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An iron evaluation story: from TALYS model parameters to validation on the ASPIS benchmark with the Monte Carlo code TRIPOLI-4®

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Engineering - Energy, Fluid dynamics and Turbo-machinery

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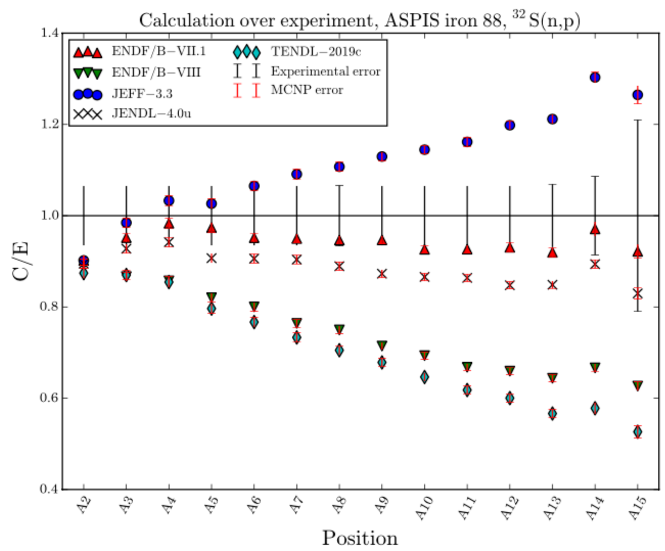
Introduction

- Iron is an important structural material for nuclear applications
- Good nuclear data are needed for correct modeling
- For most libraries, iron evaluations are still performing poorly in shielding benchmarks
- Examples are the Winfrith Iron and Iron-88 Benchmark Experiment (ASPIS)
  - TENDL-2019 underestimates certain experimental results by up to 40%!
- In this work, the code infrastructure T6 is used to produce improved iron evaluations compared to TENDL-2019
- The isotopes considered are ^{56}Fe and ^{54}Fe

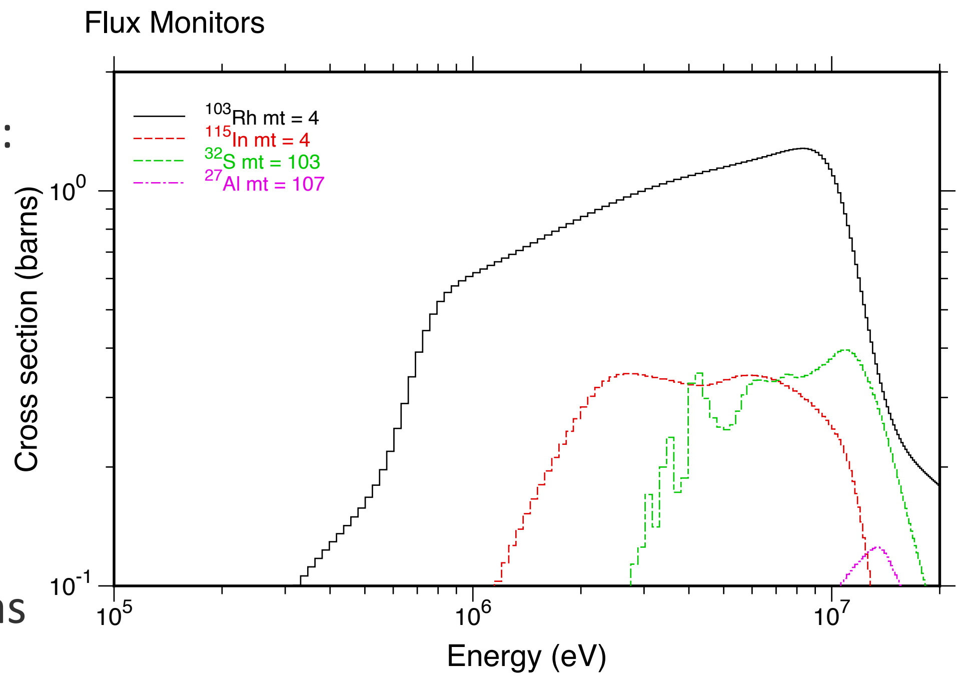


^{54}Fe	**5.85%**
^{56}Fe	**91.75%**
^{57}Fe	2.12%
^{58}Fe	0.28%

ASPIS Iron Benchmark

Fission neutron shielding benchmark

- Deep transmission in the iron bulk – up to 120 cm
- Several detectors placed at different depths:
  - ^{103}Rh(n,n') – threshold ~ 500keV
  - ^{115}In(n,n') – threshold ~ 1MeV
  - ^{32}S(n,p) – threshold ~ 2MeV
- Trying to model the high energy detector well, and progressively go down in energy, as suggested by the shielding physics
- The inelastic scattering and continuum cross section are important in the MeV range



T6, TALYS and autotalys

- T6 has been used to produce TENDL libraries since 2008
- Made of TALYS, TARES, TASMAN, TEFAL, TAFIS, TANES
  - TALYS : nucler model code, generates nuclear data beyond the resolved resonance range
  - TARES: resonance parameters computation
  - TASMAN: covariance calculation, uncertainty quantification, linear sensitivity on TALYS model parameters
  - TEFAL: processing into endf file
- The T6 codes can be run in sequence by a script called autotalys

TALYS features

- TALYS input files contain multiplication factor for the nuclear model parameter default values
- 'Best' input file
  - Contains the best parameters, according to current knowledge
  - Assembled through expert opinion
- Autonorm
  - Allows to normalise selected cross section channels to match channels from another library
  - Requires a second TALYS run, to renormalise the remaining channels for consistency

n-Fe56 'best' input TENDL-2019

```
#
# General
#
ldmodel 2
#
# (n,tot), (n,el), (n,inl)
#
#
# (n,p), (n,2n), (n,np)
#
rvadjust p 0.99
avadjust p 0.99
gnadjust 26 57 0.90
gpadjust 26 57 0.90
aadjust 25 56 1.12
pshiftadjust 26 56 -0.2
pshiftadjust 25 56 0.1
#
# (n,a)
#
cknock a 1.1
cstrip a 1.1
#
# (n,g)
#
gamgamadjust 26  57 0.60
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
```

Evaluation construction

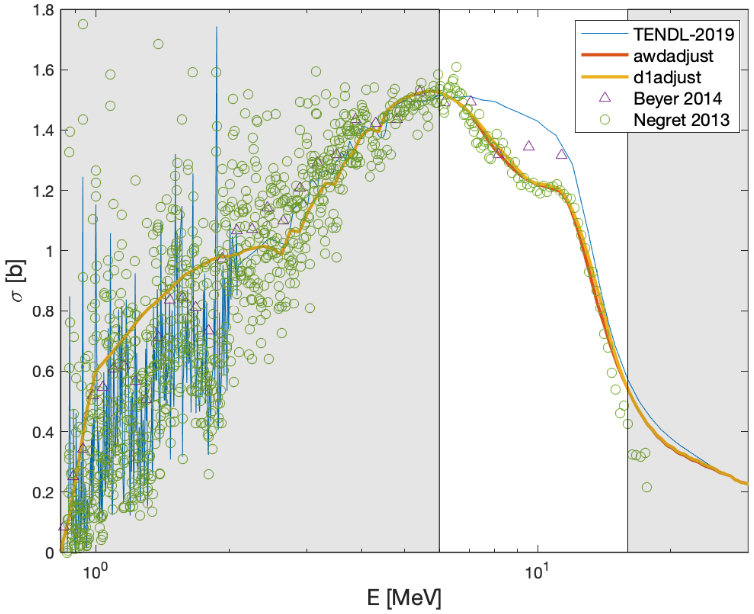
Initial attempt

- Trying to fit ^{56}Fe and ^{54}Fe total inelastic scattering cross section to experimental EXFOR data:

1. Running TASMAN linear sensitivity through autotalys
2. Identifying parameters with high sensitivity coefficients for MT=4 and low sensitivity for other reaction channels
3. Manually varying the 'best' input file, adding the parameter chosen with energy dependence

- Two parameters allowed to fit EXFOR data: *awdadjust* and *d1adjust* (from the Optical Model Potential)

^{56}Fe inelastic cross section




```
#
# General
#
ldmodel 2
#
# (n,tot), (n,el), (n,inl)
#

awdadjust n 1. awdadjust-n.table

#
# (n,p), (n,2n), (n,np)
#
rvadjust p 0.99
avadjust p 0.99
gnadjust 26 57 0.90
gpadjust 26 57 0.90
aadjust 25 56 1.12
pshiftadjust 26 56 -0.2
pshiftadjust 25 56 0.1
#
# (n,a)
#
cknock a 1.1
cstrip a 1.1
#
# (n,g)
#
gamgamadjust 26 57 0.67
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
```

awdadjust-n.table

```
6.0 1.0
7.0 0.95
8.0 0.83
9.0 0.76
9.5 0.74
10.0 0.72
11.0 0.73
12.0 0.74
13.0 0.78
14.0 1.0
```

```
#
# General
#
ldmodel 2
#
# (n,tot), (n,el), (n,inl)
#

d1adjust n 1. d1adjust-n.table

#
# (n,p), (n,2n), (n,np)
#
rvadjust p 0.99
avadjust p 0.99
gnadjust 26 57 0.90
gpadjust 26 57 0.90
aadjust 25 56 1.12
pshiftadjust 26 56 -0.2
pshiftadjust 25 56 0.1
#
# (n,a)
#
cknock a 1.1
cstrip a 1.1
#
# (n,g)
#
gamgamadjust 26 57 0.67
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
```

d1adjust-n.table

```
6.0 1.0
7.0 0.88
8.0 0.73
8.5 0.68
9.0 0.63
9.5 0.58
10.0 0.56
12.0 0.56
13.0 0.70
14.0 1.0
```

^{56}Fe TALYS input files

New input 1

```
#
# General
#
ldmodel 2
#
# (n,tot), (n,el), (n,inl)
#

awdadjust n 1. awdadjust-n.table

#
# (n,p), (n,2n), (n,np)
#
rvadjust p 0.99
avadjust p 0.99
gnadjust 26 57 0.90
gpadjust 26 57 0.90
aadjust 25 56 1.12
pshiftadjust 26 56 -0.2
pshiftadjust 25 56 0.1
#
# (n,a)
#
cknock a 1.1
cstrip a 1.1
#
# (n,g)
#
gamgamadjust 26 57 0.67
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
```

awdadjust-n.table

```
6.0 1.0
7.0 0.95
8.0 0.83
9.0 0.76
9.5 0.74
10.0 0.72
11.0 0.73
12.0 0.74
13.0 0.78
14.0 1.0
```

Energy range:
6 – 14 MeV

New input 2

```
#
# General
#
ldmodel 2
#
# (n,tot), (n,el), (n,inl)
#

d1adjust n 1. d1adjust-n.table

#
# (n,p), (n,2n), (n,np)
#
rvadjust p 0.99
avadjust p 0.99
gnadjust 26 57 0.90
gpadjust 26 57 0.90
aadjust 25 56 1.12
pshiftadjust 26 56 -0.2
pshiftadjust 25 56 0.1
#
# (n,a)
#
cknock a 1.1
cstrip a 1.1
#
# (n,g)
#
gamgamadjust 26 57 0.67
#
# Other: Isomers, (n,d), (n,t), (n,h) etc.
#
```

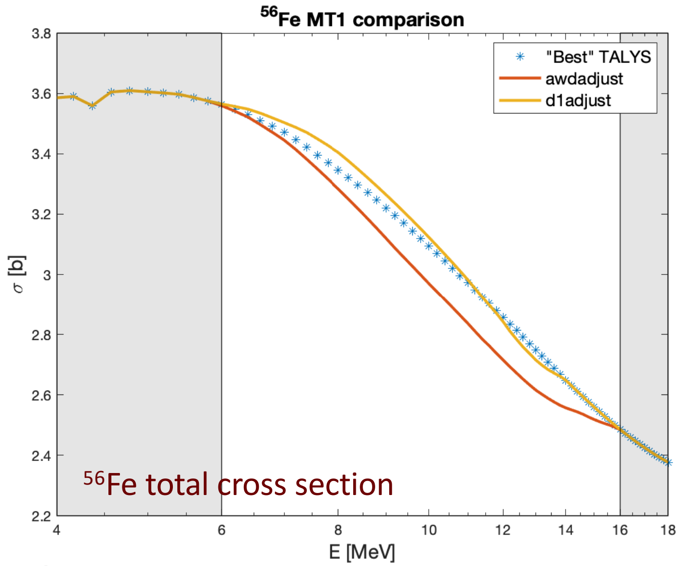
d1adjust-n.table

```
6.0 1.0
7.0 0.88
8.0 0.73
8.5 0.68
9.0 0.63
9.5 0.58
10.0 0.56
12.0 0.56
13.0 0.70
14.0 1.0
```

Energy range:
6 – 14 MeV

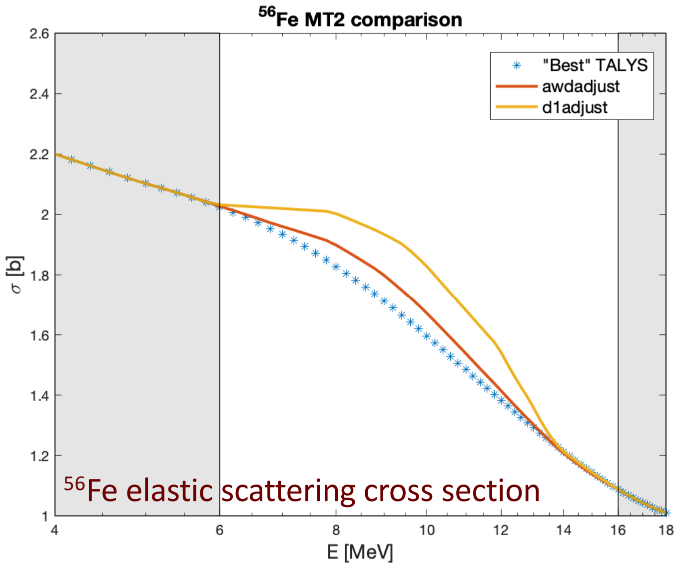
Results Fe-56

- However, other channels were modified too!
- ASPIS results got worse due to the overall modifications
- Fitting differential experimental data blindly is not enough

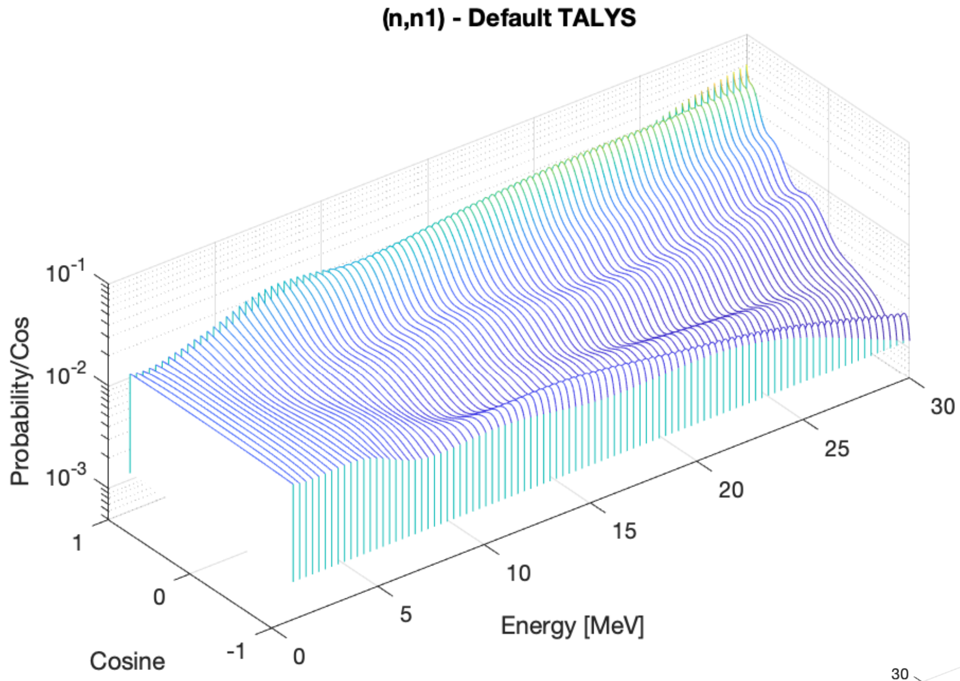


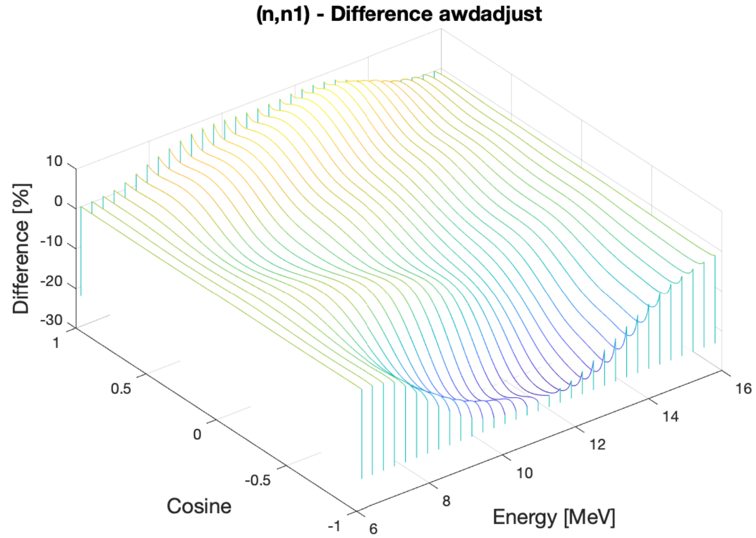
ISSUES:

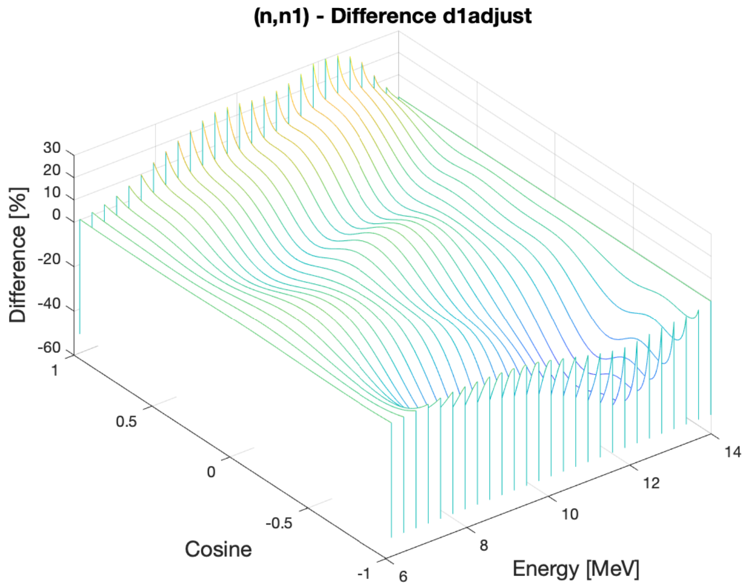
- Do data exist for that MT?
- Which data to choose?
- Are experiental data reliable?



Results Fe-56







- The impact of the parameters on the angular distributions was analysed too
- The effect on the benchmark is hard to quantify, but noticeable, not all is cross-section driven

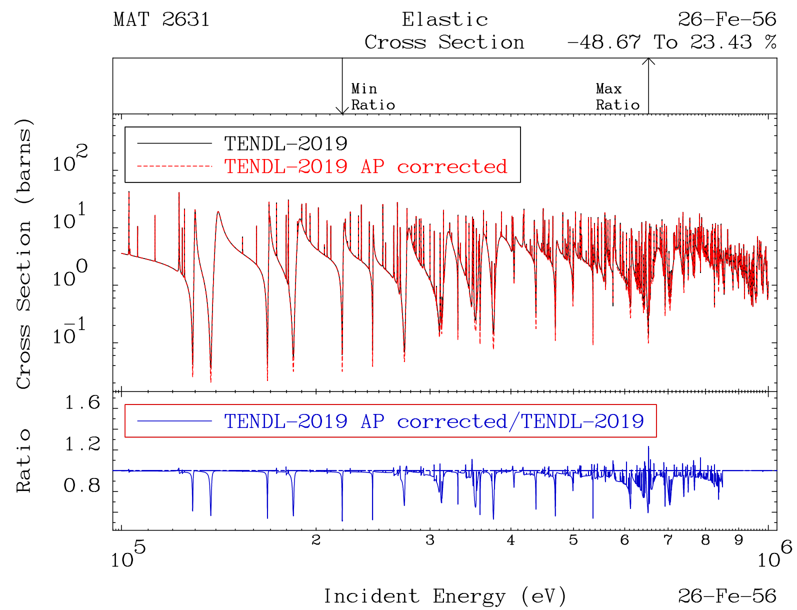
^{56}Fe evaluation

Different approach

- Using integral (benchmark) experimental data rather than differential (EXFOR) data
- Comparing TENDL-2019 with JENDL-4.0, which performs well with ASPIS

SCATTERING RADIUS

- Impacts penetrability and hard-sphere shift
- Different in TENDL-2019 and JENDL-4.0 (taken from JEF-2). Here it was corrected
- Affects heavily the resolved resonance range (up to 850 keV in ^{56}Fe), e.g. elastic scattering



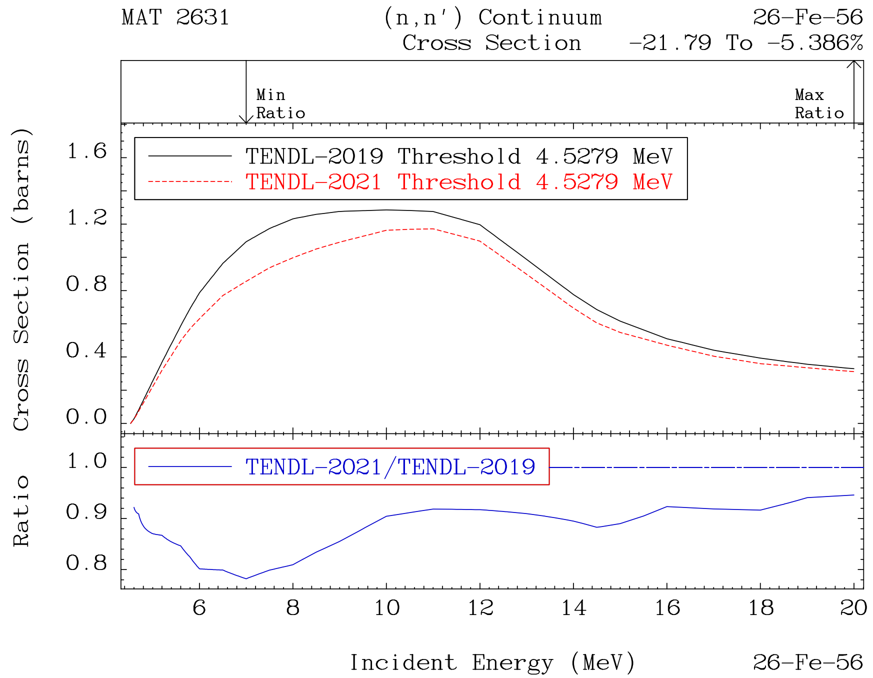
^{56}Fe evaluation

TALYS PARAMETERS

- Used to decrease the inelastic continuum cross section
- Relevant for the high energy detector ^{32}S
- Also affect other channels, like MT 2!

AUTONORM

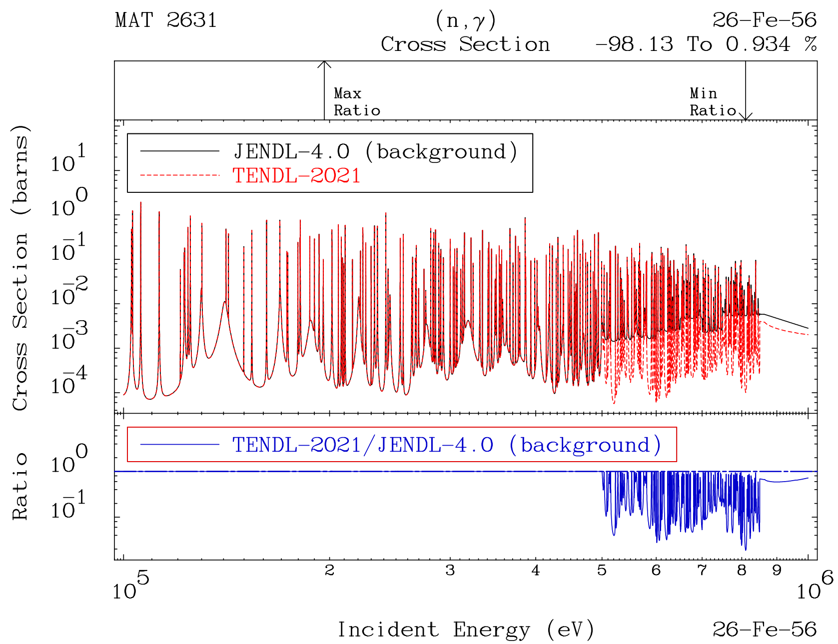
- Already used in TENDL-2019 on MT 4, MT 51-54 from 850keV up to 14 MeV
- Energy range decreased to 6MeV for those channels
- Introducing autonorm on MT 2 until 14MeV



^{56}Fe evaluation

BACKGROUND

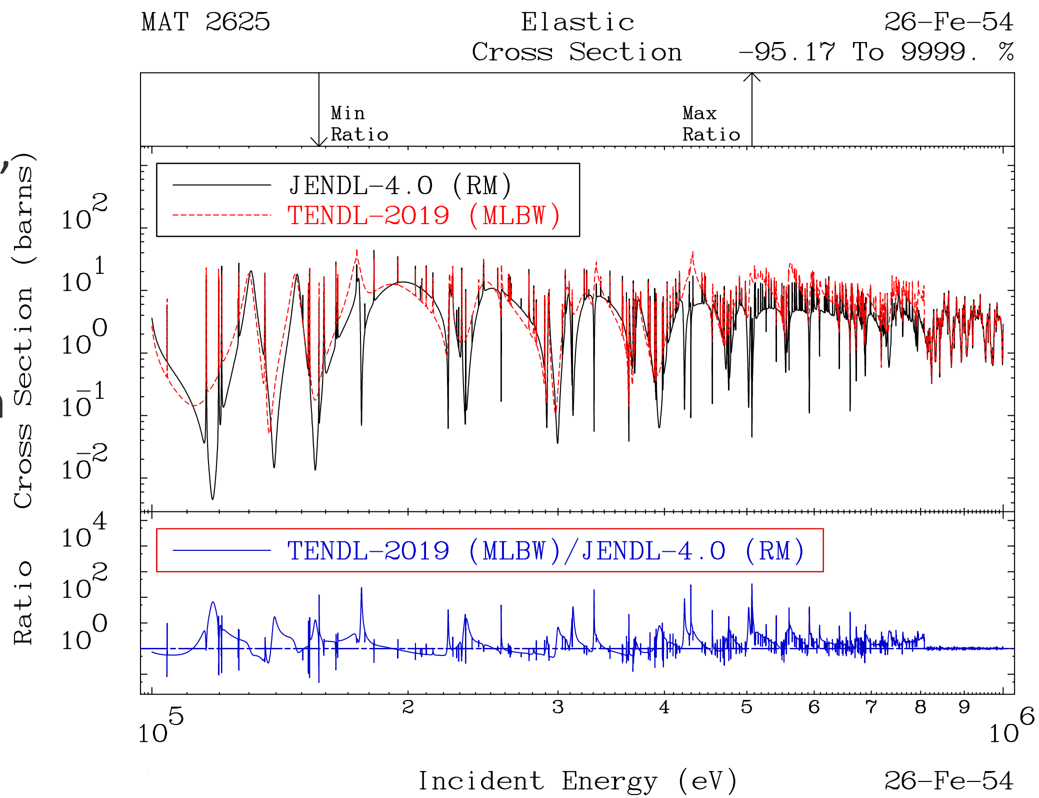
- JENDL-4.0 and TENDL-2019 use a background in the resolved resonance range for capture and total cross section from 500keV to 850keV
- A background has negative side effects when self-shielding and temperature play a role, like in a reactor
- Based on ASPIS it didn't seem necessary, thanks to the modifications in the high energy range, so it was removed



^{54}Fe evaluation

RESONANCE PARAMETERS and FORMALISM

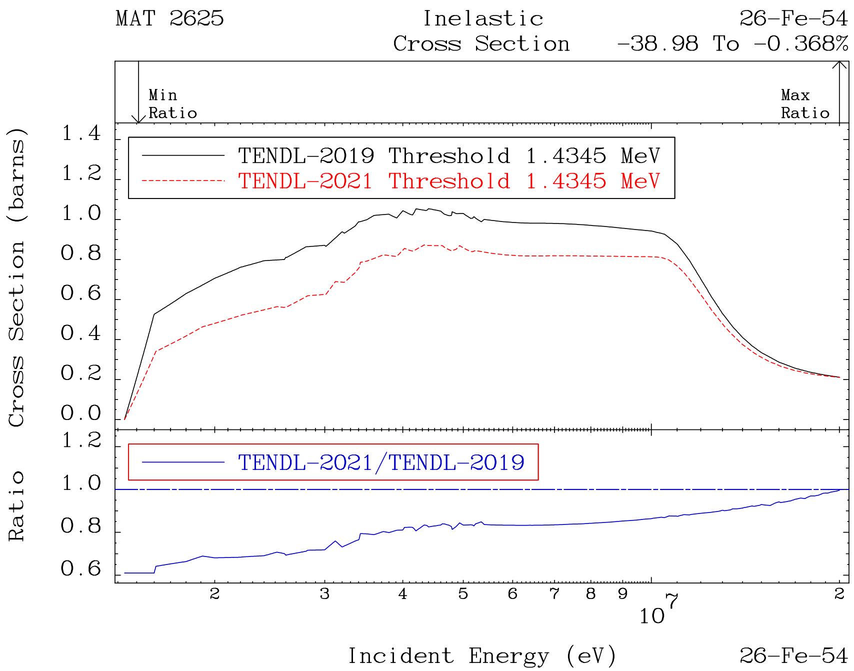
- JENDL-4.0 adopts Reich Moore formalism, TENDL-2019 uses Multi Level Breiter Wigner
- JENDL-4.0 includes more resonances than TENDL-2019
- The mf2 file has been adopted from JENDL-4.0 in this work, rather than from the Atlas like TENDL-2019

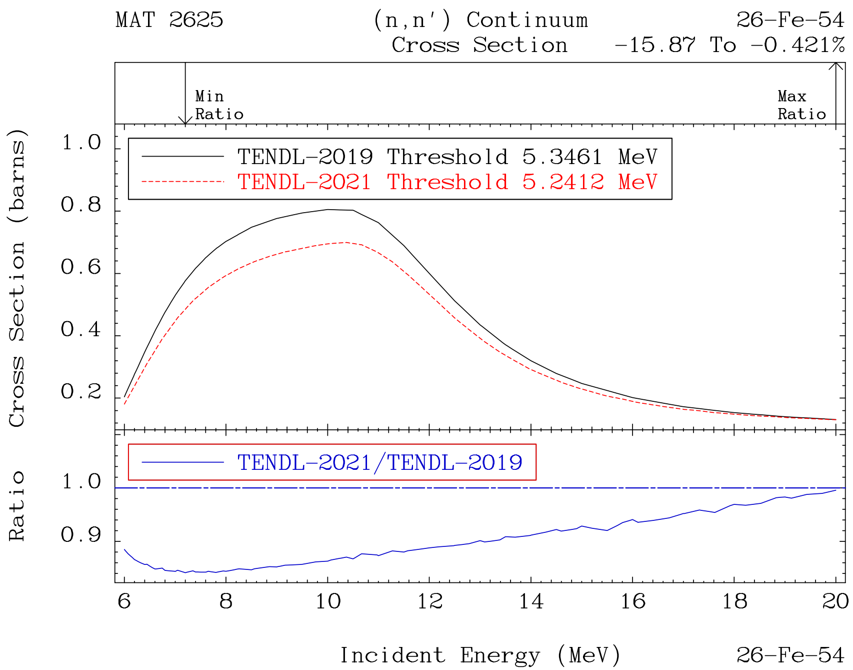


^{54}Fe evaluation

AUTONORM

- In this work, adopted for MT 4 and MT 51-53 and 55 from start of TALYS range until 6MeV
- Also adopted for MT 2 until 14 MeV
- The renormalisation performed in the second TALYS run acted on the continuum too, decreasing it. Thus, modifying TALYS parameters was not needed

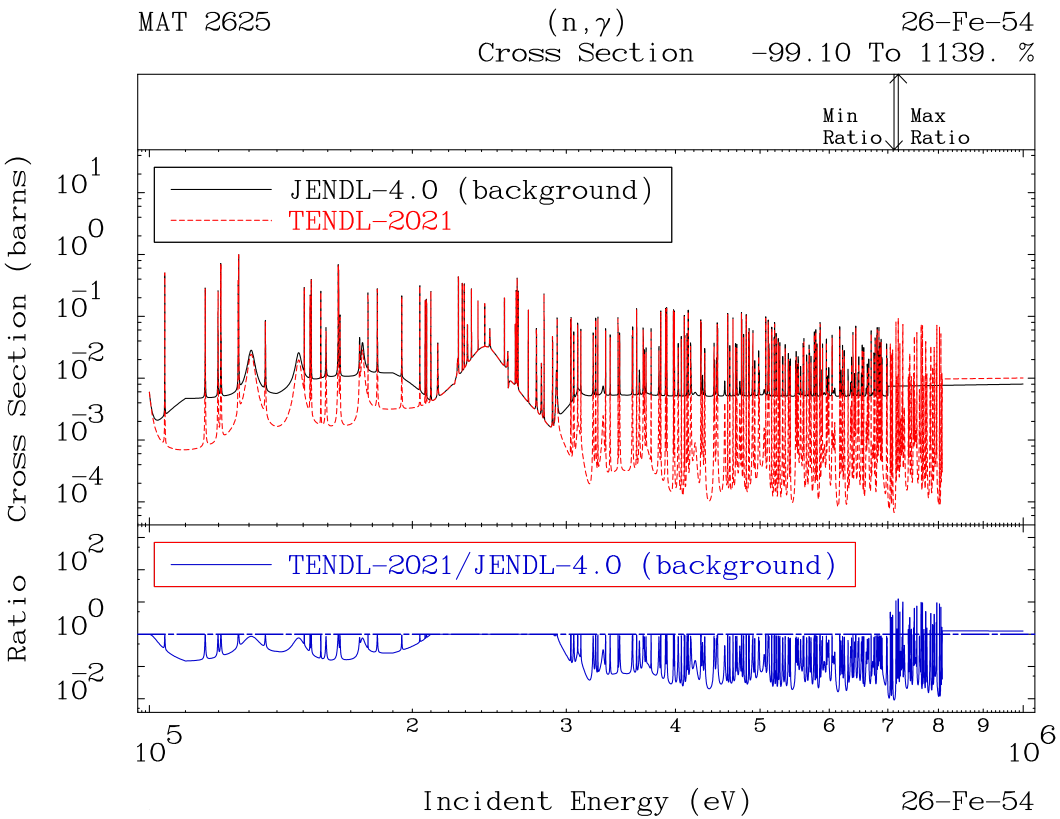




^{54}Fe evaluation

BACKGROUND

- JENDL-4.0 and TENDL-2019 use a background in the resolved resonance range for capture and total cross section
- Based on ASPIS it didn't seem necessary, so it was removed in this work



^{57}Fe evaluation?

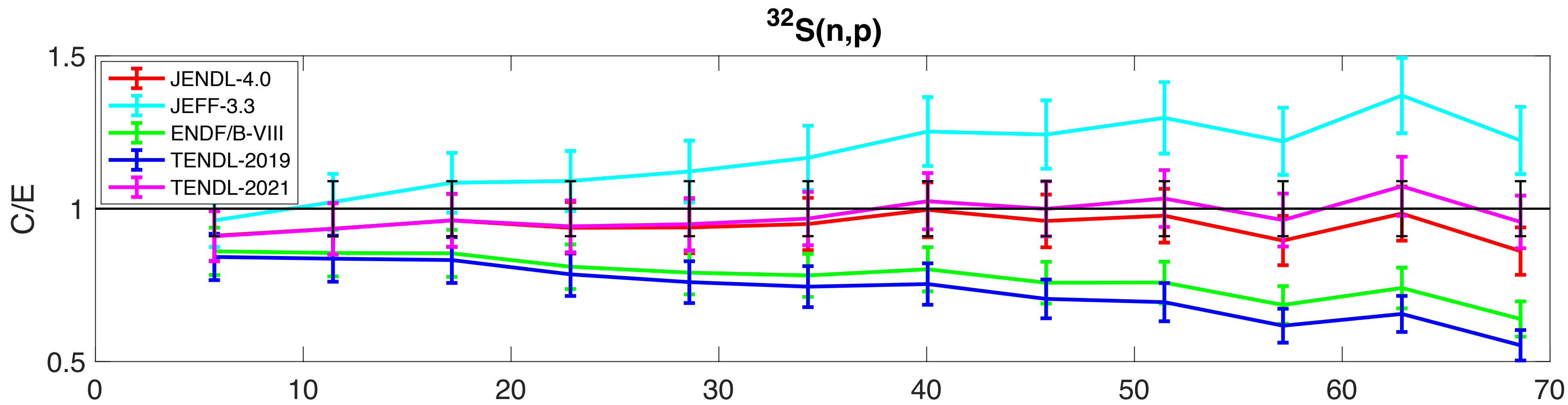
An attempt with ^{57}Fe was done too. However…

- Impact of small modifications can't be seen in integral benchmarks with natural iron
- Few differential experimental data exist
  - Mainly MT 4 (TENDL-2019 is too high) and MT 1 (TENDL-2019 seems ok, better than JENDL-4.0)
- All major libraries have significant differences in evaluation choices
  - JENDL-4.0 uses RM, TENDL-2019 uses MLBW
  - TENDL-2019 uses autonorm on MT 2,4,102 fitting ENDF/B-VIII.0
  - JENDL-4.0 uses a background for MT 102 and MT 1
  - ENDF/B-VIII.0 has oscillations in MT 51 (so in MT 4 too) and threshold around 15keV, and JENDL-4.0 takes that from ENDF/B. TENDL-2019 and JEFF-3.3 have no structure and different threshold

It is not clear in which direction to move!

Monte Carlo ASPIS results

- The ASPIS Benchmark Experiment was simulated with TRIPOLI-4®
- Big improvements at all energies compared to TENDL-2019
- The new ^{56}Fe and ^{54}Fe contributed equally to improve results from TENDL-2019
- The inelastic continuum influenced strongly the ^{32}S detector only



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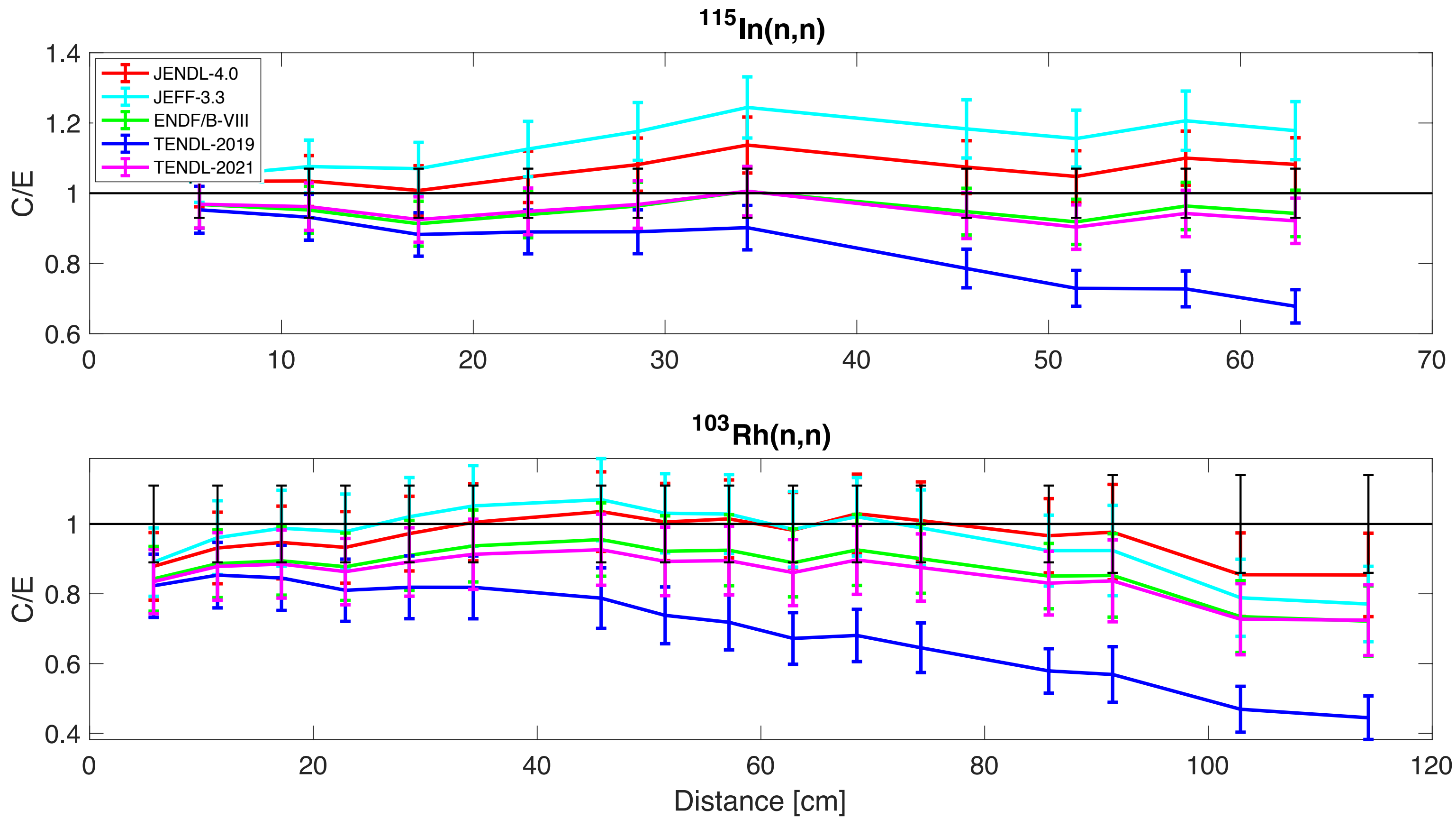
Monte Carlo ASPIS results

- The resonance parameters only impacted the two low energy detector



Lessons learnt

- Differential experimental data are not always the best reference for cross sections – especially for scattering, tricky to measure
- TALYS parameters cannot do all the heavy lifting by themself
- The devil is in the detail: resonance parameters make a huge difference and should be double checked
- The use of a background is dangerous, and often goes unnoticed. It should be unnecessary, if the high energy data has been modelled properly

Conclusions and Future Work

CONCLUSIONS

- New evaluation files were produced with T6 for ^{56}Fe and ^{54}Fe
- They perform extremely well on the ASPIS Iron Benchmark Experiment
- The new input files will be the ‘best’ inputs of TENDL-2021

FUTURE WORK

- Run MCNP to corroborate TRIPOLI-4®’s results
- Test the files on different benchmarks, e.g. at high energies, like TIARA, and fusion benchmarks

THANK YOU FOR YOUR ATTENTION