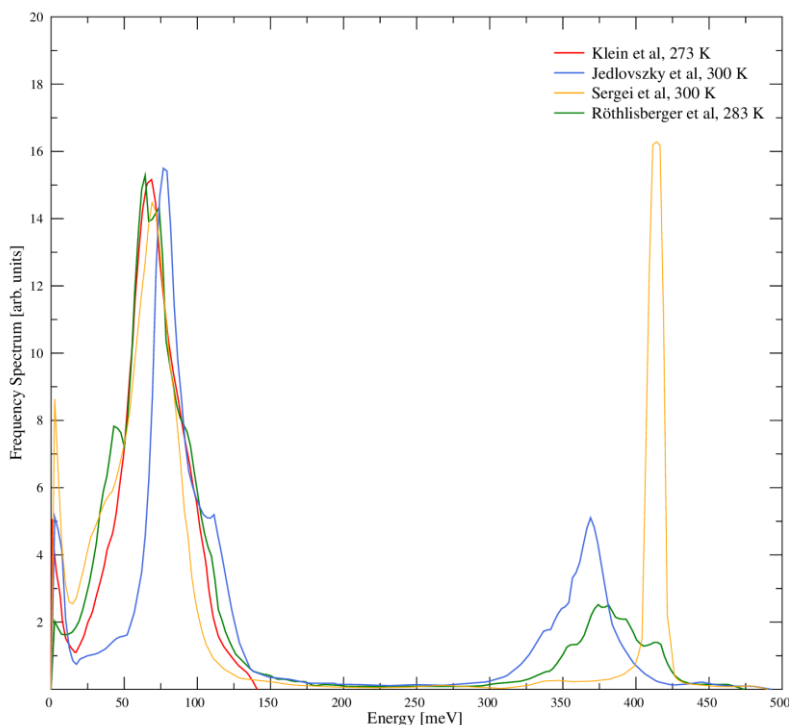


Figure 3: Phonon spectrum of H in HF based on simulation data.

As can be seen in Fig. 3., the phonon spectrum varies as a function of temperature and is also influenced by the different simulation methodologies included in the data simulation. The variation in the peaks of various vibrational modes is also evident due to the different interacting potential used in these simulations. The bibliography study highlights the need for carrying out new time-of-flight inelastic neutron scattering experiments with HF. These experiments are essential to have a better understanding on the dynamics of HF and an improved comprehension on the different interaction modes in the phonon spectrum. This new experimental data will also serve as complimentary information to validate the existing/new simulation results.

The shape and the peaks of the vibrational modes in the phonon spectrum influence the accuracy of the developed TSL. It is thus important to have a choice on the most appropriate atomistic simulation type and the interacting potential used to carry out new simulations for HF at different temperatures. For the present work, molecular dynamics simulation was chosen as an appropriate method to generate the phonon spectrum of liquid HF. A recent study carried out by Elija et al [11] also indicates that molecular dynamics simulations are able to provide reliable results and reproduce the properties of liquid HF for a series of temperatures.

4 MOLECULAR DYNAMICS SIMULATION FOR HF

Molecular dynamics (MD) simulation for hydrogen fluoride has been carried out using the open-source GROMACS-2021.2 [12] molecular dynamics code. About 270 HF molecules in an isothermal-isobaric ensemble were simulated in a cubical box of 2.1 nm with a periodic boundary condition and a time step of 1 fs. The classical potential utilized to carry out the simulation has been adopted from the work carried out by Jedlovsky et al., which is a 3-site polarizable potential fitted correctly to the experimental and simulation data. Following a minimization step, two equilibration runs of two nanoseconds each were carried out using the Nose-Hoover thermocouple and Parrinello-Rahman barostat, respectively. The final production run was carried out for five ns.

Table I. Thermodynamic conditions for the MD simulation of HF

Temperature (K)	273.15	283.15	300.15	323.15	348.15	367.45
Pressure (bar)	1.0	1.0	1.5	2.0	6.0	6.0

Table I, presents the thermodynamic conditions of the simulations carried out for liquid HF. The MD simulations at different temperatures were validated with the diffusion coefficient obtained from the simulations and compared with the experimental diffusion coefficient from the literature, providing acceptable results. The Velocity Auto Correlation Function (VACF) was further obtained for each temperature and Fourier transformed to generate the phonon spectrum. Figure 4 shows the obtained phonon spectrum of H in HF for a series of temperatures between 273.15 - 367.45 K. The peak of the intermolecular stretching region can be seen around 70 meV and the intramolecular stretching region is not captured due to the choice of the potential used.

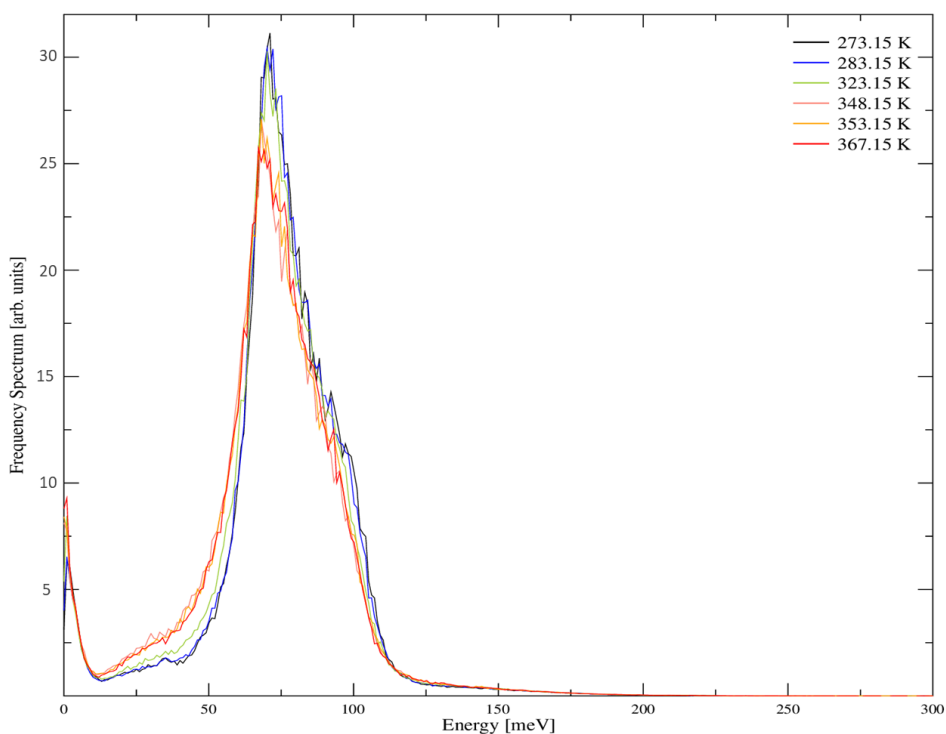


Figure 4: Phonon spectrum of H in HF for a series of temperature obtained from GROMACS simulation.

The amplitude of the phonon spectrum in Fig. 3 and Fig. 4 are not to be compared as the phonon spectrum is normalized to the weights of the individual interacting region while preparing the TSL data. For the preparation of H in HF TSL, the intramolecular stretching region of the phonon spectrum was approximated using a discrete oscillator at 410 meV based on the experimental data by Sheft et al [9], and a corresponding weight was associated to it. The frequency spectrum of H in HF and F in HF obtained from the GROMACS simulations, the weights corresponding to each interacting region in the frequency spectrum, and other necessary parameters were used to generate H in HF and F in HF TSL using the LEAPR module of NJOY. The newly developed TSL for HF was tested on critical benchmarks and is presented in the next section.

5 BENCHMARK AND VALIDATION

Verifying and validating the newly generated TSL for both H in HF and F in HF is important before using it in criticality safety assessment. As mentioned in the previous sections, the motivation to carry out the present work was driven by the differences observed on the HEU-SOL-THERM-039 (HST-039) benchmark available in the ICSBEP database [13]. In addition, a second test was carried out to study the impact of HF TSL for the estimation of uranium critical mass in criticality safety assessment.

5.1 HEU-SOL-THERM-039 ICSBEP Benchmark:

HEU-SOL-THERM-039 (HST-039) is a series of experiments carried out at the VALDUC facility of CEA, France, in the mid-60s. This benchmark includes a hot water reflected spherical tank containing uranium hexafluoride and hydrofluoric acid in its interior. The temperature range of the experiment was between 348.15 K to 367.45 K. The experiments were carried out in a way to obtain high uranium concentrations and low H/U ratio, and the experimental multiplication factor was close to 1. Out of the twelve experiments carried out, only six were considered as they achieved the critical height without filling the tank, and the rest did not achieve criticality even when the tank was full of the mixture. The experimental configuration of the six selected benchmarks is provided in Table 2. For further information about the benchmarks, readers are suggested to refer to [13]. As shown in Table II, these six cases have low H/U concentrations, and despite a minimal change in the temperature, the multiplication factor varies significantly in the modeling. From case 1 to case 6, the H/U increases, and the energy corresponding to average neutron lethargy causing fission (EALF) decreases, thus changing the thermal and epithermal neutron spectrum drastically. Along with the uncertainty in the modeling of the benchmark, another source of this discrepancy is believed to be linked to the cross-sections used. It should be noted that free gas cross-sections at 300 K were used for all the isotopes and the HF cross-section was approximated by the free-gas cross-section of H and F.

Table II. Experimental configuration of the HST-039 benchmark as reported in [13]

Case	1	2	3	4	5	6	
Temperature (K)	348.15	367.45	347.45	348.15	348.75	348.45	
H/U	9.9	16.9	21.0	26.0	38.0	82.0	
EALF (eV)	10.8	2.49	1.48	0.913	0.427	0.133	
Flux %	Thermal	1.5	2.9	3.5	4.3	6.1	11.2
	Epithermal	37.0	38.2	38.6	38.8	39.0	38.1
	Fast	61.5	58.9	57.9	56.9	54.9	50.7
Fission %	Thermal	41.2	55.1	59.9	64.8	72.5	84.4
	Epithermal	49.9	39.4	35.5	31.4	24.8	14.3
	Fast	8.8	5.5	4.6	3.8	2.7	1.3
k_{eff}	Experimental	1.0000 ± 0.0057	1.0000 ± 0.0051	1.0000 ± 0.0045	1.0000 ± 0.0045	1.0000 ± 0.0045	1.0000 ± 0.0045

The IRSN Monte Carlo code MORET 5.D.1 has been used to carry out the validation of the new TSL evaluation of HF. It is believed that using TSL for both H in HF and F in HF in this type of thermal benchmark involving HF as a moderator would improve the C/E of k_{eff} and indicate the accuracy of the newly developed HF TSL. As a first approach and to have a better insight on the impact of HF TSL, a new set of cross-sections were processed using the in-house GAIA-1.2.0 code system [14] to regenerate the free gas cross-sections at the required temperature for the benchmark, i.e., 348 K and 367 K. The SAB module [15] was also used to generate TSL for H in H₂O for the required temperatures.

Table III. Benchmark results for the HST-039 ICSBEP benchmark using new HF TSL. The Monte Carlo standard deviation for all the calculations is 15 pcm.

Case	1	2	3	4	5	6	
Temperature (K)	348.15	367.45	347.45	348.15	348.75	348.45	
Experimental k_{eff}	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	
JEFF-3.3 XS + H-H ₂ O	k_{eff}	1.04505	1.03797	1.03333	1.03670	1.04756	1.03049
	Δk_{eff} (pcm)	4505	3797	3333	3670	4756	3049
JEFF-3.3 XS+ H-H ₂ O + H- HF + F-HF	k_{eff}	1.04217	1.03370	1.02856	1.03170	1.04183	1.02495
	Δk_{eff} (pcm)	4217	3370	2856	3170	4183	2495
Impact from HF TSL (pcm)	-288	-427	-477	-500	-573	-554	

As can be seen in Table III, by adapting the correct temperatures of all the free gas cross sections and the TSL for H in H₂O, there still exists significant differences in the C/E of the effective multiplication factor. Further calculations using both, H in HF and F in HF TSL to study its impact on the benchmark were carried out. It has been observed that using the new HF TSL and the updated cross sections at the required temperatures, there is a decrease in the difference between the modeling and experimental k_{eff} (Table III). Improvements linked to the usage of H in HF and F in HF is around 300 pcm to 600 pcm depending on different benchmark cases from 1-6. The EALF decreases from case 1 to case 6 (ref. Table II), i.e., from 10.8 eV to 0.133 eV. Hence case 6, being a more thermal system sees a bigger impact from HF TSL rather than case 1. Individual calculations using H in HF and F in HF showed that the impact of F in HF is small.

5.2 Impact of HF TSL on the Estimation of Uranium Critical Mass

Results obtained for HST-039 benchmark are not enough to conclude on the impact of HF TSL in criticality safety assessment. Unfortunately, there is just a single series of benchmark using HF as moderator in the ICSBEP handbook. To evaluate the interest of using HF TSL, and possibly the need to perform new critical experiments with HF, the impact of these TSL on the minimal critical mass of uranium was studied. The modeling is a UF₆-xHF sphere surrounded by 30 cm of water. The calculation was done at 300 K at moderation optimum for the mass, H/U = 30, and a uranium enrichment of 6 wt. %. The minimal critical mass was estimated to be around 71 kg of uranium. No TSL for HF was considered in this calculation and the nuclear data cross-section library was JEFF-3.1.1. The calculation performed with MORET 5.D.1 code with JEFF 3.3 at 300 K highlighted the following impact of the use of HF TSL:

- Increase of k_{eff} value of + 807 pcm;
- Decrease of the minimal critical mass of U of -4.99 %.

These first results show that it is not conservative to not consider the IRSN HF TSL evaluation in criticality safety calculations.

A second calculation at the moderation ratio corresponding with the minimal mass, at $H/U = 300$ and a uranium enrichment of 93.5 wt. % was then performed at 300 K; the critical mass of UF_6 moderated by HF was estimated from a criticality standards calculation to be around 2.2 kg of uranium. No TSL for HF was considered in this calculation and the nuclear data cross-section library was JEFF-3.1.1. The MORET 5.D.1 code was then used to model this configuration at 300 K with JEFF-3.3 library and it was observed that using HF TSL there is a significant increase in the k_{eff} indicating a decrease in the critical mass. The studied case with a k_{eff} of 0.99612 using free gas cross sections, changes to about 0.99878 with the use of HF TSL and a new criticality calculation allowed estimating the change of mass. A +266 pcm increase of k_{eff} results in a decrease of uranium mass of -1.2 % (reference mass of 2.2 kg).

These results highlight a significant impact of HF TSL. A similar work carried out by the North Carolina State University, towards the development of TSL for HF [16] would serve as a reference in the future comparison of the developed TSL in this present work. Following further tests on integral benchmarks, the present evaluation will be submitted to the upcoming JEFF nuclear data library. Likewise, the HF TSL could be obtained by requesting the authors for further testing with other benchmarks or new TSL evaluations.

6 CONCLUSIONS AND PERSPECTIVES

Hydrogen Fluoride is an important moderator in nuclear criticality safety studies and other nuclear applications. The development of a new thermal scattering law for hydrogen fluoride using molecular dynamic simulations has been discussed. A bibliographic study of the available experimental and simulation data in the literature is performed to have better insights on the phonon spectrum of hydrogen fluoride and different methodologies to obtain accurate phonon spectra for temperatures required for criticality safety applications. It was observed that the frequency spectrum of both H in HF and F in HF varies significantly depending on the type of experiments and the choice of interacting potentials used to carry out the simulation. A series of new molecular dynamic simulations for HF have been carried out for different temperatures between 273 K and 367 K. The phonon spectrum obtained from these simulations and other necessary parameters have been used to generate the TSL for HF using the LEAPR module of NJOY. The verification and validation of the newly developed TSL have been carried out using the IRSN Monte Carlo code MORET 5.D.1 on two cases, first on an ICSBEP benchmark namely, HST-039, and a standard calculation using HF as a moderator. Significant improvements were observed in the C/E of the effective multiplication factor of the HST-039 benchmark, suggesting the validity of the generated cross-sections. Regarding standard calculations, testing of the newly generated TSL indicates significant changes in the k_{eff} and hence a change in the critical mass, that may influence criticality safety assessment. Nevertheless, the present work also highlights the need for carrying out new time-of-flight inelastic neutron scattering experiments with HF to have a better understanding on the dynamics of HF and new integral experiments to support the generated TSLs.

7 ACKNOWLEDGMENTS

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