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FISPACT-II & TENDL: developments to model high-energy activation, transmutation processes and radiation damage source terms

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Research Councils UK Energy For a Low Carbon Future

IAEA 60 Years Atoms for Peace and Development

CCFE CULHAM CENTRE FOR FUSION ENERGY

Nuclear landscape: elemental periodic table

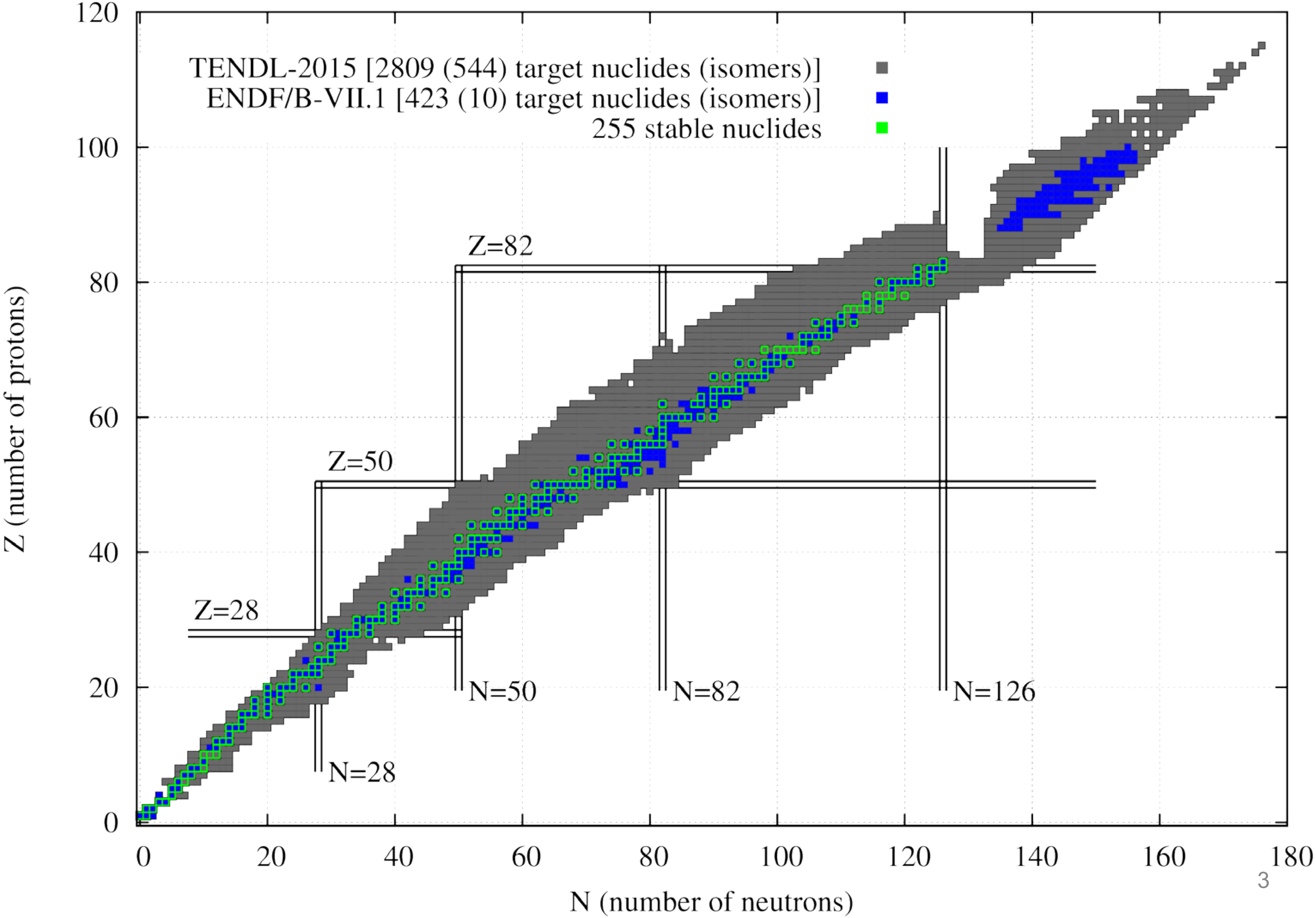
Periodic Table of the Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.732	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 84.798
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71 Lanthanides	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103 Actinides	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [278]	110 Ds Darmstadtium [281]	111 Rg Roentgenium [280]	112 Cn Copernicium [285]	113 Nh Nihonium [286]	114 Fl Flerovium [289]	115 Mc Moscovium [289]	116 Lv Livermorium [293]	117 Ts Tennessine [294]	118 Og Oganesson [294]

57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.243	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967
89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]

Alkali Metal | Alkaline Earth | Transition Metal | Basic Metal | Semimetal | Nonmetal | Halogen | Noble Gas | Lanthanide | Actinide

Nuclear landscape: Isotopic targets



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TENDL: from MF-1 to MF-40, 200 MeV

- MF-1: Description + fission parameters
- MF-2: Resonance parameters (Reich-Moore or Multi-level Breit Wigner)
- MF-3: Cross sections (n,tot), (n,el), (n,non), (n,inl$_i$), …, (n,γ), (n,p$_i$), (n,α_i)
- MF-4: Elastic angular distribution (Legendre Polynomials)
- MF-5: Fission neutron spectrum
- MF-6: Double differential distributions and spectra for (n,2n), …, (n,α_i)
- MF- 8-10: Isomeric cross sections
- MF- 12-15: Gamma yields, angular distributions and spectra
- MF- 31-32-33-34-35, 40: nubar, Resonance parameter, cross section, angular distribution and fission neutron spectrum, radionuclide production.

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Nuclear Data Sheets 113 (2012) 2841–2934

Nuclear Data Sheets

www.elsevier.com/locate/nds

Modern Nuclear Data Evaluation with the TALYS Code System

A.J. Koning* and D. Rochman

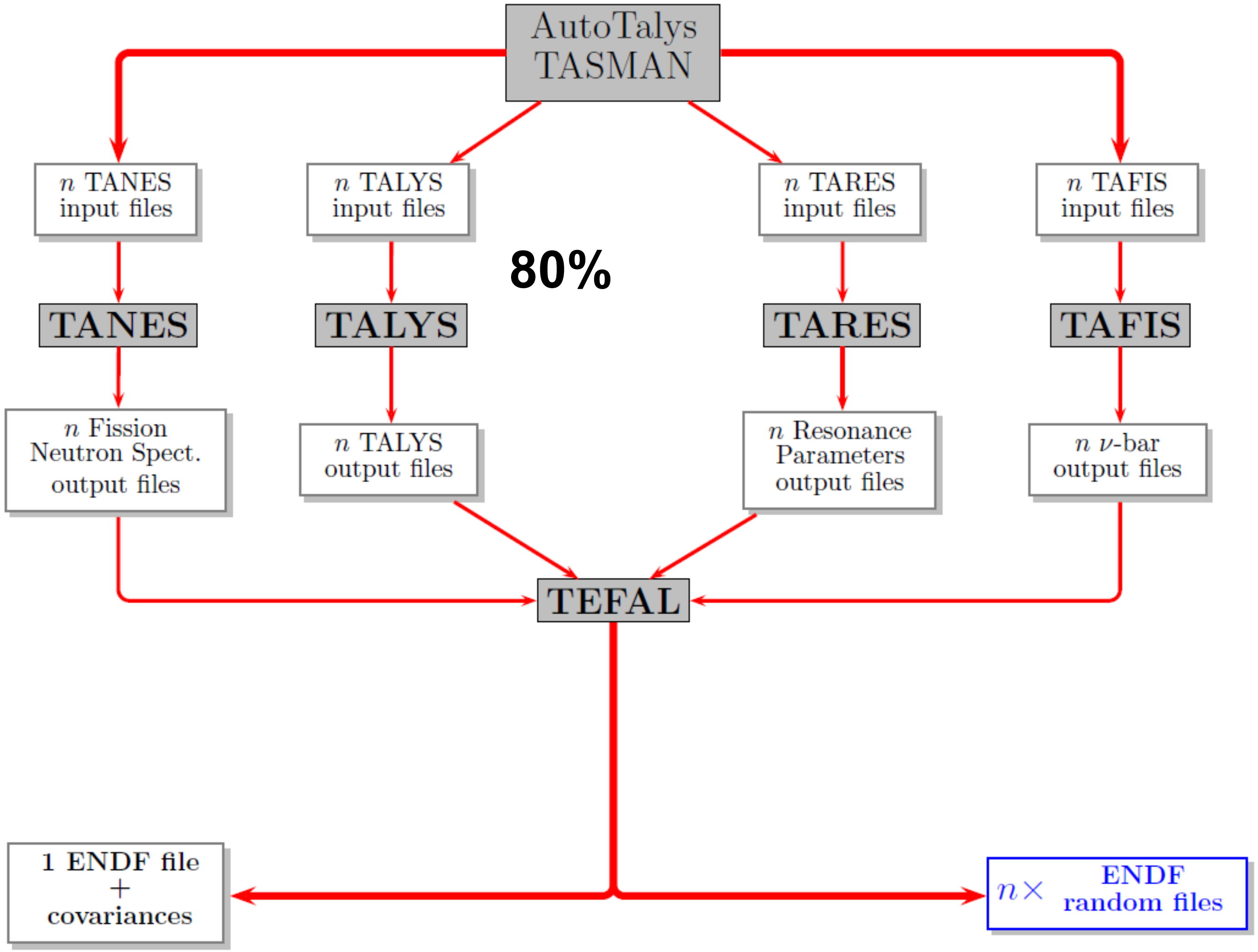
Most Cited Articles

The most cited articles published since 2011, extracted from Scopus .

1. ENDF/B-VII.1 nuclear data for science and technology: Cross sections, covariances, fission product yields and decay data
   M. B. Chadwick | M. Herman | ...
2. Modern Nuclear Data Evaluation with the TALYS Code System
   A. J. Koning | D. Rochman

The making of TENDL: T6 infrastructures

- T6: at the origin of TENDL: combination of 6 codes plus utilities
- Allow to loops over nuclear science ➔ variance-covariance



TENDL's advantages

- All targets isotopes in the same evaluated data forms, 10^{-5} eV to 200 MeV, with variance-covariance (MF-31 to 40), isomers as target ($T_{1/2}$ > 1 s) and daughters ($T_{1/2}$ > 0.1 s)
- 8th version, "putting 69 nuclear physics codes to work"

	Neutron	Proton	Deuteron	Triton	Alpha	Helium3	Photon	Fi. Yields	Covariances
TENDL-2015	**2809**	**2804**	**2804**	**2803**	**2804**	**2804**	**2804**	**16**	**2805**
TENDL-2014	**2632**	**2629**	**2629**	**2629**	**2629**	**2629**	**2629**	**-**	**2632**
TENDL-2013	**2630**	**2625**	**2625**	**2625**	**2624**	**2624**	**2626**	**-**	**2630**
TENDL-2012	**2435**	**2429**	**2428**	**2348**	**2429**	**2429**	**2430**	**-**	**2338**
TENDL-2011	**2425**	**2429**	**2419**	**2431**	**2429**	**2428**	**2428**	**574**	**2416**
TENDL-2010	**2394**	**1157**	**1159**	**1156**	**1159**	**1140**	**1152**	**529**	**1086**
TENDL-2009	**2375**	**1163**	**1164**	**1116**	**1163**	**1127**	**1165**	**509**	**1141**
TENDL-2008	348	344	336	339	342	338	327		**342**
(JEFF-3.2)	*472*								*218*
(ENDF/B-VII.1)	*423*	*47*	*5*	*3*		2	*163*	*80*	*146*
(JENDL-4.0)	*406*								*90*

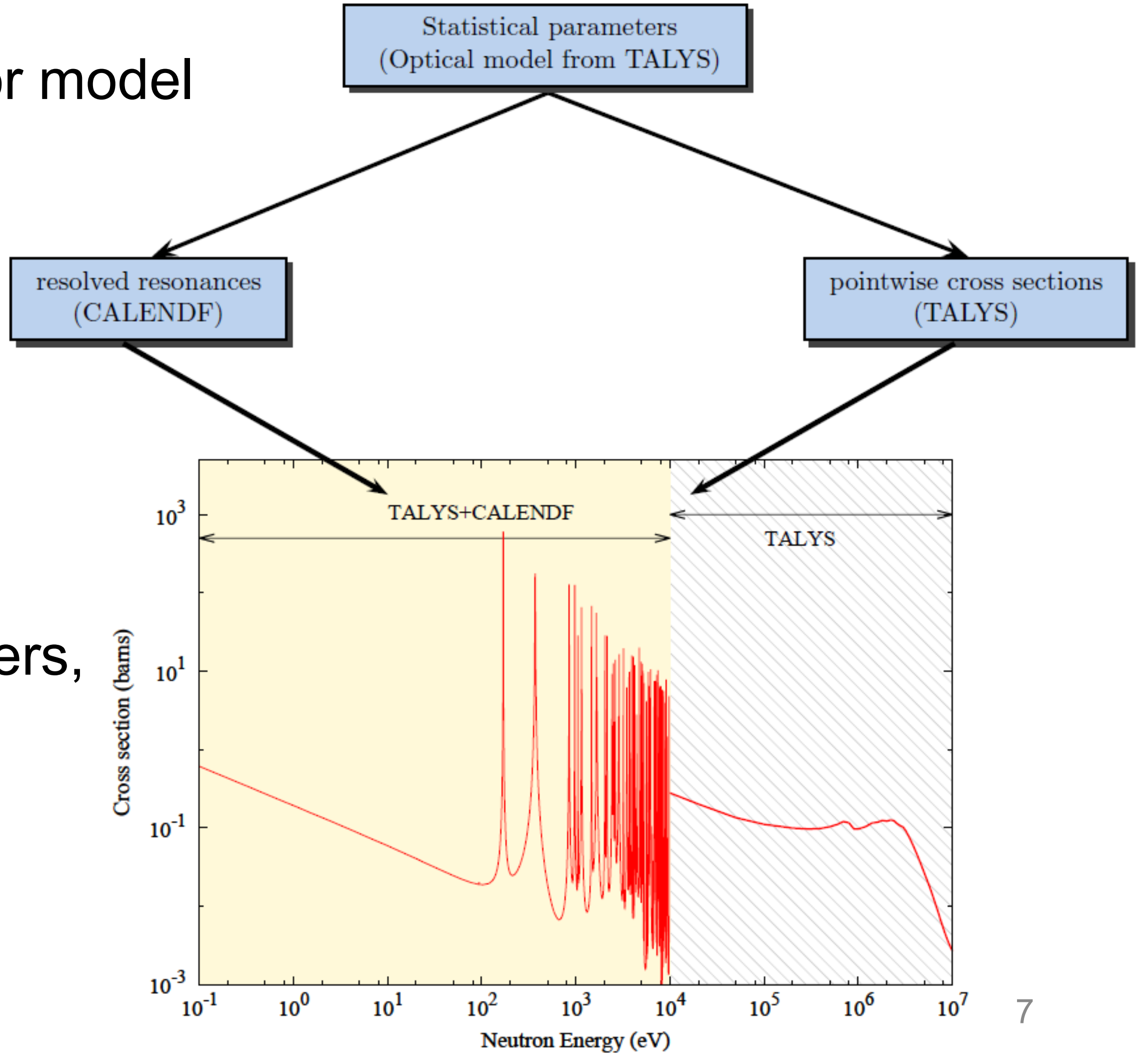
T6 infrastructures

The TENDL infrastructure combines other methods:

- (fast) TMC: Total Monte Carlo for uncertainty propagation

- BMC: Bayesian Monte Carlo for model parameter updates and sampling

- HFR: Resonance parameters for all targets isotopes consistent with the fast neutron range : Level Densities, Optical Model Parameters, Gamma-ray Strength Function,…



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Processing steps: three codes

ENDF file

- **NJOY12-082**
  - reconr
  - broadr
  - unresr
  - thermr
  - heatr
  - gaspr
    - purr
    - acer
    - groupr

ACE file

cross-check

- **PREPRO-2015**
  - **linear**
  - **recent**
  - **sigma1**
  - **sixpack**
  - **activate**
  - **merger**
  - **dictin**
  - **groupie**

Processed ENDF file

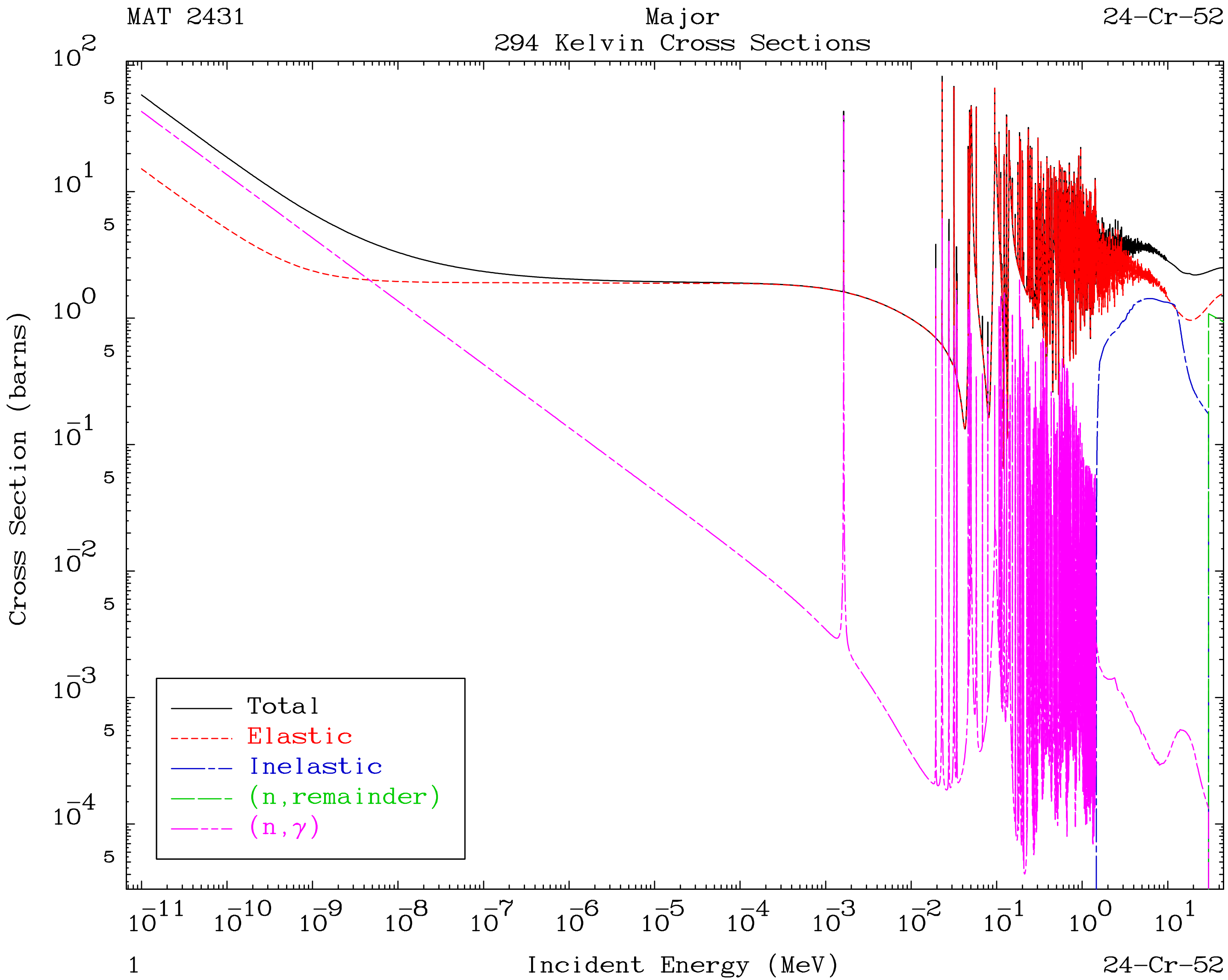
cross-check

- **CALENDF-2010**
  - calendf
  - regroutp
  - lecritp
  - ….

PT file

Single script for an entire library

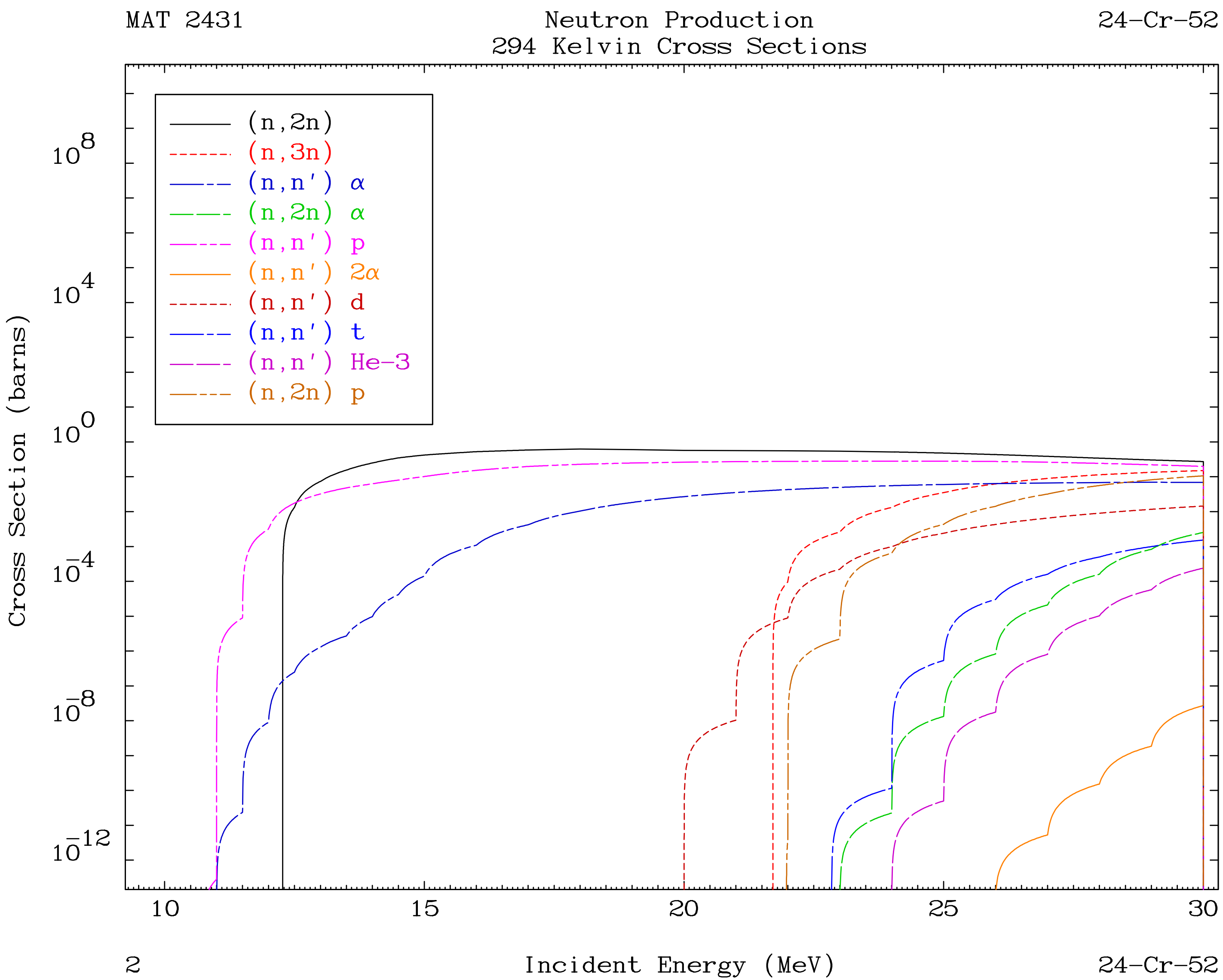
TENDL-2015 pendf, 200 MeV



90 reaction types

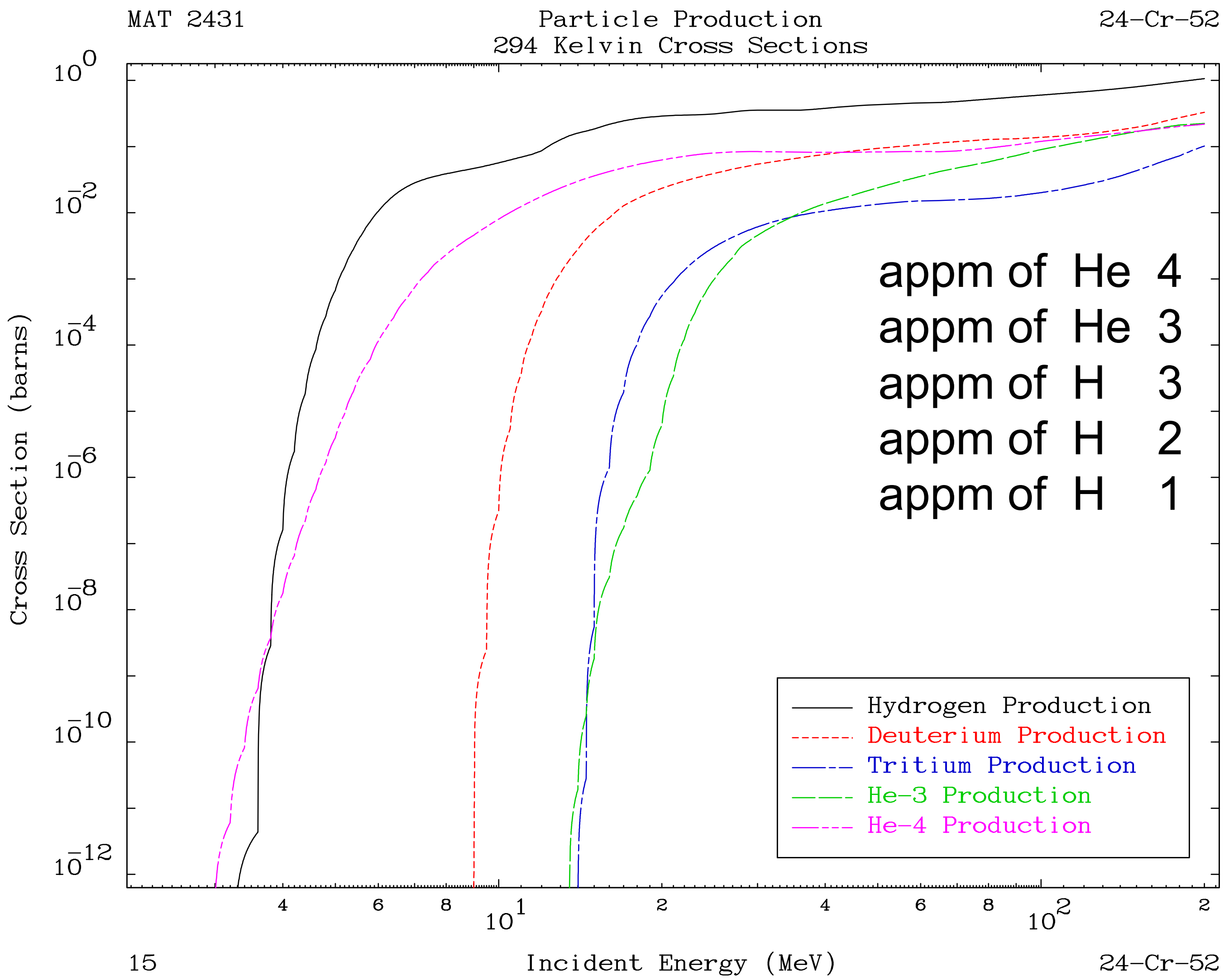
(n, remainder) =mf3-mt5*mf6 above 30 MeV

TENDL-2015 pendf, below 30 MeV



TENDL-2015 pendf, 200 MeV

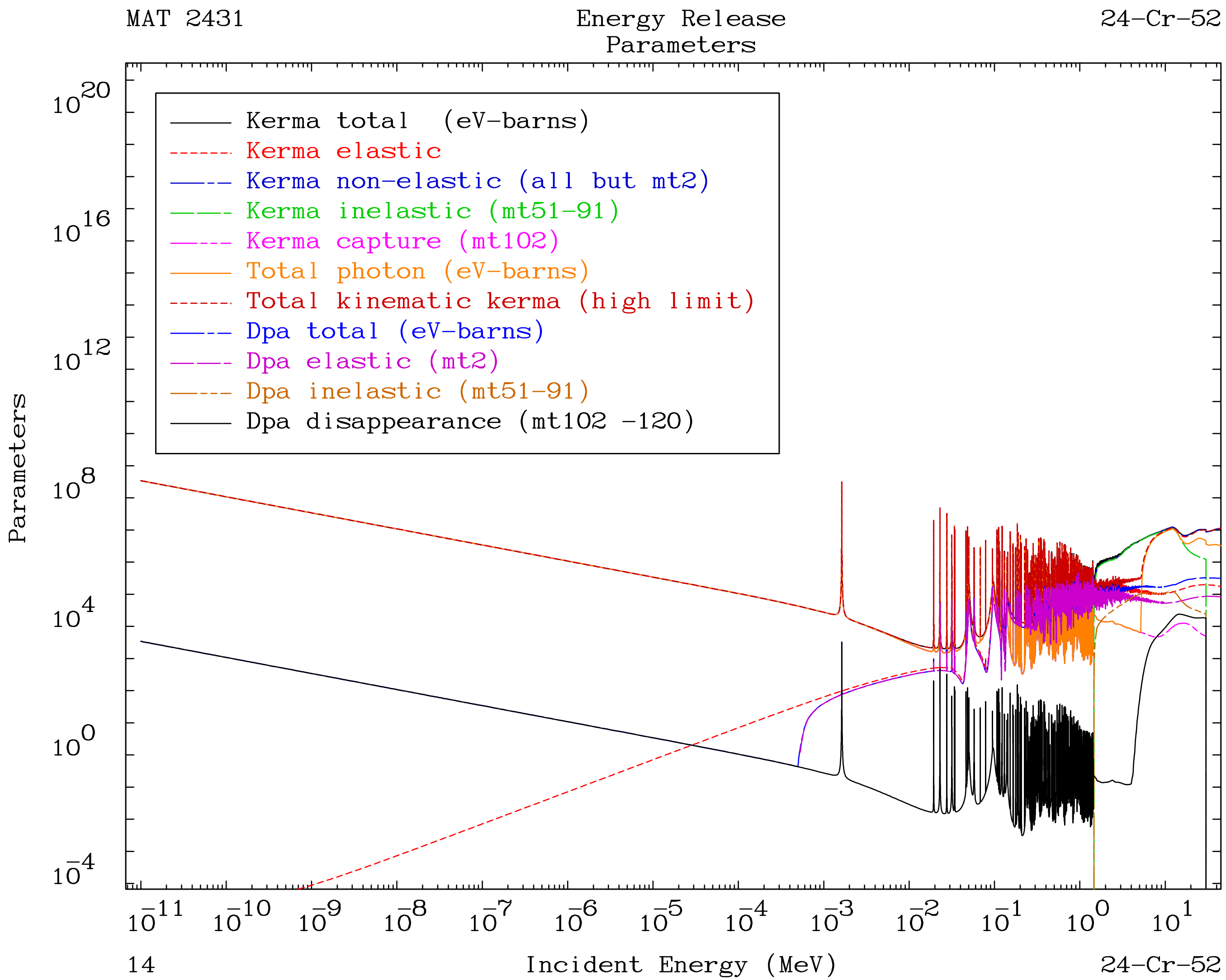
Gas production



appm of He 4 = 1.13E+03
appm of He 3 = 1.30E-02
appm of H 3 = 1.43E-18
appm of H 2 = 2.07E+01
appm of H 1 = 1.18E+03

NJOY generated Gas production MT's displayed by PREPRO

TENDL-2015 pendf, 200 MeV



Total, partials Kerma

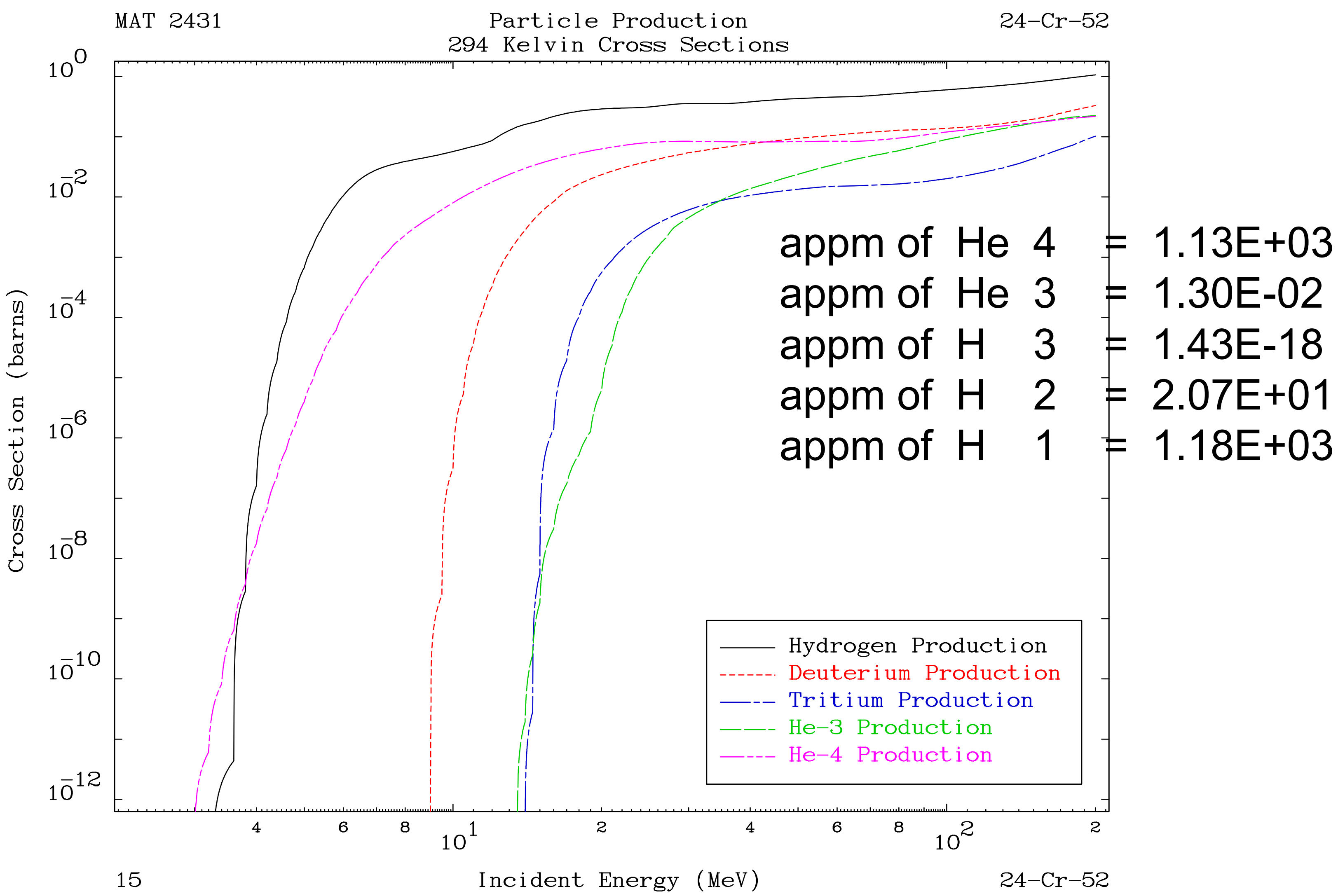
Total, partials Dpa

Only from fully populated files

NJOY generated KERMA and DPA MT's displayed by PREPRO

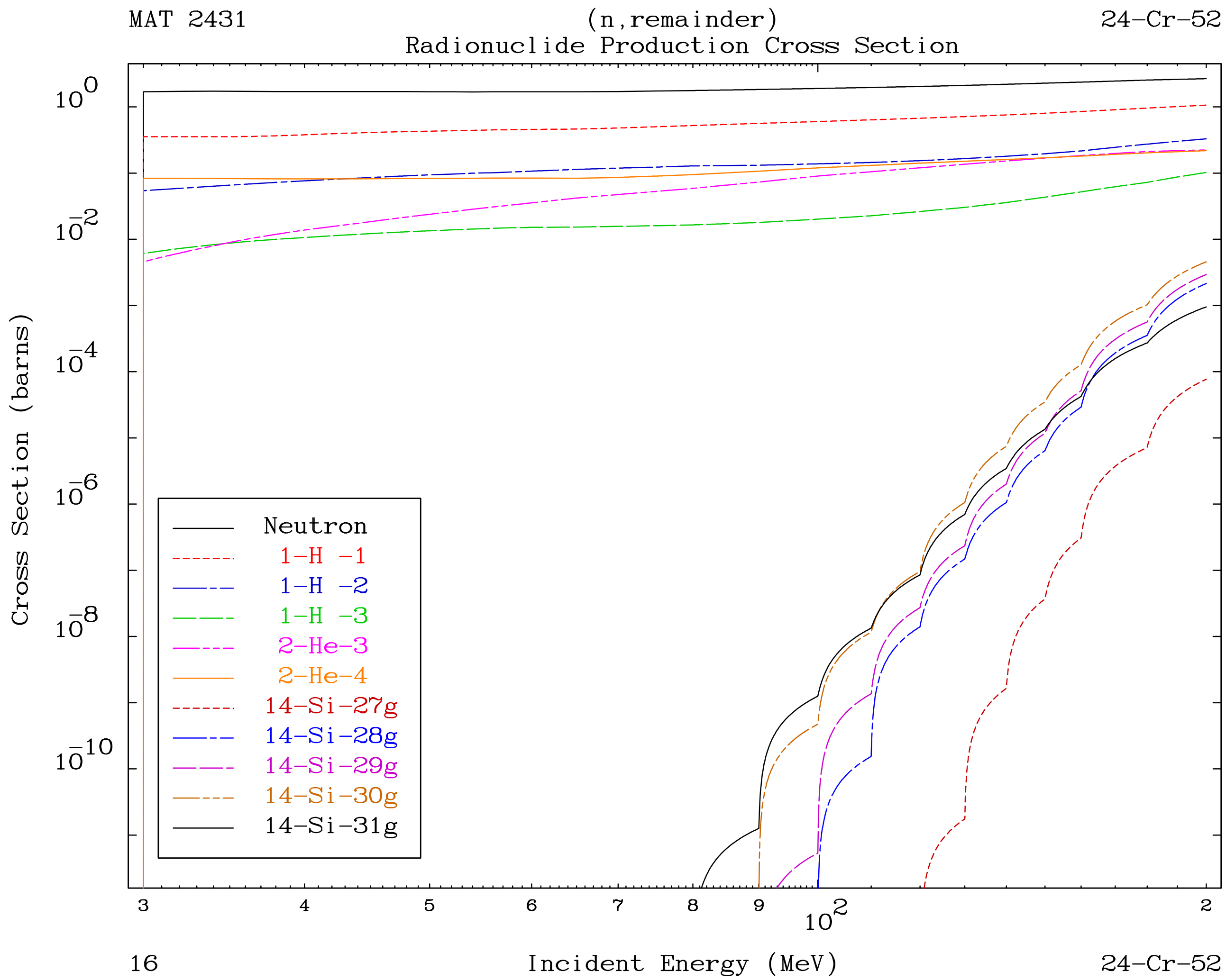
TENDL-2015 pendf, 200 MeV

Gas production



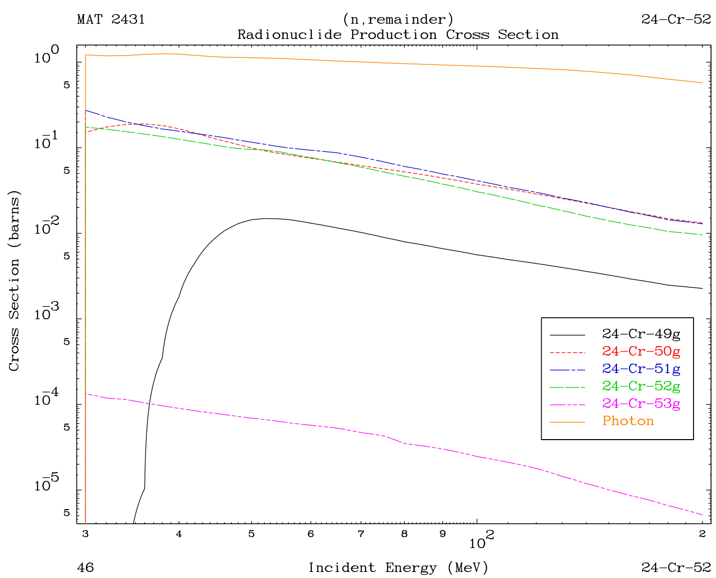
NJOY generated gas production MT's displayed by PREPRO

TENDL-2015 pendf from mf3*mf6



Cross section channels above 30 MeV

A < 4 and A > 4 productions cross sections



Unique processing to PREPRO-2015 mf10-mt5, with isomers

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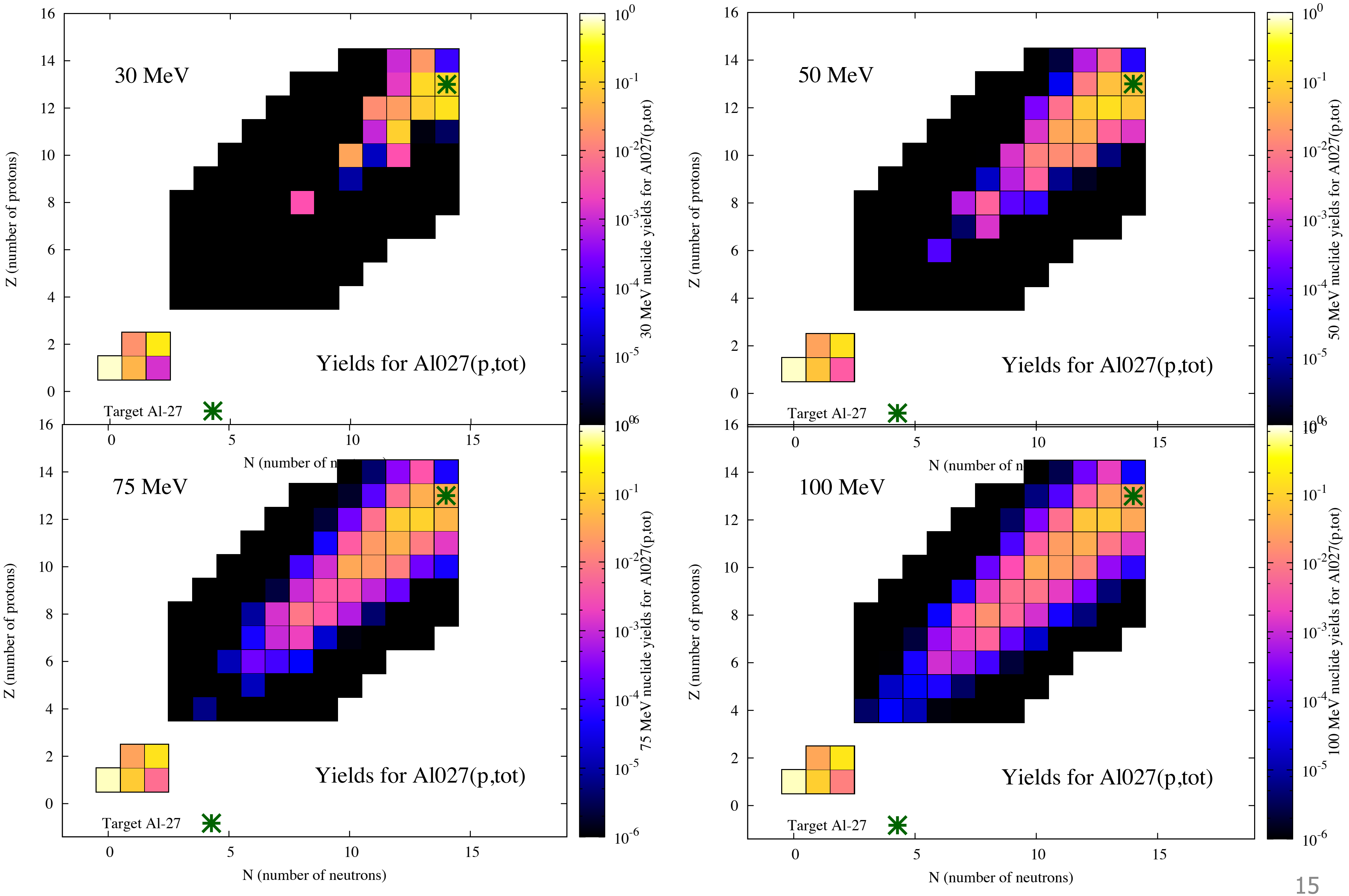
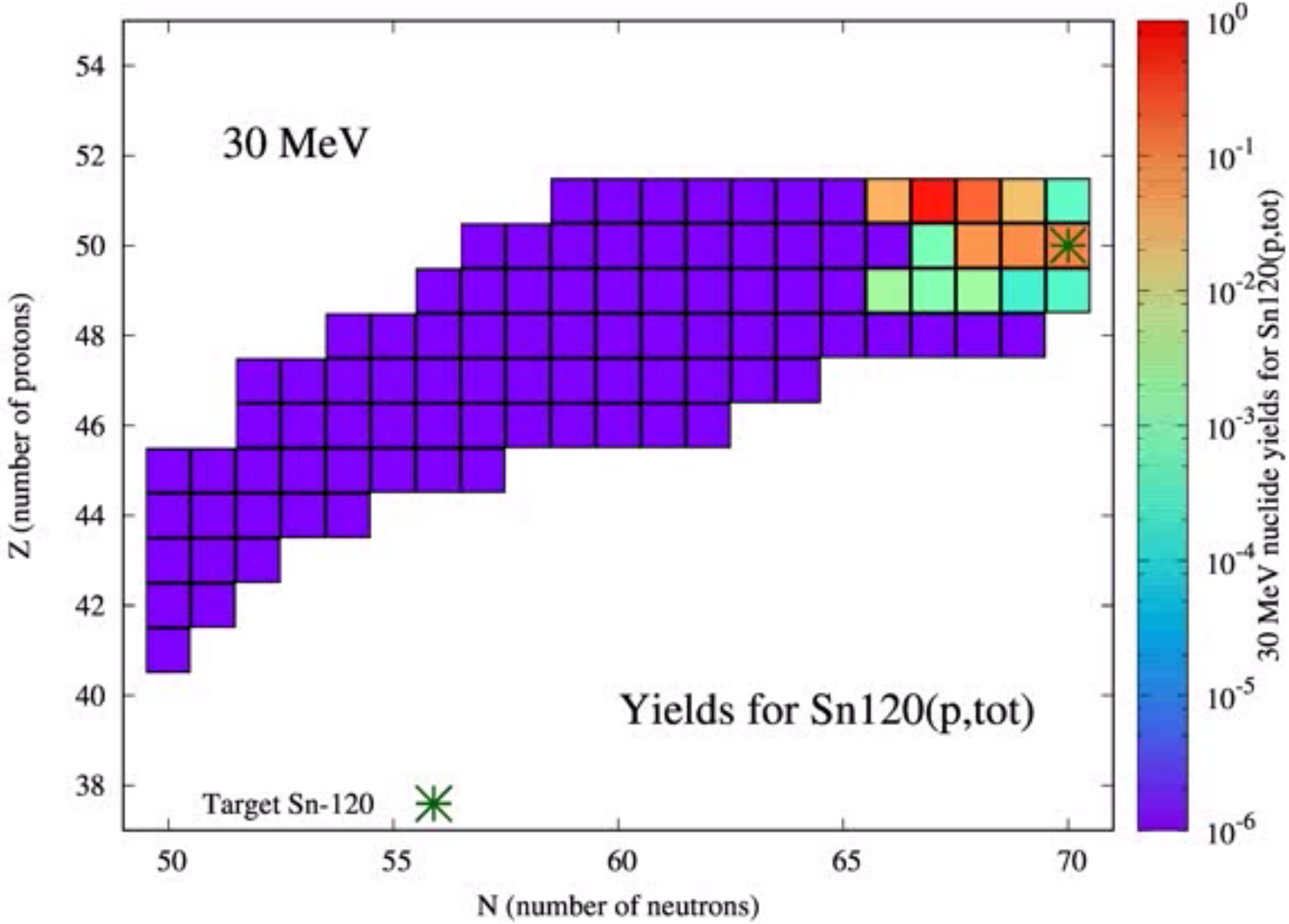
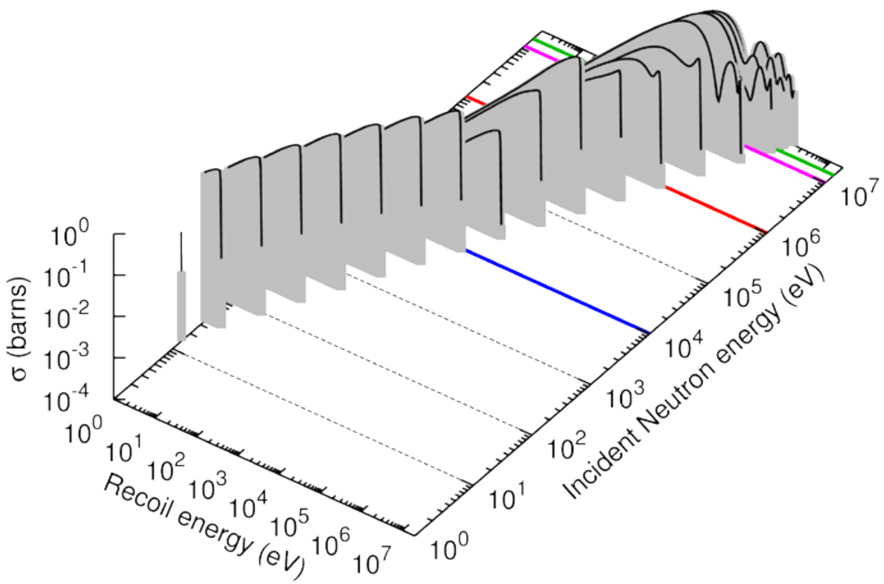
TENDL-2015 proton [Al27]

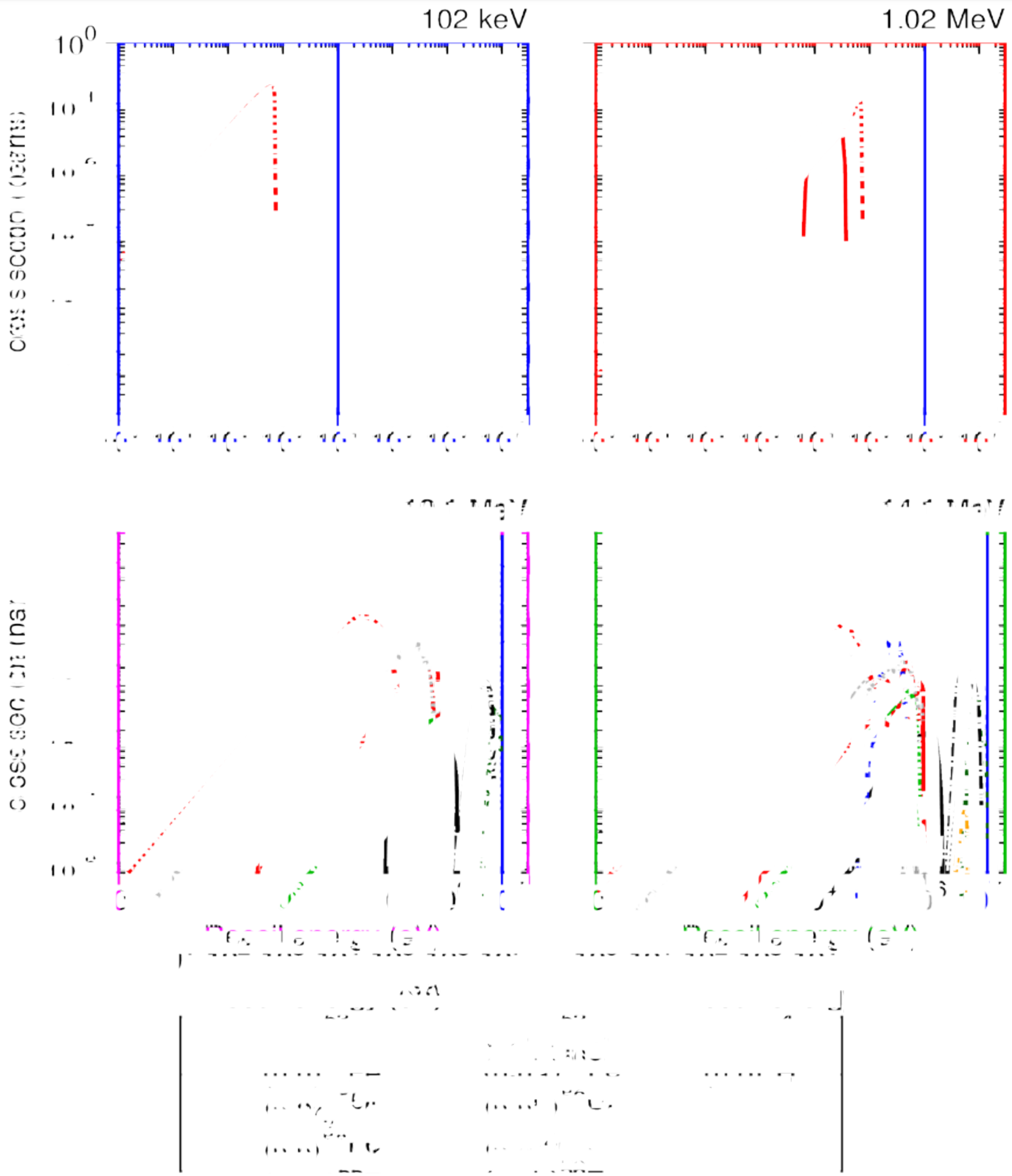


TENDL-2015 proton [Sn120]



PKA spectra – recoil matrices & vectors



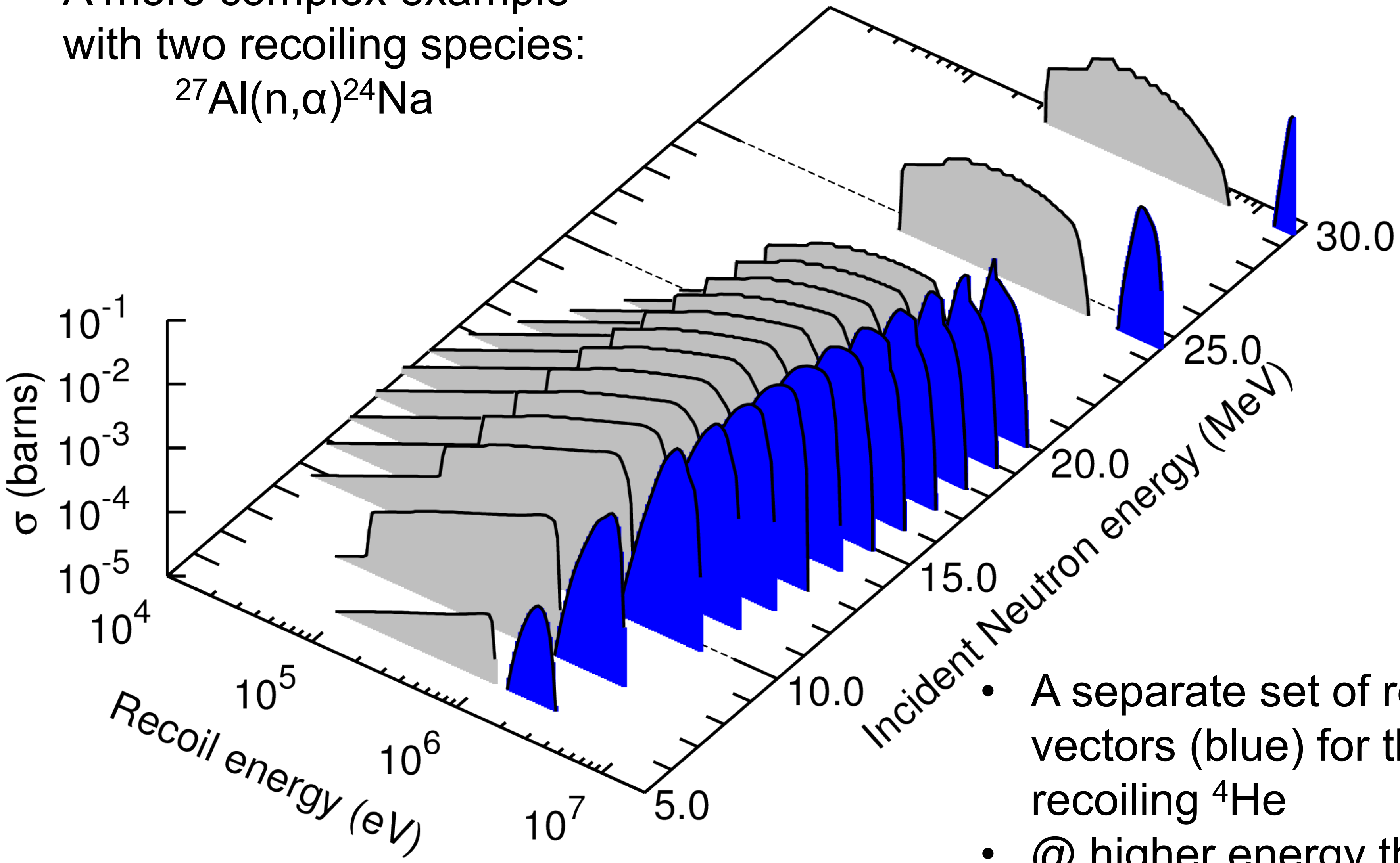


- In ^{56}Fe: at low incident energy only elastic channels is important
- Number of contributing channels increases dramatically at higher energies (MeV range)

TENDL results

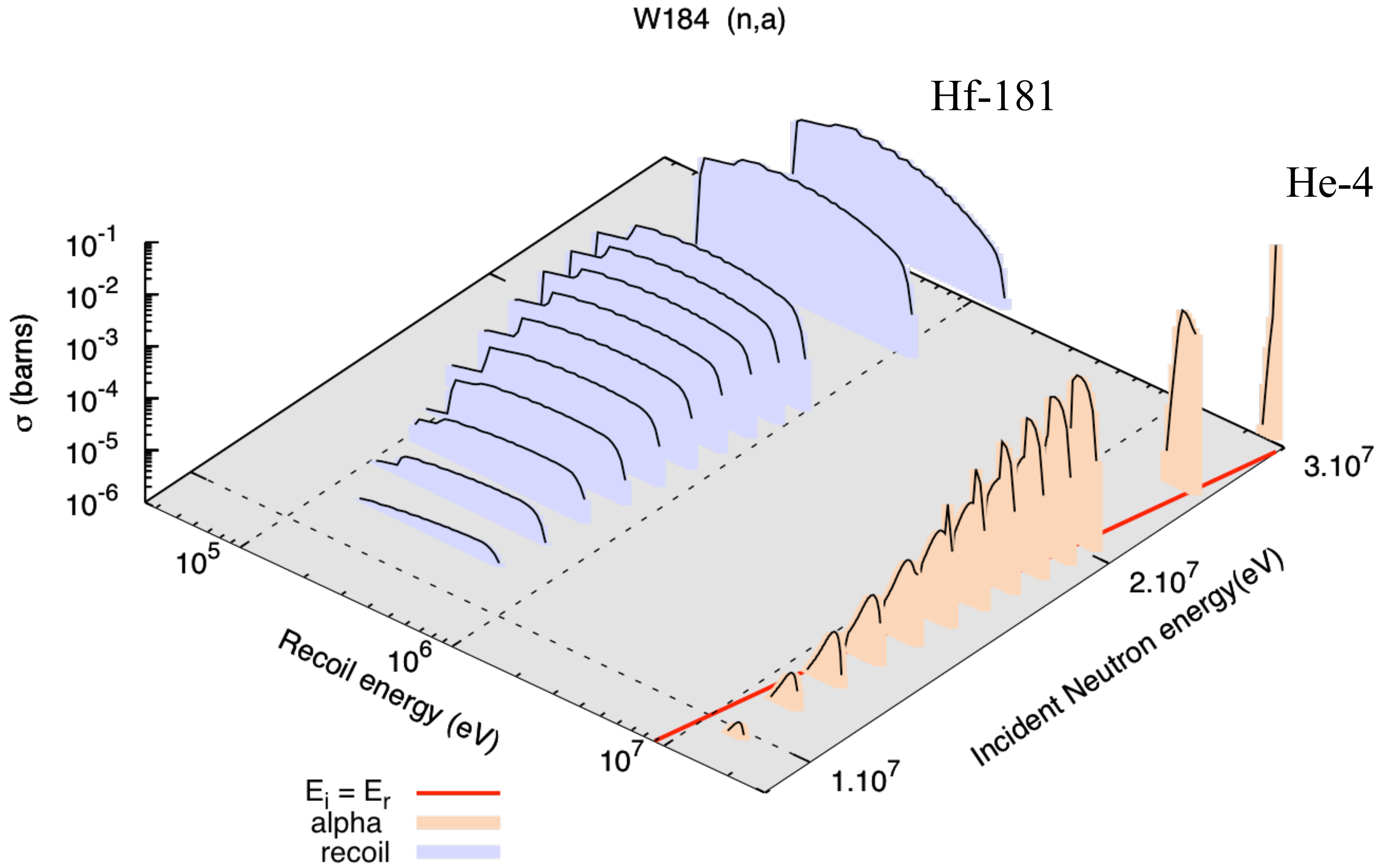
PKA spectra – recoil matrices

- A more complex example with two recoiling species: $^{27}Al(n,\alpha)^{24}Na$



- A separate set of recoil vectors (blue) for the recoiling ^{4}He
- @ higher energy than heavy ^{24}Na recoil (mass partition)

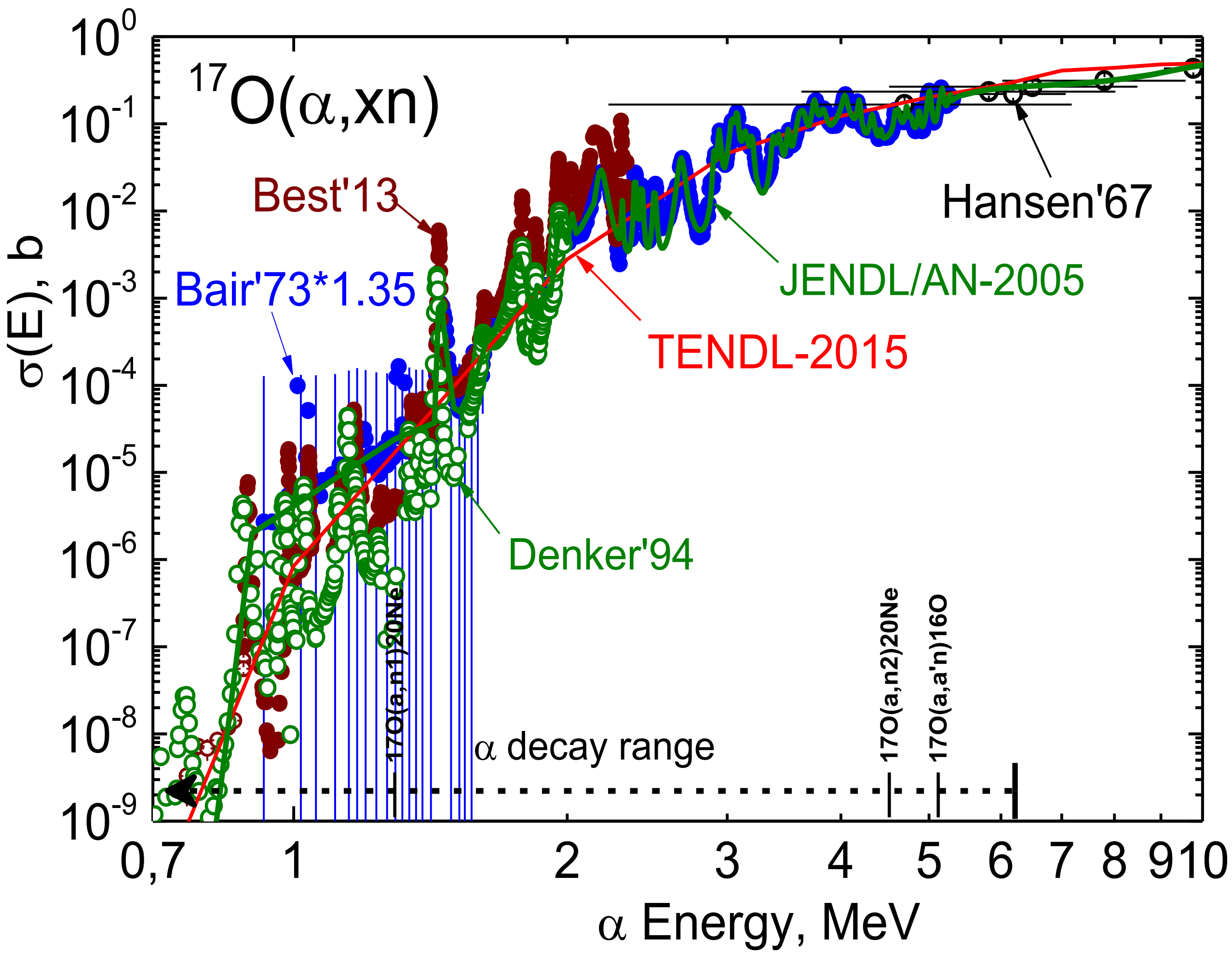
W-184 TENDL example



Q positive (7.3 MeV) means that the alpha energy can be much higher than the energy of the incident neutron

TENDL-2015 α-incident

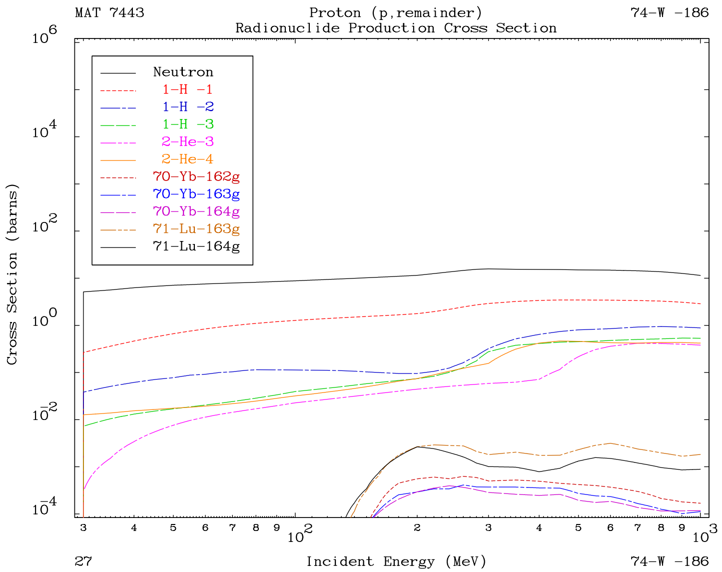
Actinide decays and consequent (α,xn) reactions for reactor fuel materials UO_2, UC, UF_6, PuO_2 and PuF_4

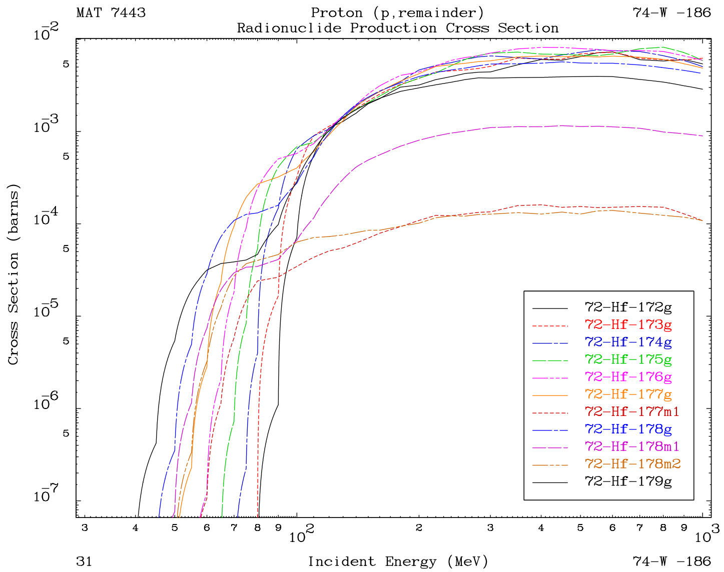


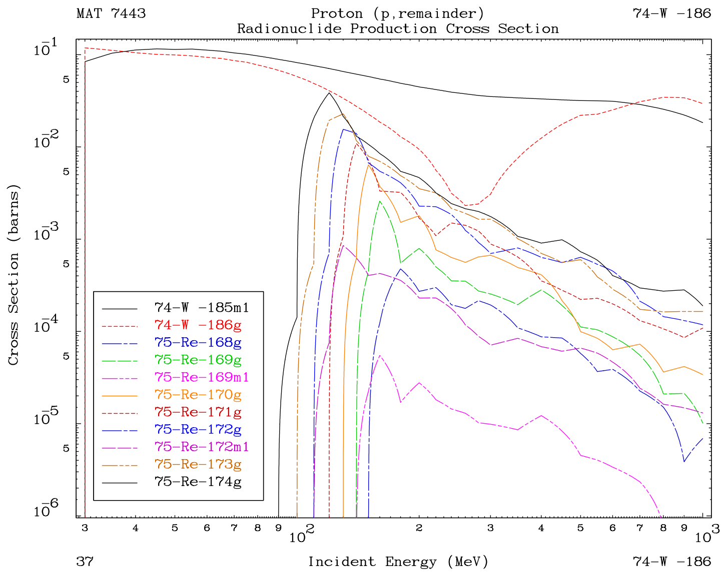
Only two libraries for Alpha induced!
17 targets in JENDL

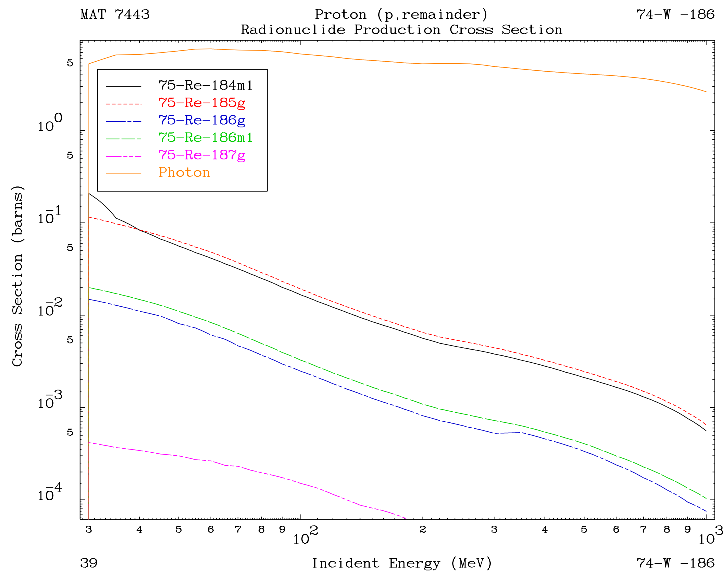
TENDL-2015 is also been used in fuel denaturing studies

TENDL-2015 p-incident up to GeV



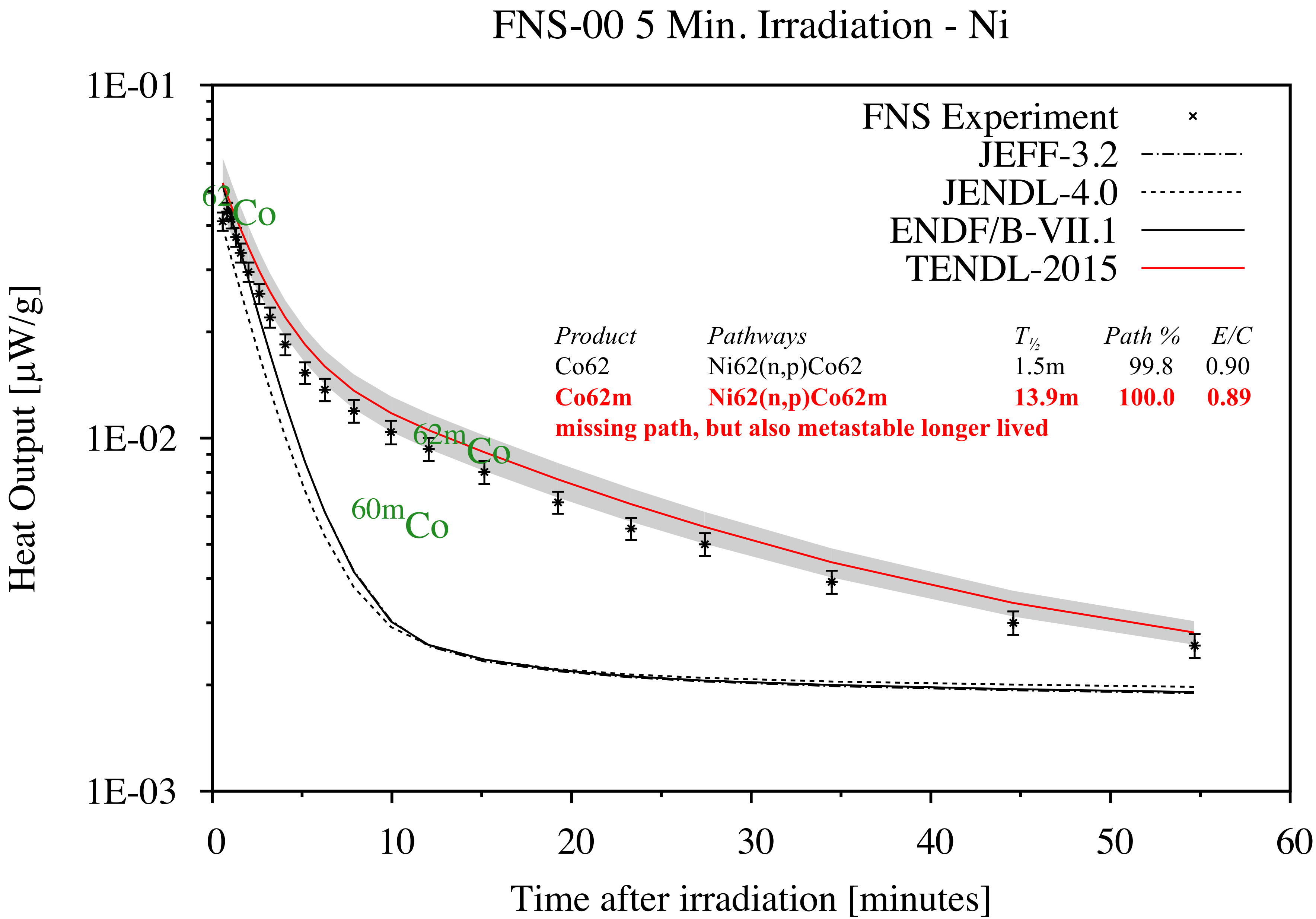






Decay power: FNS JAERI

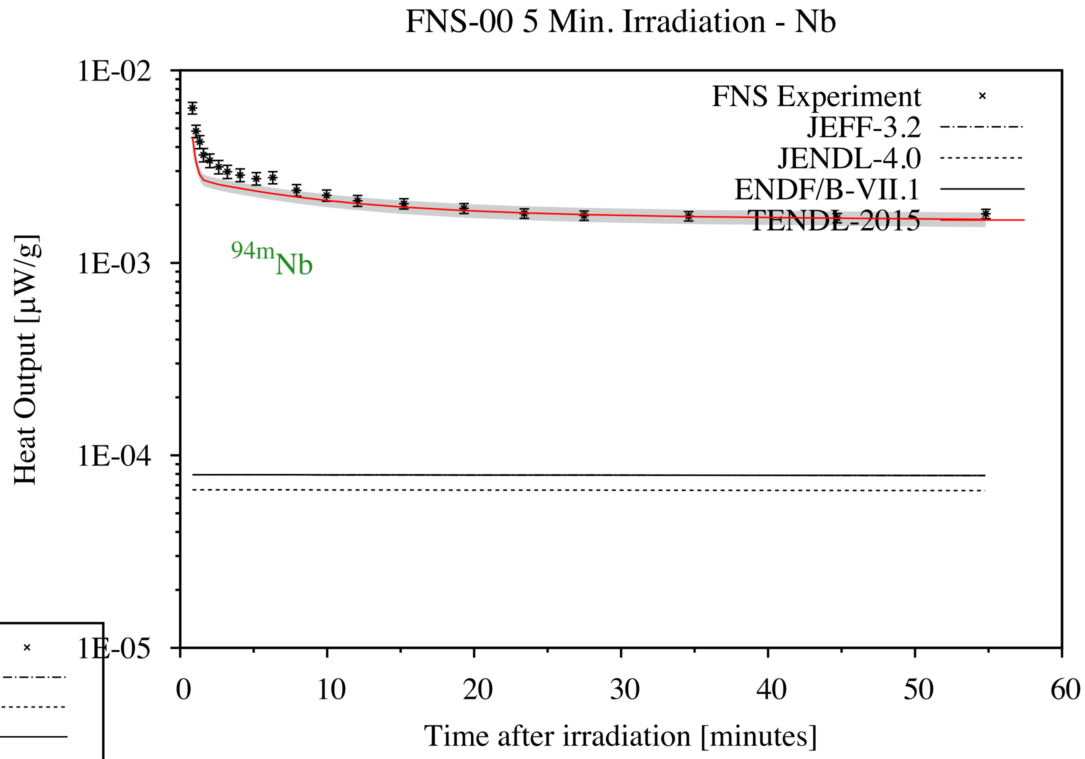
Random walk uncertainty

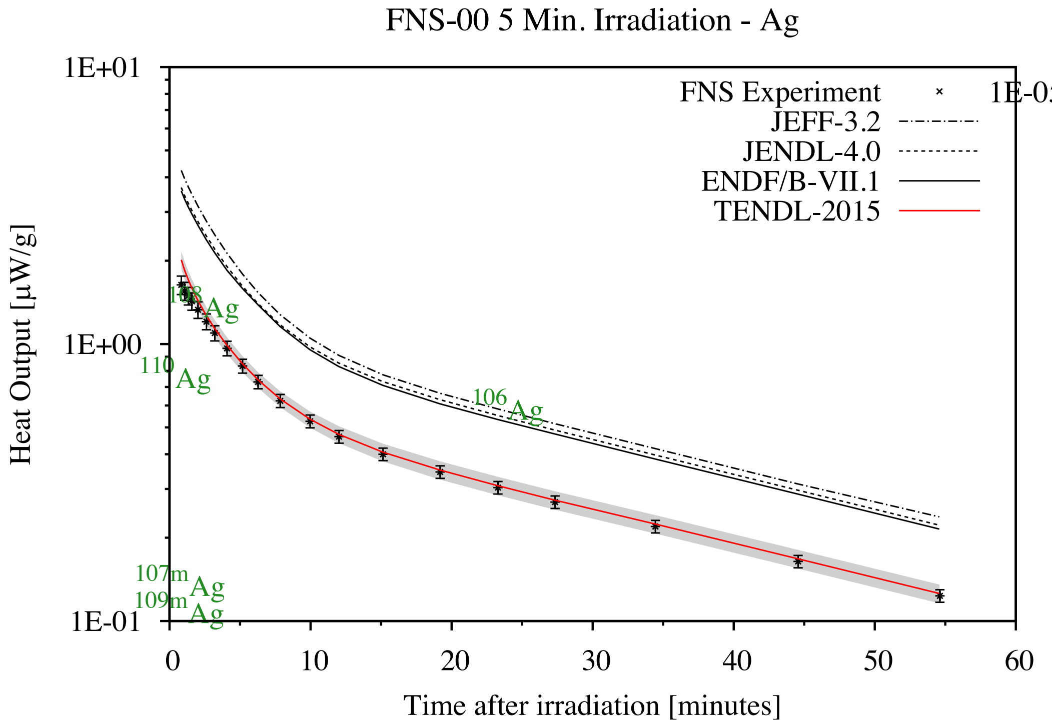


Decay power: FNS JAERI

When you do not account for isomer production channels….

The responses are missed entirely !!



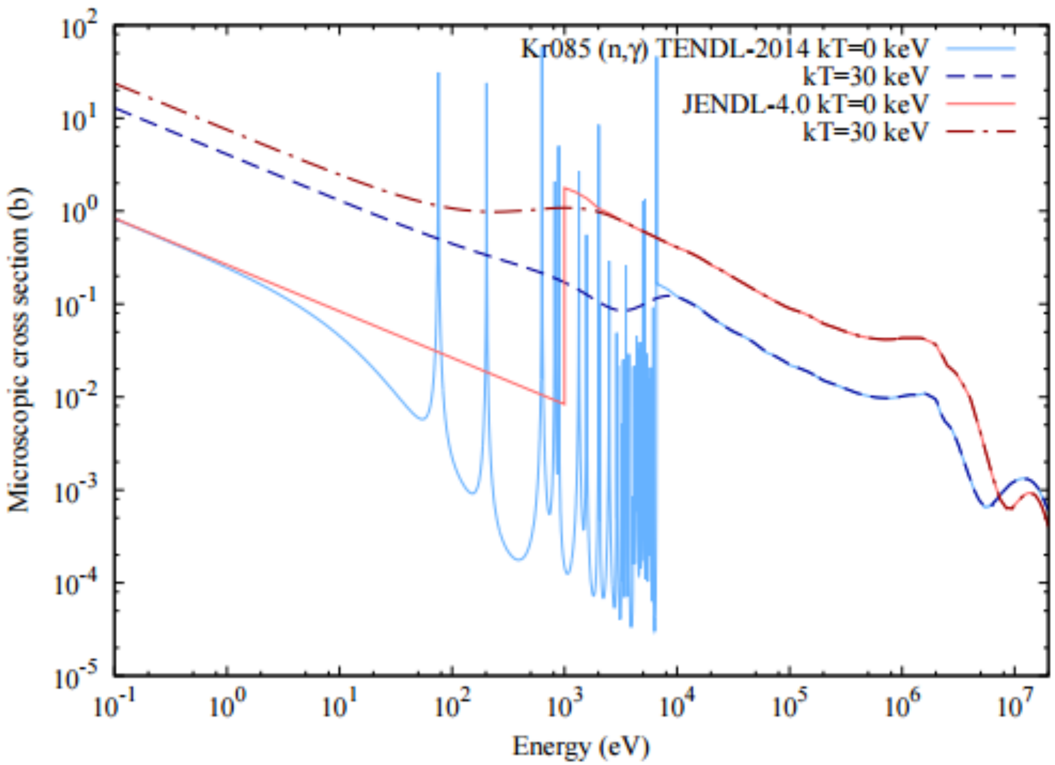


Hunt for the isomers

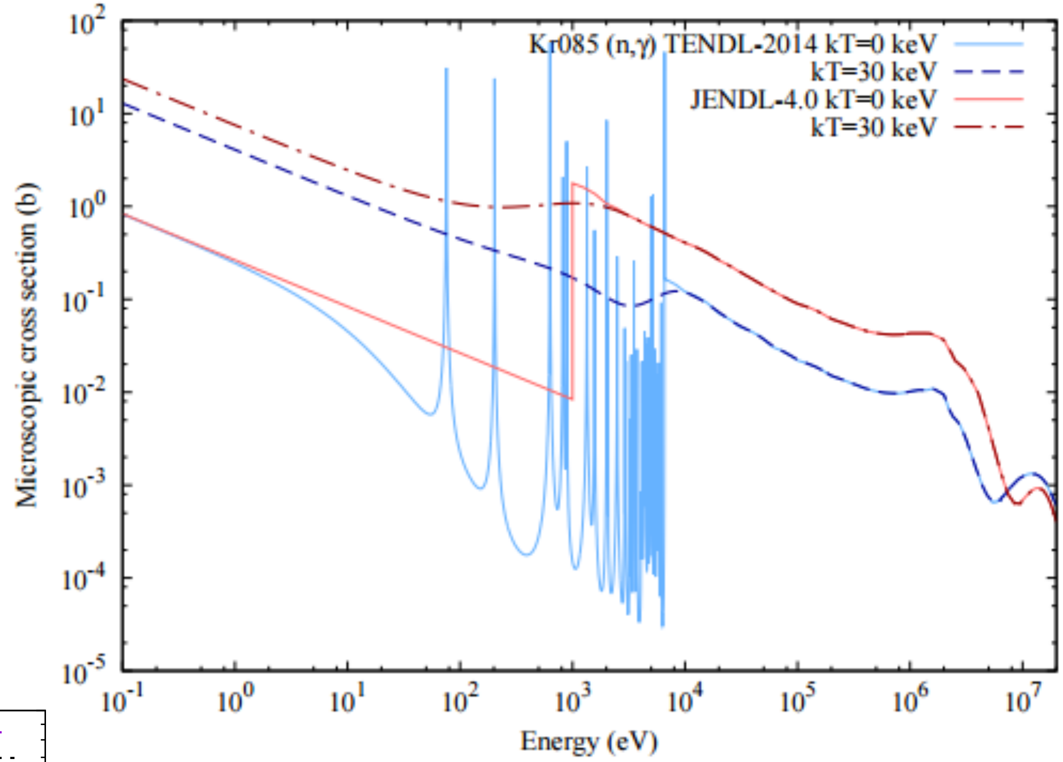
Most are lost in seconds, minutes…

Capture reactions

- Neutron capture and other reactions are exothermic, allowing the reaction at any incident energy
- These reactions possess resonance structure which often determines reaction rate (aside from thermal spectra systems)
- Either the resonances have been measured, we statistically resolve them or (in non-TENDL) we get unphysical straight lines…

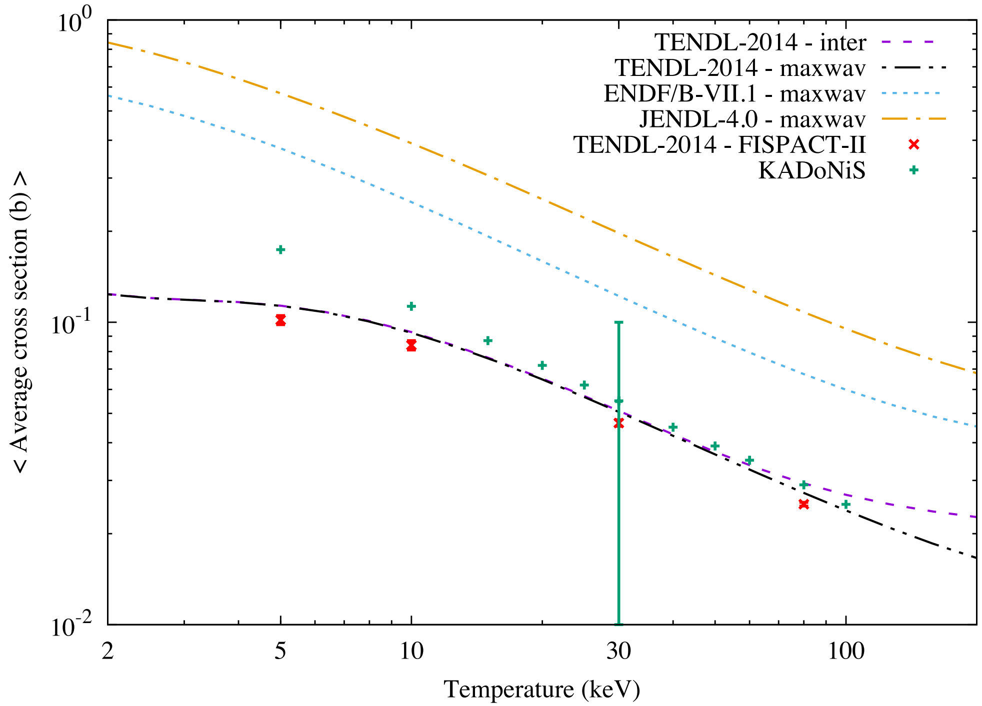


Astrophysics reaction rates



0 Kelvin and kT=30 keV broadened cross-sections

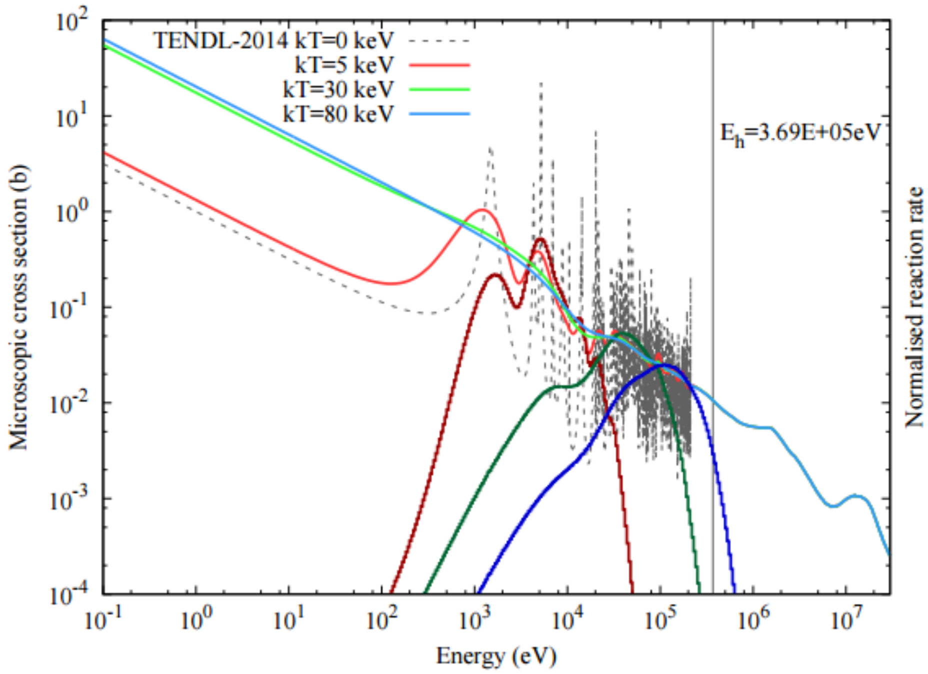
ENDF/B-VII.1 and JENDL-4.0 seriously overestimate whatever the temperature



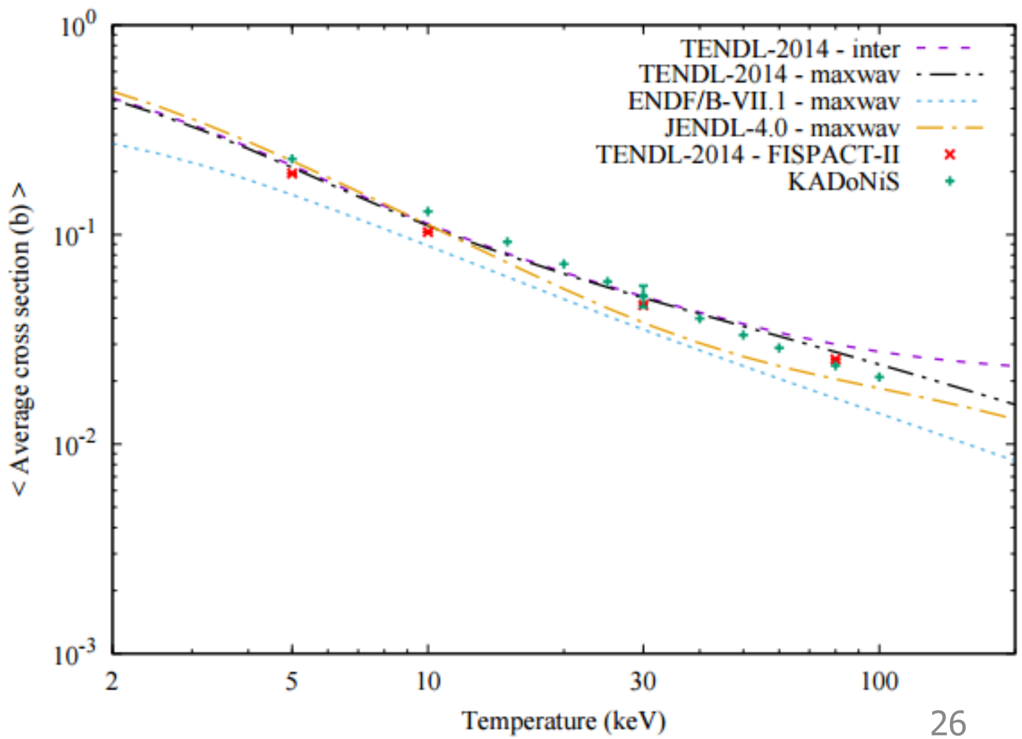
Temperature-dependent averaged cross-sections:
Astrophysical 5-80 keV

FISPACT-II forms: 1102 groups

- The KADoNiS database includes some 357 nuclides over 11 Maxwellian-averaged temperatures for RR comparison



Broadened cross-sections



Temperature-dependent averaged cross-sections

FISPACT-II 3.20

- Provide the user with the most sophisticated incident-particle nuclear data from the TENDL-2015, ENDF/B.VII.1, JENDL-4.0, CENDL-3.1 and JEFF-3.2 international libraries, which are complemented with the latest decay and fission yield data, including the most recent GEFY-5.2 libraries.

- Code features include self-shielding factors, broad temperature dependence, thin/thick target yields, robust pathway analysis, Monte-Carlo sensitivity and uncertainty quantification and propagation using full covariance data.

New features

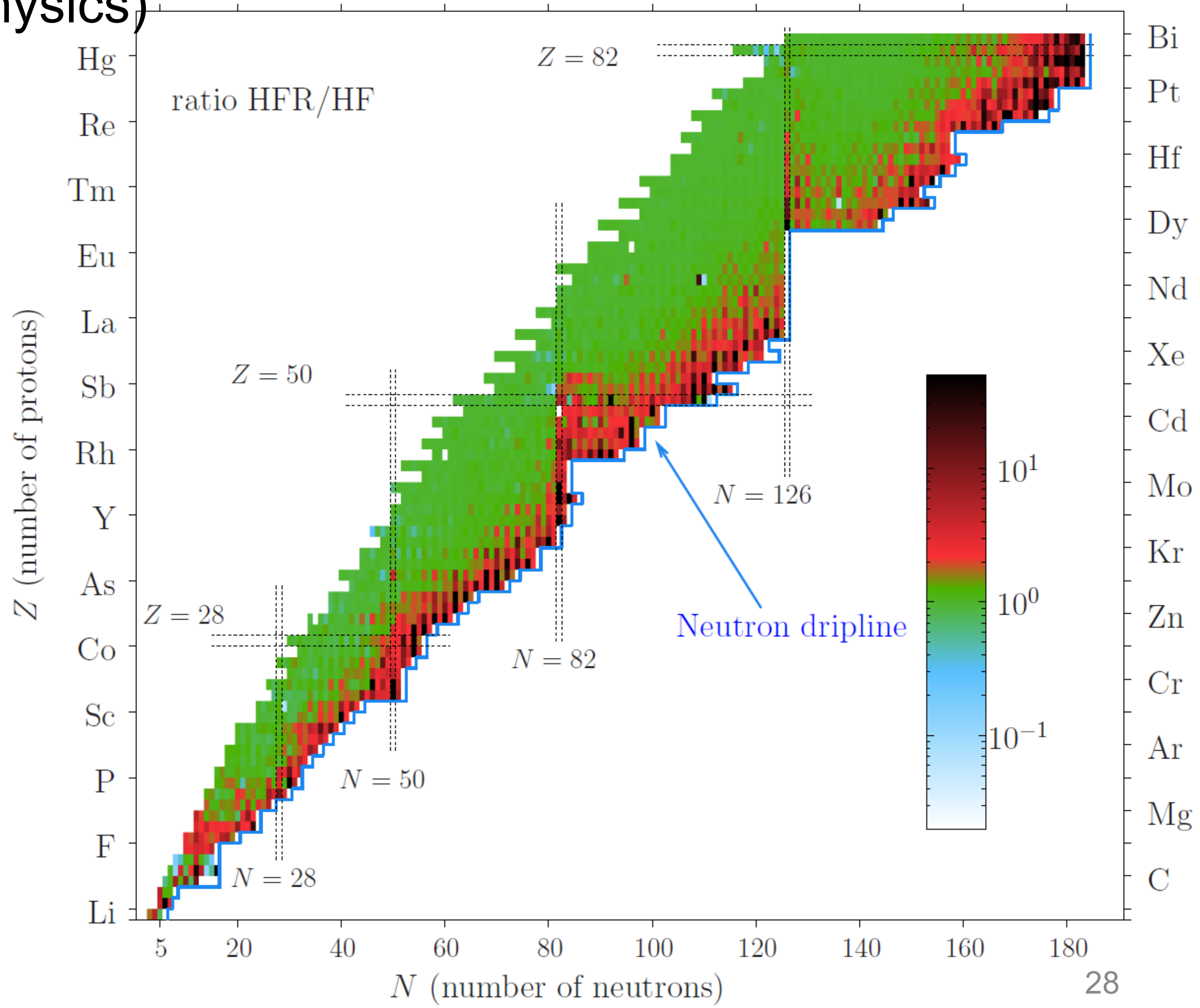
- Allows the user to specify any output gamma group structure for decay sources
- Now with the ability to use arbitrary (ebins) incident group structure
- FISPACT-II to output the uncertainty from all depletion processes for a set of specified nuclides
- Creates data outputs and plot scripts with break-downs for all individual dominant nuclides

(as opposed to integral quantities) http://fispact.ukaea.uk/

Moving forward

- TENDL-2015 includes about 2809 isotopes, why not going beyond ?
  - Understanding that nuclear data are pdf and not only σ ± Δσ,
  - Develop T6 to include other evaluation tools ?
  - 8000 isotopes (astrophysics)
  - 1 GeV ?

Example of what happens when model goes to the neutron drip line (Hauser Feshbach is not applicable anymore)



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Summary

- Completeness, predictability, simultaneity
  - 6 incident particles, number of targets, isomers (targets and daughters), energy range (10^{-5} eV to 200 MeV) total and partials cross section, with variance-covariance, double differential data, all emitted spectra (particles and recoils)
- Reliability, regularity, robustness
  - For all applications (not a particular one) extensive V&V: fission, fusion, astrophysics, medical, high energy, earth explorations, safeguard, safety, security, …
- The only nuclear data library able to go outside the proverbial validations domains (differential and integral), scout the nuclear landscapes, fulfil the (often difficult to specified) data needs