Trend Analysis of CENDL-3.2 Criticality Benchmark Test Results Based on Reaction Channel Sensitivity

——Al and Cr

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Introduction

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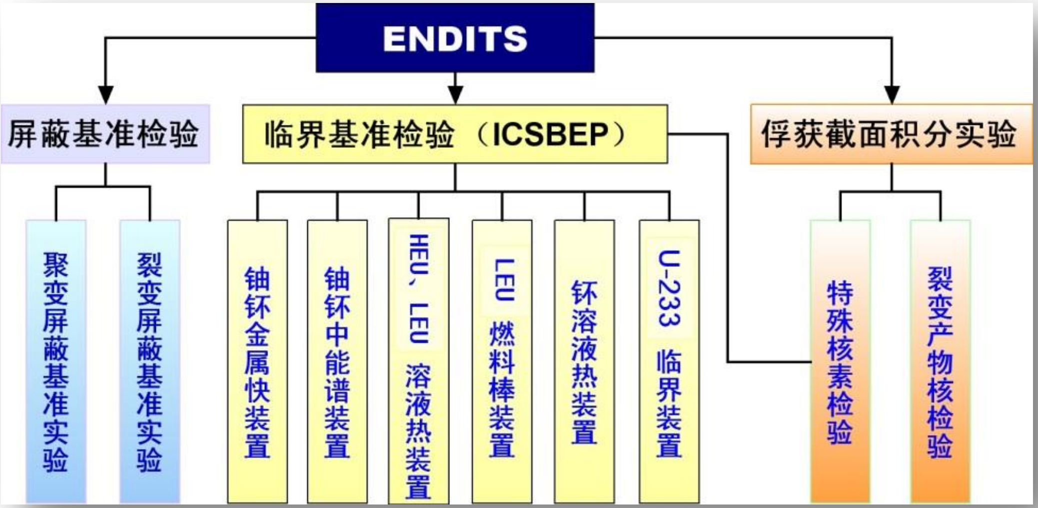
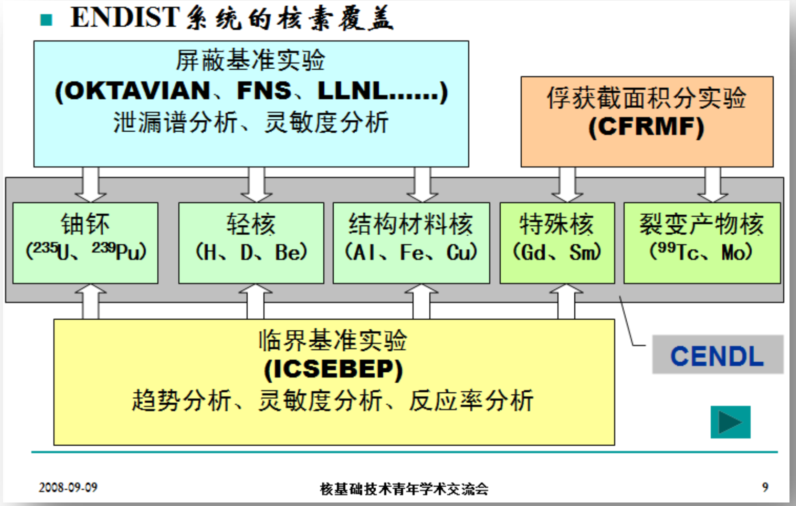
1 Introduction

☐ The concept of systematic integral validation for evaluated nuclear data library

- Different types of benchmark experiments can be utilized to achieve nuclide coverage and energy spectrum coverage for the integral validation of evaluated nuclear data libraries.
- During analysis, different criticality benchmarks are correlated with the characteristic parameters of the experiments.





1 Introduction

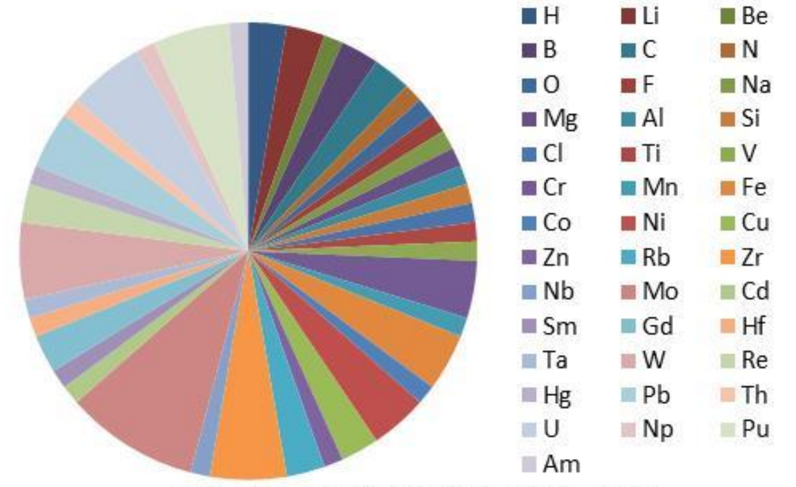
- ENDITS-2.1 was developed in 2020, which includes 2,237 criticality benchmarks from the ICSBEP.

Fuel	From	Spectrum	ICSBEP2006	ENDITS-2.1
HEU	MET	FAST	304	330
		INTER	14	14
		THERM	127	140
		MIXED	32	**33**
	SOL	INTER	3	**3**
		THERM	463	472
	COMP	FAST	8	5
		INTER	14	14
		THERM	216	214
		MIXED	45	48
	MISC	THERM	7	**7**
IEU	MET	FAST	20	20
	SOL	THERM	5	**5**
	COMP	FAST	2	2
		INTER	14	16
		THERM	41	34
		MIXED	3	**14**
LEU	MET	THERM	65	26
	SOL	THERM	104	67
	COMP	THERM	1066	136
	MISC	THERM	11	0

Fuel	From	Spectrum	ICSBE P2006	ENDITS-2.1
PU	MET	FAST	87	72
		INTER	4	1
		THERM	2	0
		MIXED	1	0
	SOL	THERM	529	307
	COMP	FAST	6	0
		INTER	1	**1**
		THERM	21	0
		MIXED	7	0
U233	MET	FAST	10	10
		THERM	1	0
	SOL	INTER	29	29
		THERM	192	113
		MIXED	8	8
	COMP	THERM	5	5

Fuel	From	Spectrum	ICSBE P2006	ENDITS-2.1
MIX	MET	FAST	45	5
		INTER	2	0
		MIXED	1	0
	SOL	THERM	72	**16**
	COMP	FAST	2	2
		INTER	3	0
		THERM	255	65
		MIXED	17	0
	MISC	FAST	8	0
		THERM	56	0
		MIXED	8	0
SPEC	MET	FAST	20	3
Total			3955	2237

Sensitive nuclide: 75
Sensitive element: 40



Sensitive elements

1 Introduction

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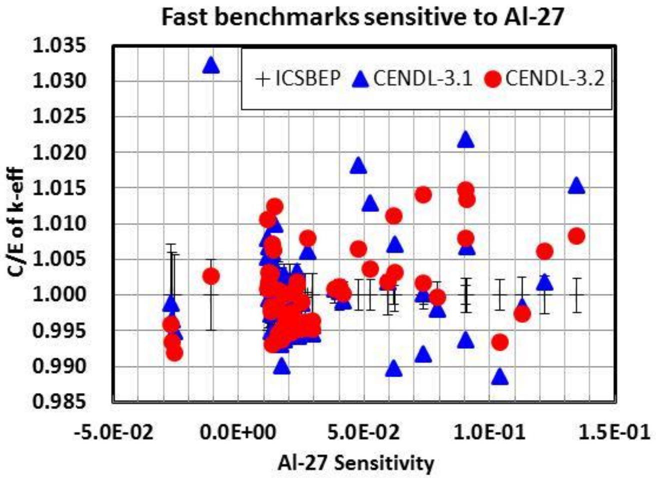
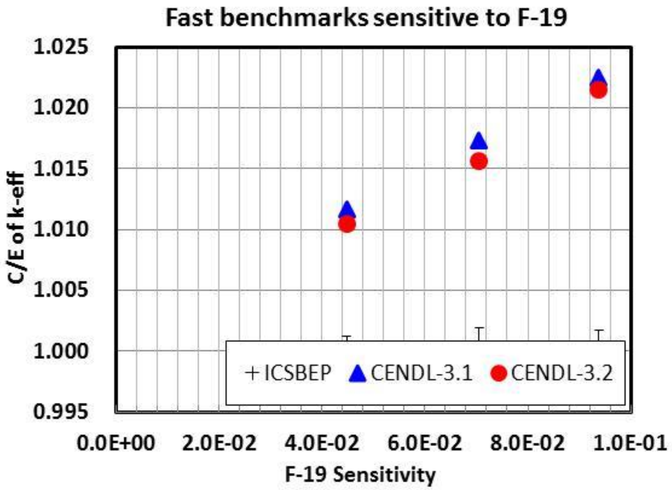
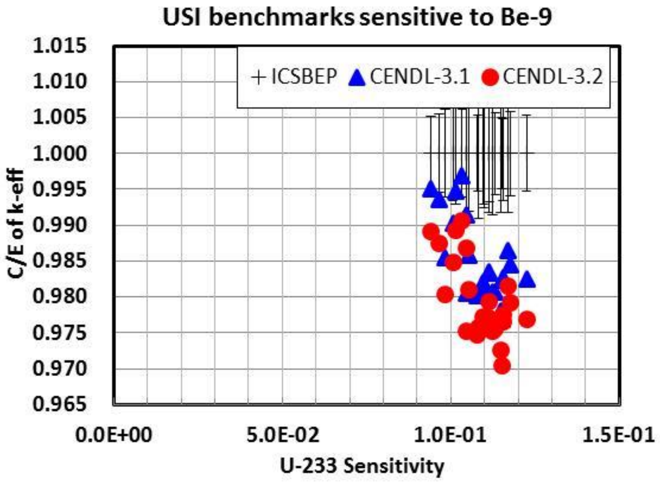
□ 2023, CENDL-3.2 library was tested with the ENDITS-2.1.

- By introducing the cumulative chi-square, normalized chi-square, and Pearson's chi-square test related to sensitive nuclides, 16 major nuclides causing criticality calculation deviations were identified: Al-27、F-19、Th-232、Be-9、C-12、Fe-56、Pu-239,240、U-235,238、N-14、Mo-95、Nb-93、Zr-90,94、Cd-113.







□ Sensitivity-related statistical analysis and trend analysis can only identify the nuclides that cause criticality calculation deviations. Thus, further identifying the sources of these deviations is the core problem need to be solved.

02

Methodology of trend analysis based on reaction channel sensitivity

2 Methodology

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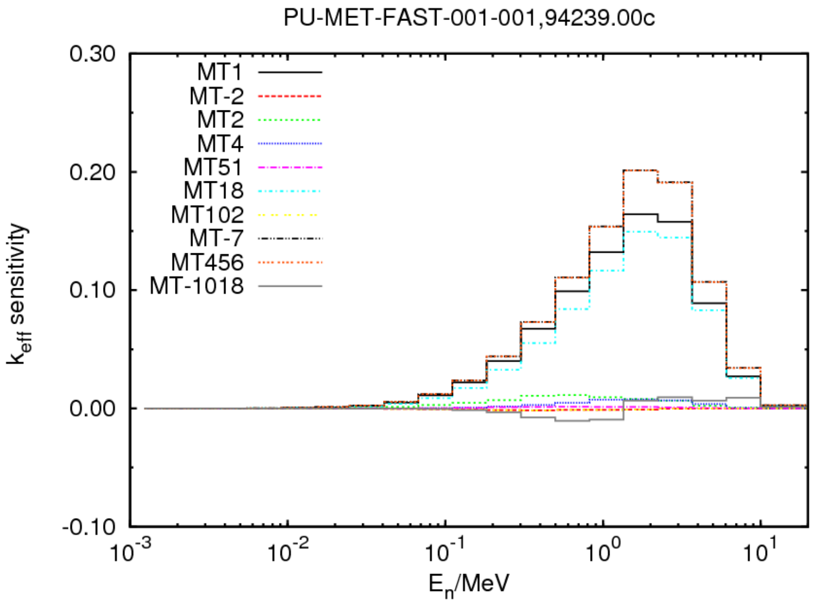
□ Sensitivity database of criticality benchmarks, ENDITS-SEN-2.1

- □ The sensitivities of k_{eff} in groups were calculated using the MCNP/JMCT code.
- □ Reaction channels： (n,tot), (n,el), (n,inl), (n,f), (n,γ), nubar, PFNS, TSL and et al.
- □ Sensitive nuclides： $|k_{eff}$ sensitivity to (n,tot) reaction$|$ > 1%.

Table： sen_mat_mt

case	mat	mt	sensitivity
PMF001_01	94239	-1018	-3.7718E-07
PMF001_01	94239	-7	0.964619
PMF001_01	94239	-2	-0.00886138
PMF001_01	94239	1	0.820482
PMF001_01	94239	2	0.0660574
PMF001_01	94239	4	0.0362481
PMF001_01	94239	18	0.726546
PMF001_01	94239	102	-0.00886108
PMF001_01	94239	456	0.963031



2 Methodology

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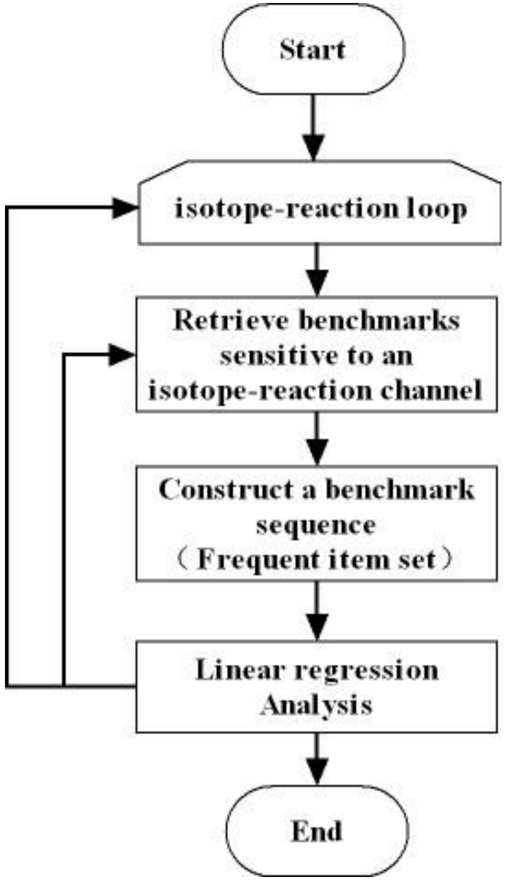
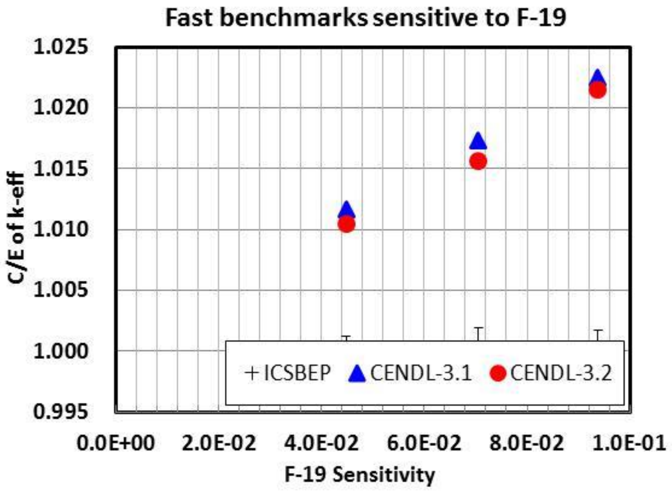
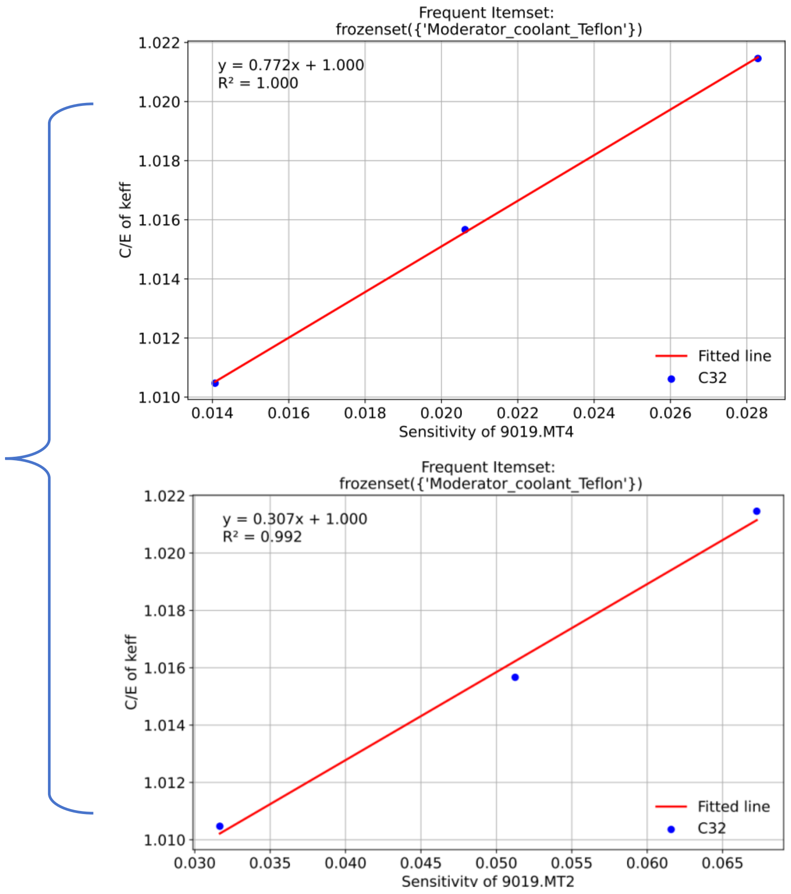
- To further pinpoint the sources of criticality calculation deviations at the reaction channel level, the Apriori algorithm was applied to establish a trend analysis method based on reaction channel sensitivity.







03

Trend Analysis of Benchmark Test Results for Al and Cr in the CENDL-3.2 Library

3.1 Al-27

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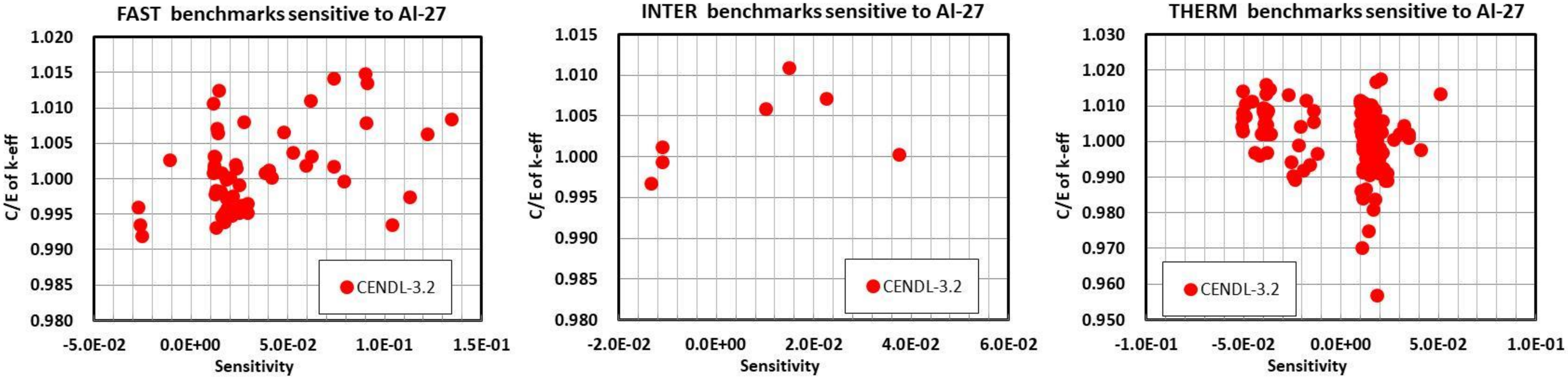
☐ The testing results for criticality benchmarks sensitive to Al-27 reaction data.

- When conducting trend analysis against Al-27 sensitivity by energy spectrum classification, it is difficult to identify any relationship between k_{eff} value calculation deviations and nuclear data.



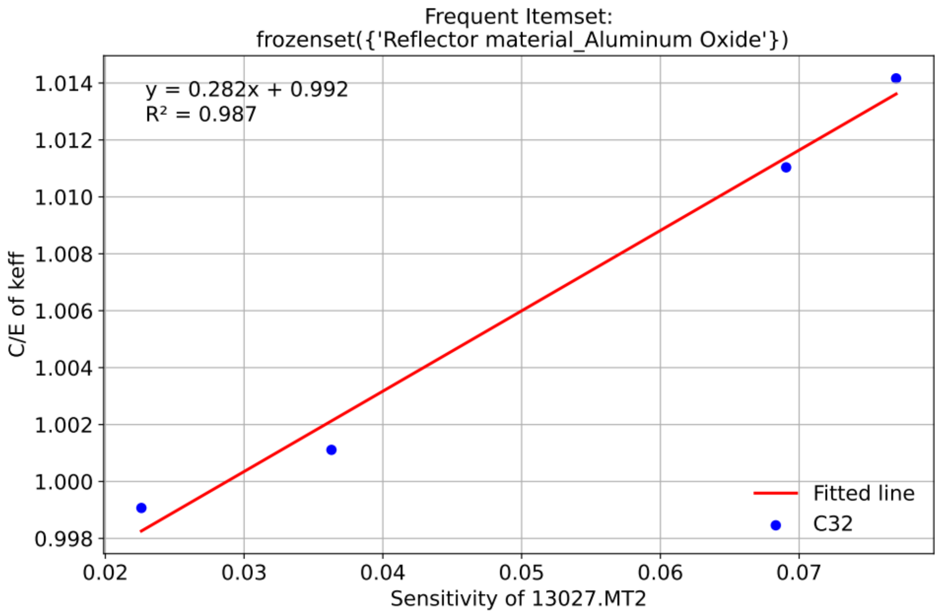
3.1.1 Al-27(n,el)

No.	Frequent Itemset	Support	R^2	Cases
1	['Separator_Stainless Steel (Fe, Cr, Ni)']	0.013158	0.999487	HST008_02, HST008_06, HST008_10
2	['Reflector material_Aluminum Oxide']	0.017544	0.987124	HMF070_01, 03, HMF084_02, 15
3	['Reflector material_Borated Uranyl Nitrate (B, U, N, H, O), Uranyl Nitrate, Water (Light Water)']	0.017544	0.975849	HMCT001_20-23
4	['Reflector material_Depleted Uranium', 'Fuel type_IEU']	0.013158	0.835649	IMF012_01, IMF017_01-03
5	['Cladding material_Stainless Steel']	0.035088	0.80535	HCT011_01-03, HCT012_01-02, HCT013_01-02, HCT014_01
6	['Solid poison_Stainless Steel (Fe, Cr, Ni)']	0.017544	0.795676	SHMT002_01-04
7	['Solid poison_Cadmium']	0.017544	0.774065	HMT006_17-20
8	['Reflector material_Aluminum', 'Fuel type_IEU']	0.013158	0.745362	IMF013_01, IMF014_01, IMF014_02
9	['Moderator_coolant_Polyethylene', 'Spectrum_FAST']	0.013158	0.709716	HMF034_02, HMF047_01, IMF017_01-03
10	['Reflector material_Depleted Uranium']	0.013158	0.6605	HMF055_01, IMF012_01, IMF017_01-03
11	['Moderator_coolant_Polyethylene', 'Reflector material_Depleted Uranium']	0.013158	0.653823	IMF017_01, IMF017_02, IMF017_03
12	['Reflector material_Iron']	0.013158	0.650477	PMF045_06D, PMF045_07D, SMF014_D
13	['Spectrum_INTER']	0.013158	0.631799	HMI001_01, HMI005_05, HMI008_02
14	['Separator_Tantalum']	0.013158	0.530989	PMF045_03D, PMF045_04D, PMF045_06D

3.1.1 Al-27(n,el)

□ Reflector material _ Aluminum Oxide

HMF070_01, HMF070_03,
HMF084_02, HMF084_15



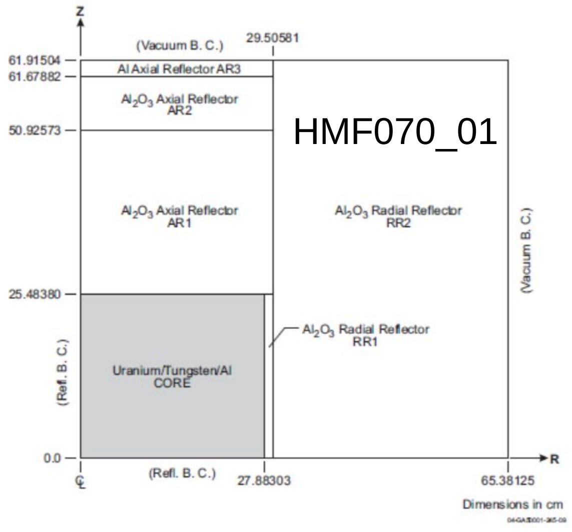
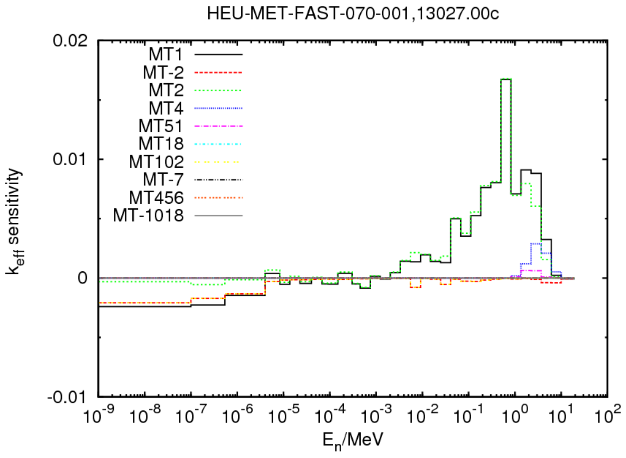
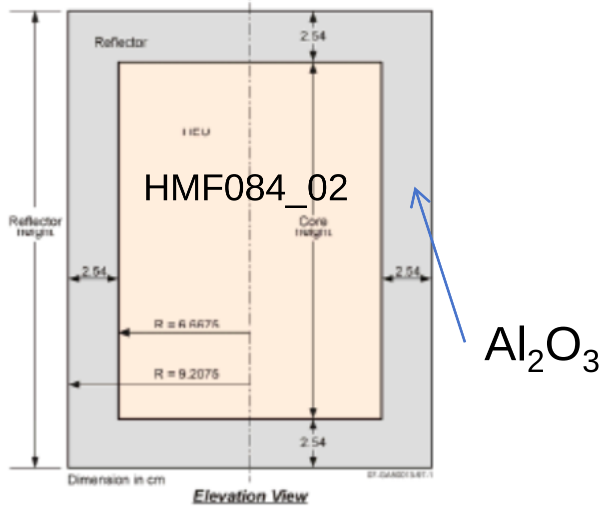
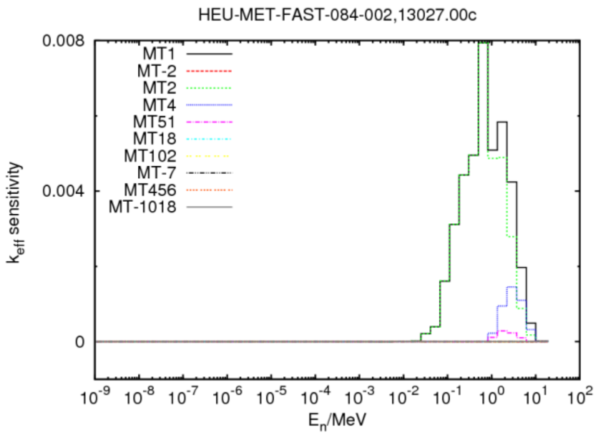


Figure 11. Benchmark-Model Geometry for ZPR-9/7.







True trend: Based on physical judgment, it is confirmed that the positive trend is related to the ^{27}Al(n,el) reaction from 0.1 to 3 MeV energy range.

3.1.1 Al-27(n,el)

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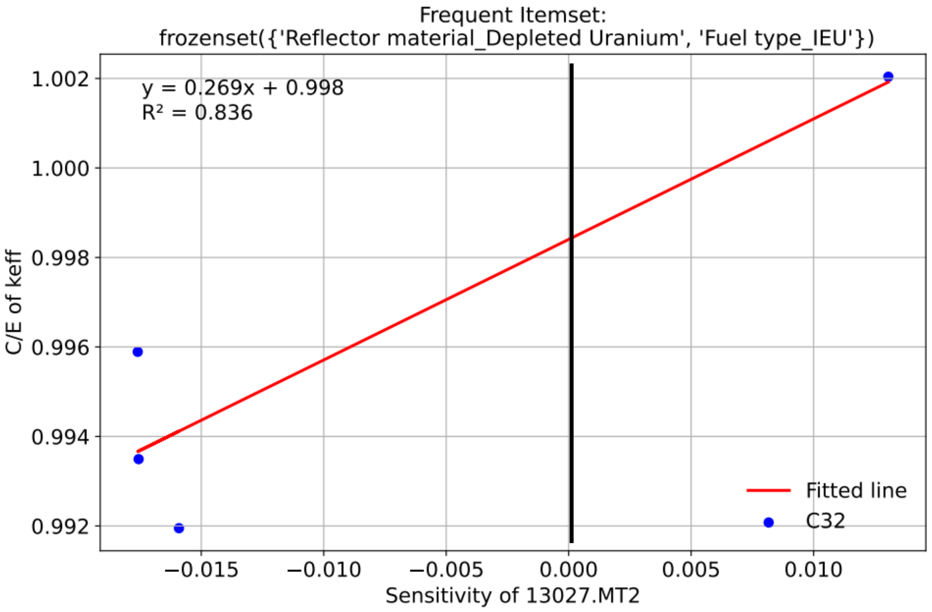
◻ Reflector material_Depleted Uranium, Fuel type_IEU

IMF012_01, IMF017_01-03



Spurious trend: An abnormal linear trend that is merely a mathematical coincidence.

IMF012_01

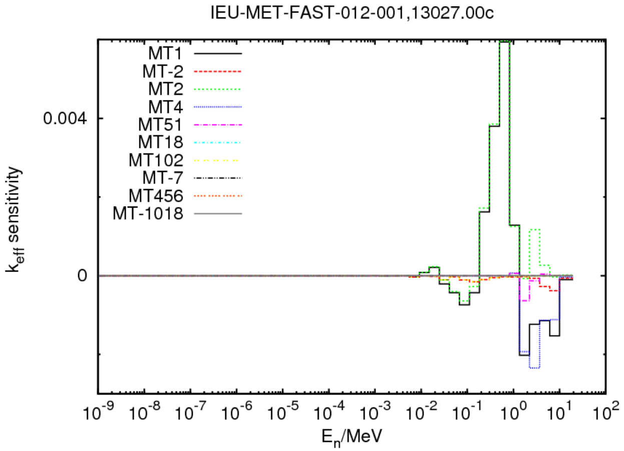
Table 14. Compositions of the Benchmark-Model (atoms/barn-cm)

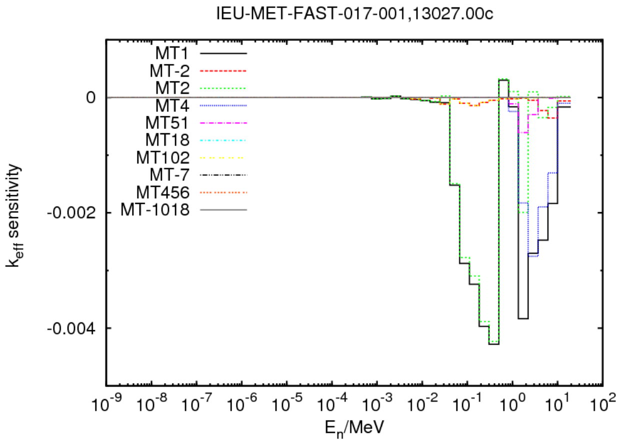
Nuclide	Core	Reflector
^{234}U	2.77890 x 10^{-5}	
^{235}U	2.86319 x 10^{-3}	8.30614 x 10^{-5}
^{236}U	1.33175 x 10^{-5}	
^{238}U	1.39681 x 10^{-2}	3.97356 x 10^{-2}
Al	1.07829 x 10^{-2}	
Fe	8.71333 x 10^{-5}	4.85493 x 10^{-3}
Ni	9.22671 x 10^{-4}	4.99615 x 10^{-4}
Cr	2.18244 x 10^{-3}	1.21570 x 10^{-3}
Mn	8.82621 x 10^{-5}	4.78958 x 10^{-5}
Si	1.13424 x 10^{-4}	6.60492 x 10^{-5}
C		1.27162 x 10^{-6}

IMF017_01

Table 10. Atom Densities.

Pellet or Tube	Structural Element	Inner Dimensions, cm	Outer Dimensions, cm	Den g/c
U(d) (Depleted Uranium Metal Pellet)	Core		D = 4.46 H = 1.01	18.9
	Aluminum Can	D = 4.46 H = 1.01	D = 4.55 H = 1.07	2.71





3.1.1 Al-27(n,el)

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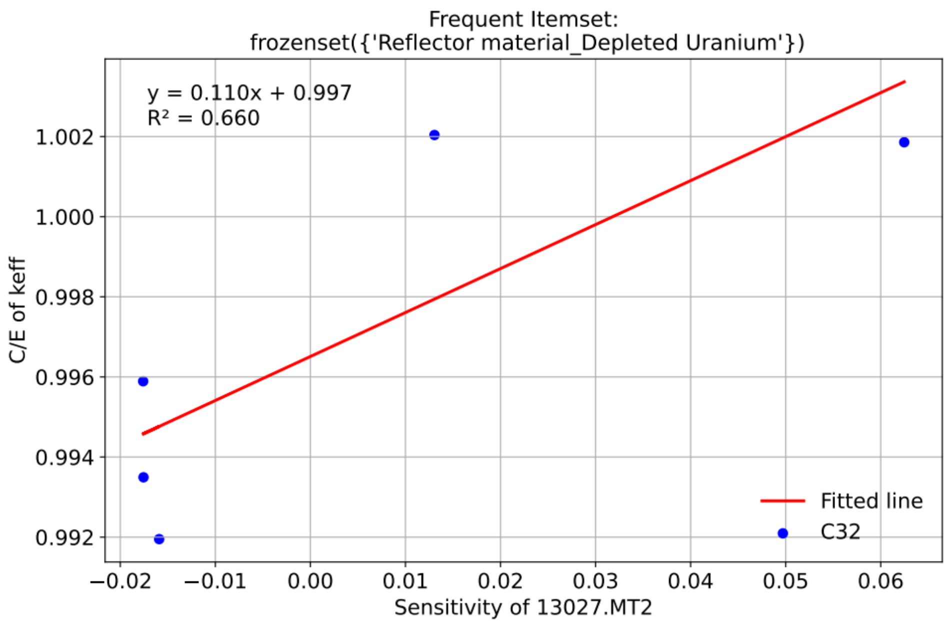
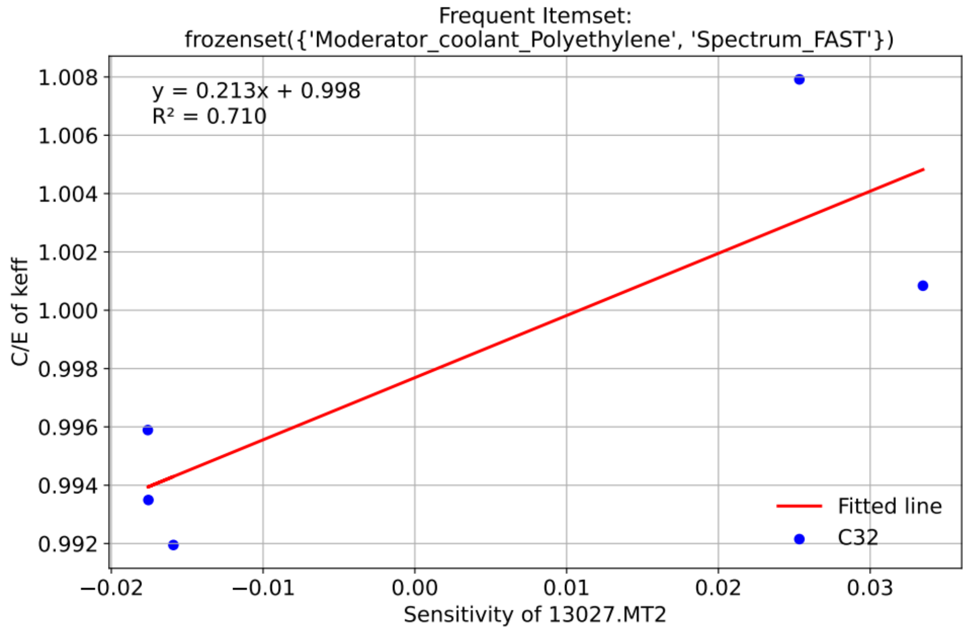
☐ Reflector material_Depleted Uranium

HMF055_01, IMF012_01, IMF017_01-03



☐ Moderator_coolant_Polyethylene, Spectrum_FAST

HMF034_02, HMF047_01, IMF017_01-03

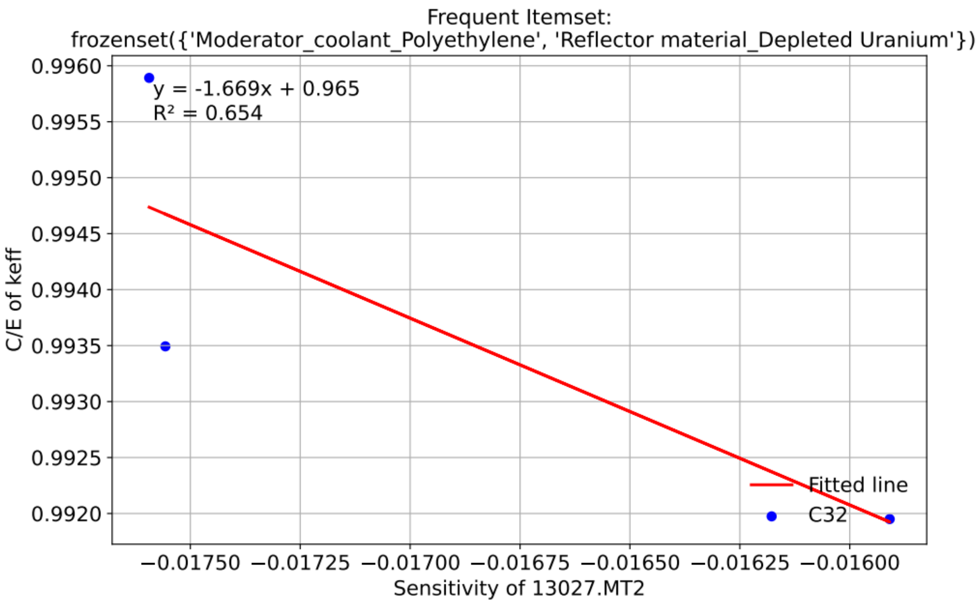


Spurious trend: An abnormal linear trend that is merely a mathematical coincidence.

3.1.1 Al-27(n,el)

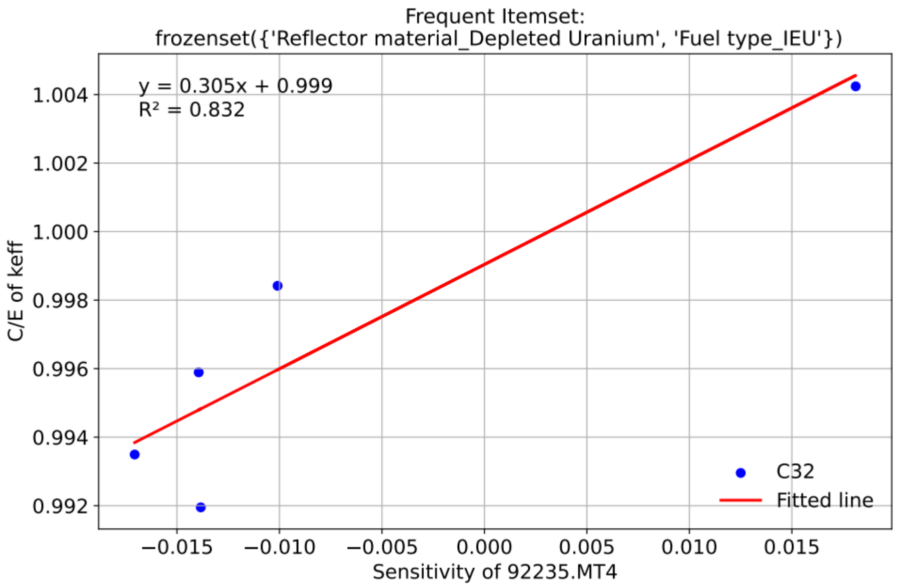
- **Moderator_coolant_Polyethylene, Reflector material_Depleted Uranium**
- **Reflector material_Depleted Uranium, Fuel type_IEU**

IMF017_01-03



Spurious trend: The benchmarks are similar, and there is a negative correlation between C/E values and ^{27}Al(n,el); due to the existence of competition, the deviation maybe not correlated to ^{27}Al(n,el).

IMF007_01S, IMF008_01, IMF017_01-03

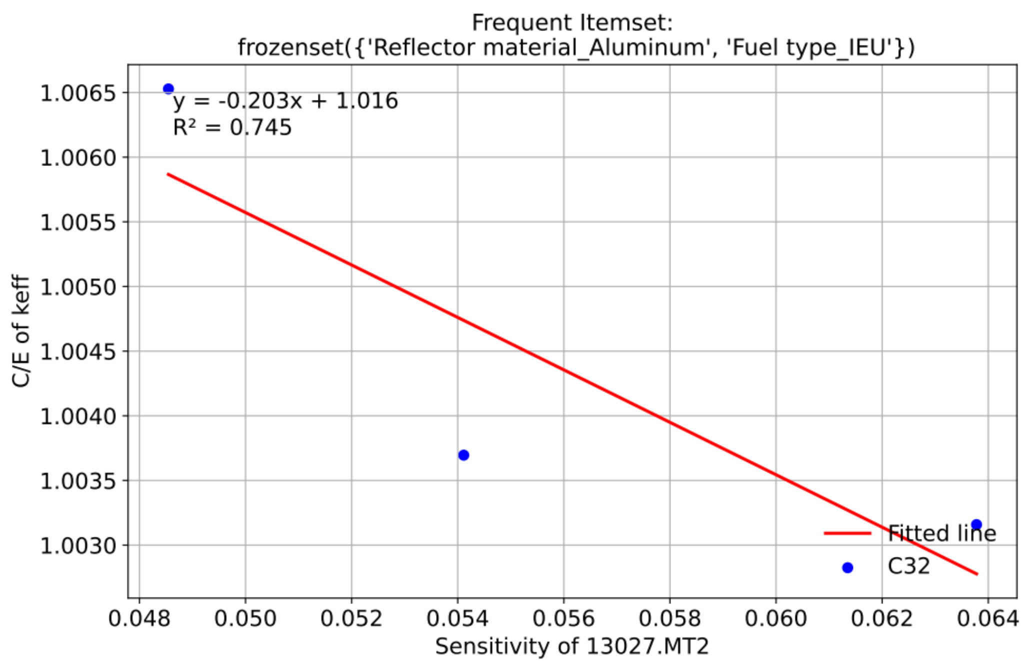


There is a positive correlation between C/E values and ^{235}U(n,inl), which may be either a mathematical coincidence or a true trend.

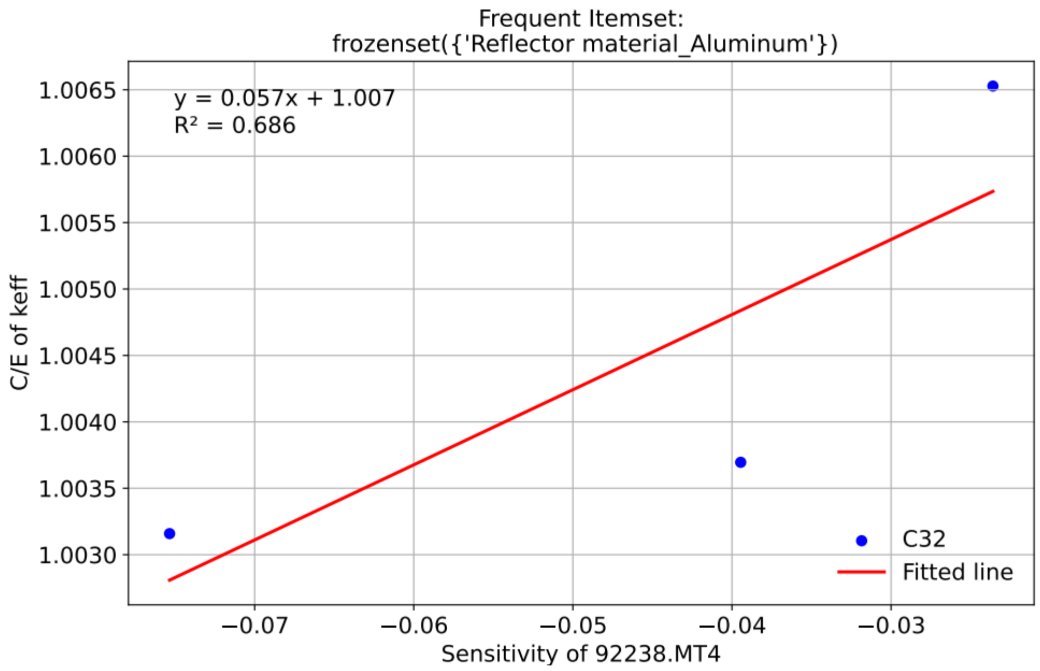
3.1.1 Al-27(n,el)

Reflector material_Aluminum, Fuel type_IEU

IMF013_01, IMF014_01-02



Spurious trend: There is a negative correlation between C/E values and ^{27}Al(n,el), which means the deviation maybe not correlated to ^{27}Al(n,el).

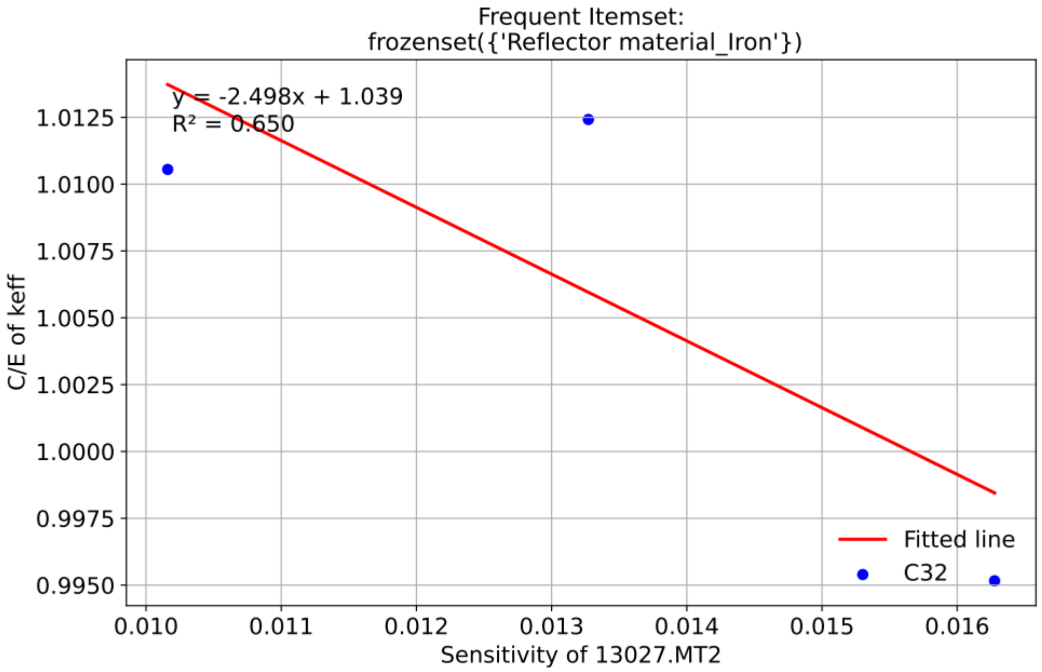


True trend: There is a positive correlation between C/E values and ^{238}U(n,inl). A decreasing of ^{238}U(n,inl) XS will get slope smaller.

3.1.1 Al-27(n,el)

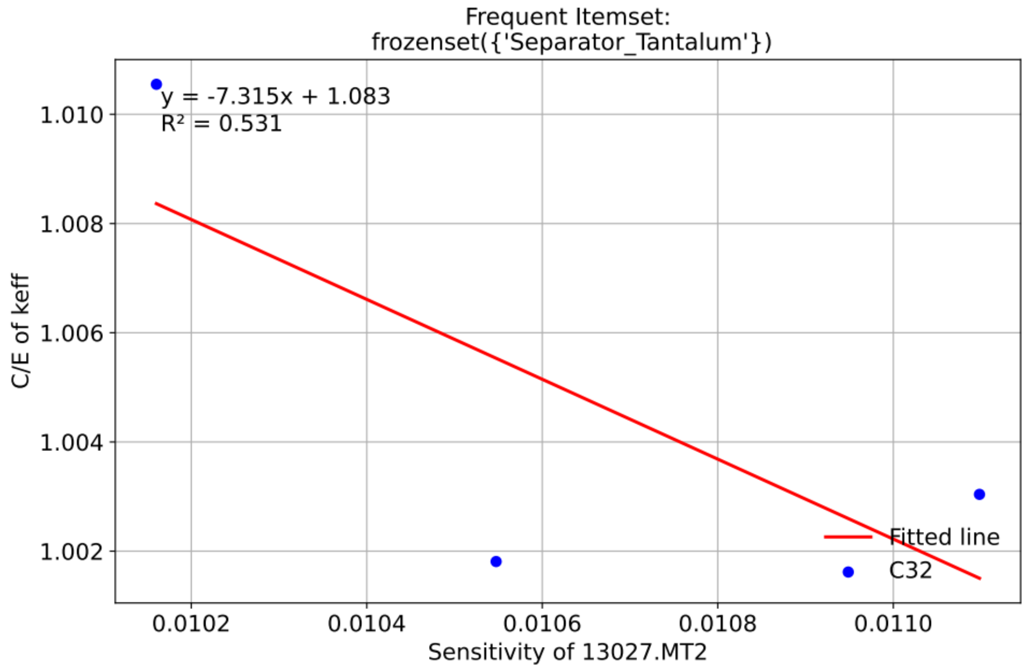
- **Reflector material_Iron**

PMF045_06D, PMF045_07D, SMF014_D



- **Separator_Tantalum**

PMF045_03D, PMF045_04D, PMF045_06D



Spurious trend: There is a negative correlation between C/E values and ^{27}Al(n,el) sensitivity, and the deviation maybe not correlated to ^{27}Al(n,el).

3.1.1 Al-27(n,el)

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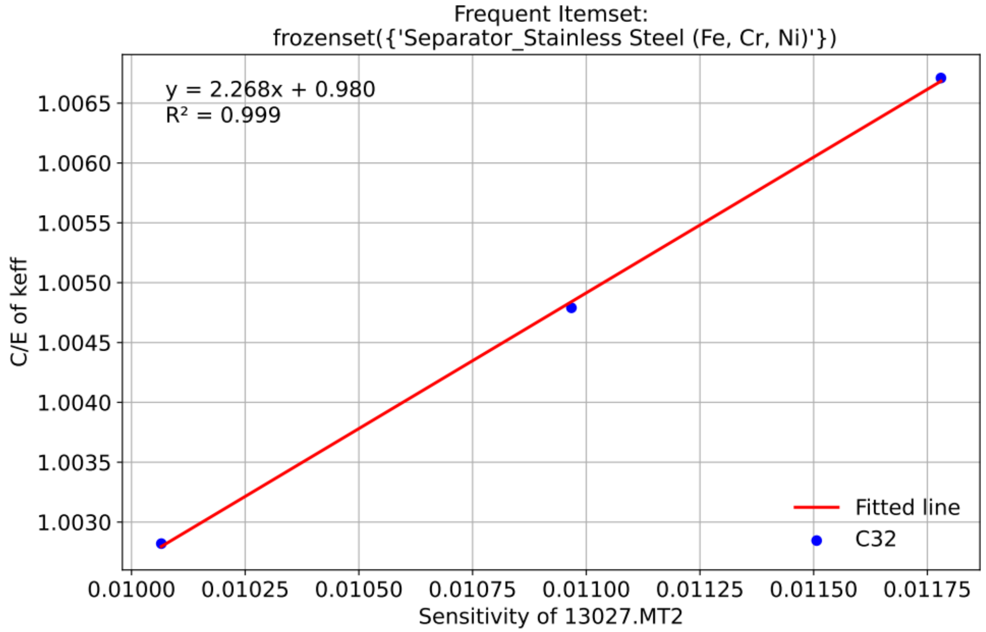
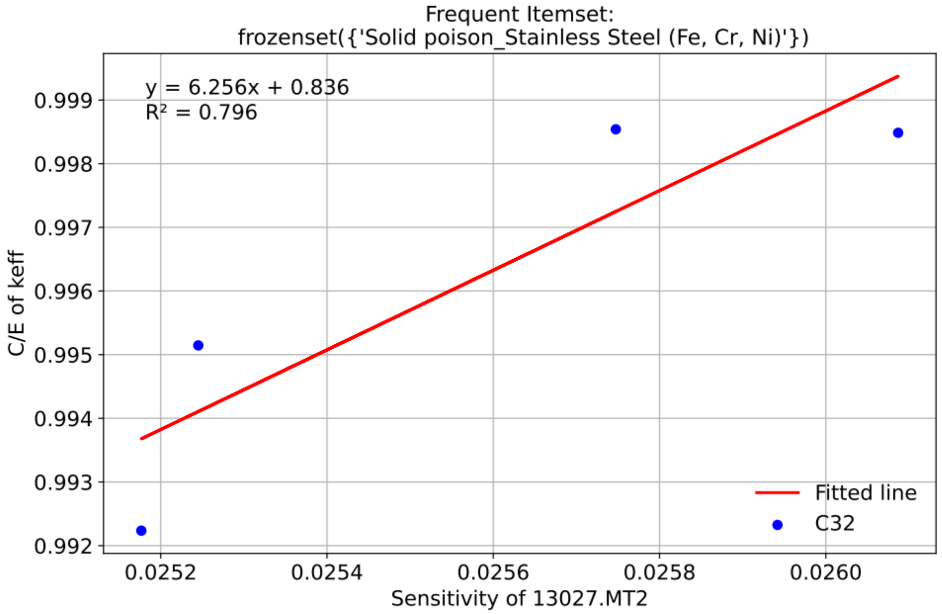
- Separator_Stainless Steel (Fe, Cr, Ni)

HST008_02, 06, 10



- Solid poison_Stainless Steel (Fe, Cr, Ni)

SHMT002_01-04



True trend: The benchmarks are similar, and there is a positive correlation between C/E values and ^{27}Al(n,el) sensitivity.

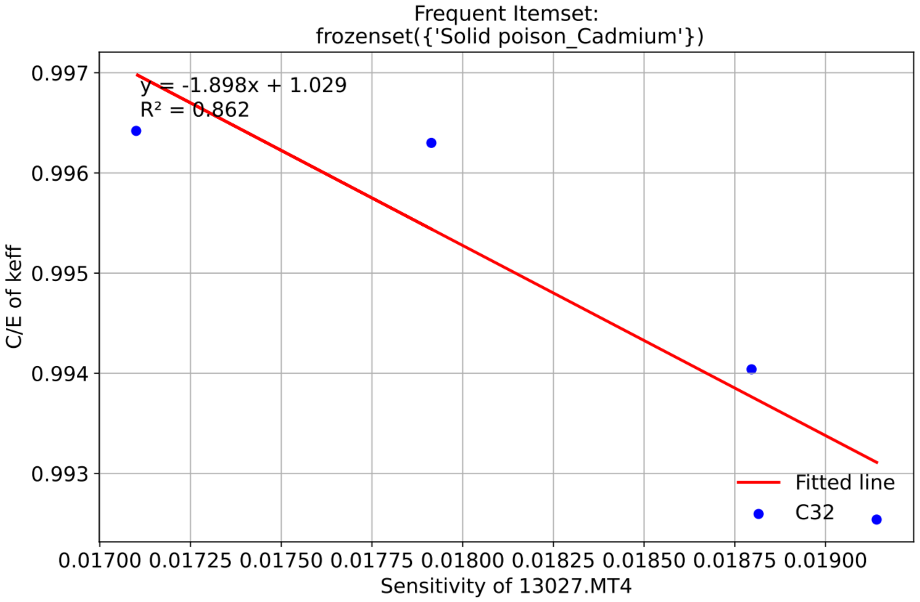
3.1.2 Al-27(n,inl)

No.	Frequent Itemset	Support	R^2	Cases
1	['Solid poison_Cadmium']	0.095238	0.861808	HMT006_17-20
2	['Reflector material_Light Water']	0.119048	0.806487	HMT006_19-23
3	['Reflector material_Borated Uranyl Nitrate (B, U, N, H, O), Uranyl Nitrate, Water (Light Water)']	0.095238	0.666641	HMCT001_20-23
4	['Form_MISC']	0.119048	0.643419	HMCT001_19-23

3.1.2 Al-27(n,inl)

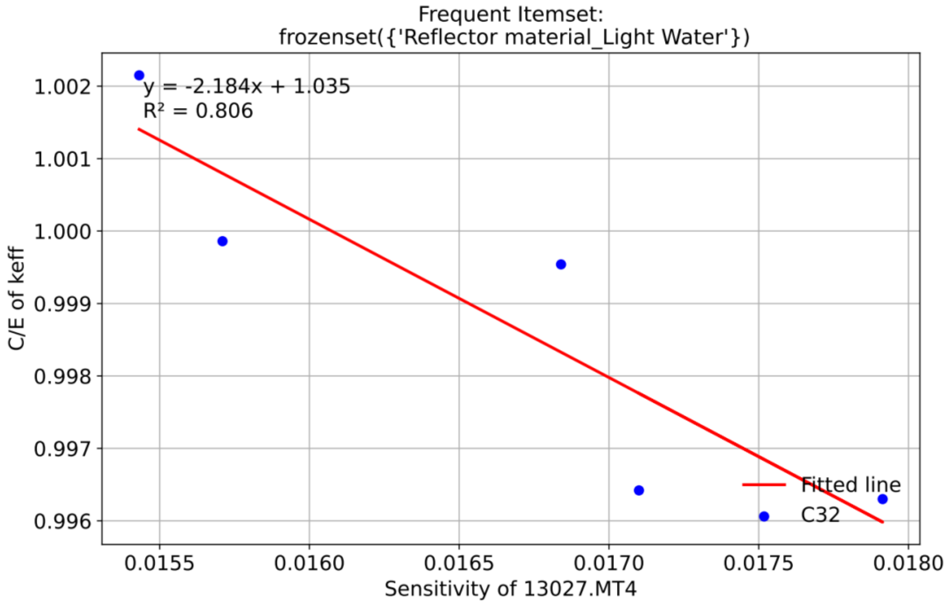
◻ Solid poison_Cadmium

HMT006_17-20



◻ Reflector material_Light Water

HMT006_19-23



Spurious trend: The benchmarks are similar, and there is a negative correlation between C/E values and ^{27}Al(n,inl); due to the existence of competition, the deviation is unrelated to ^{27}Al(n,inl).

3.1.2 Al-27(n,inl)

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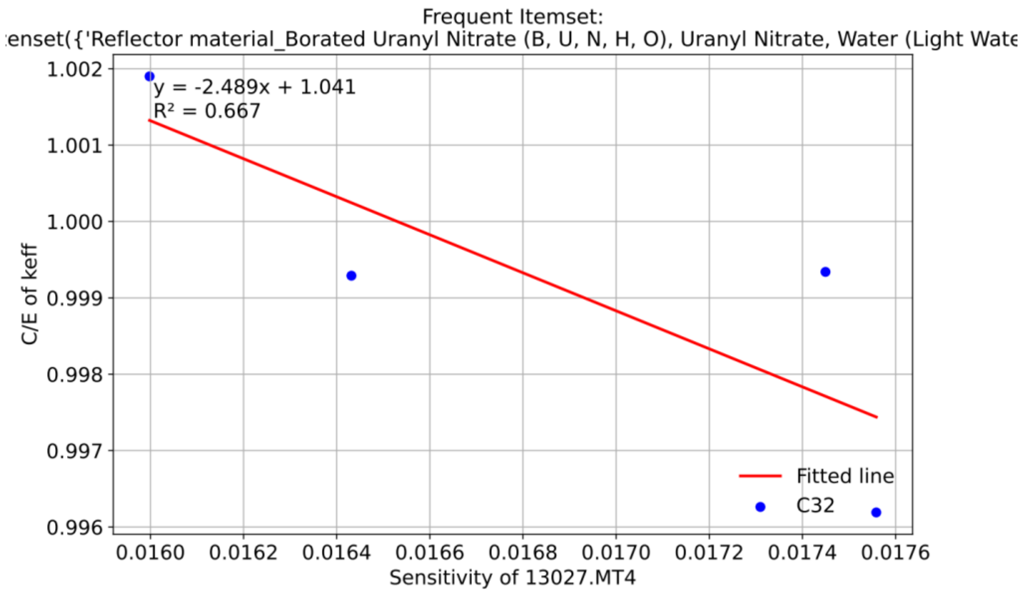
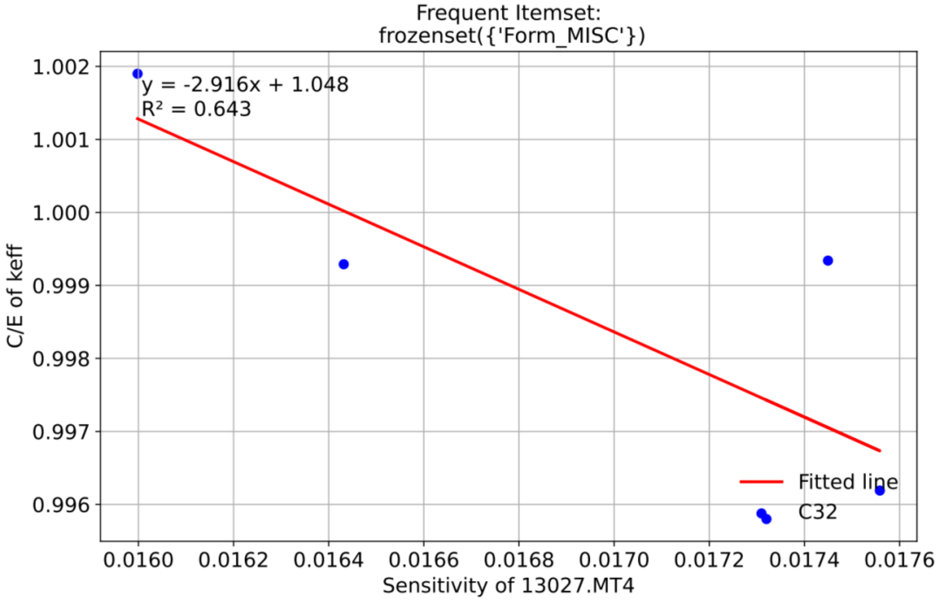
- Reflector material_Borated Uranyl Nitrate (B, U, N, H, O), Uranyl Nitrate, Water (Light Water)
- Form_MISC

HMCT001_20-23



HMCT001_19-23



Spurious trend: a negative correlation found, and the deviation may be not correlated to ^{27}Al(n,inl).

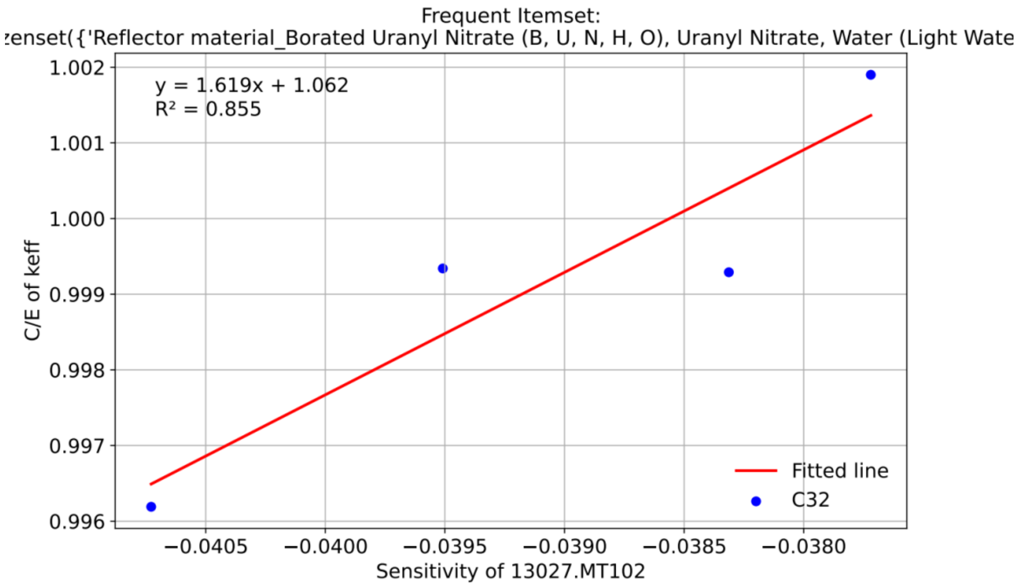
3.1.3 Al-27(n,g)

No.	Frequent Itemset	Support	R^2	Cases
1	['Form_COMP', 'Reflector material_Water (Light Water)']	0.119565	0.894945	HCT021_04, 05, 94-100, LCT003_07, 08
2	['Solid poison_Boral (B, Al, Na, Si)']	0.032609	0.859832	SHMT002_05-07
3	['Reflector material_Borated Uranyl Nitrate (B, U, N, H, O), Uranyl Nitrate, Water (Light Water)']	0.043478	0.854661	HMCT001_20-23
4	['Fuel type_HEU', 'Reflector material_Heavy Water (D, O)']	0.097826	0.852167	HCT017_01-09
5	['Solid poison_Cadmium']	0.043478	0.848747	HMT006_17-20
6	['Reflector material_Light Water']	0.054348	0.806163	HMT006_19-23
7	['Moderator_coolant_Polyethylene']	0.021739	0.682061	HMT006_01, HMT008_01S, HMT012_01D
8	['Fuel type_LEU', 'Reflector material_Heavy Water (D, O)']	0.271739	0.596201	LMT002_01-12, LMT015_01-13

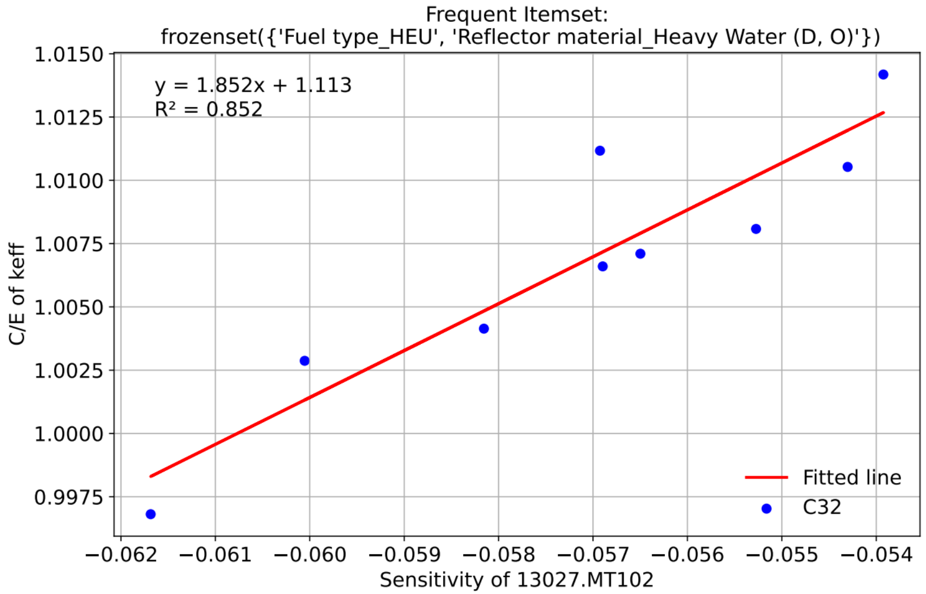
3.1.3 Al-27(n,g)

- Reflector material_Borated Uranyl Nitrate (B, U, N, H, O), Uranyl Nitrate, Water (Light Water)
- Fuel type_HEU, Reflector material_Heavy Water (D, O)

HMCT001_20-23



HCT017_01-09



True trend: The devices are similar, and there is a positive linear correlation between C/E values and ^{27}Al(n,g) reaction sensitivity.

3.1.3 Al-27(n,g)

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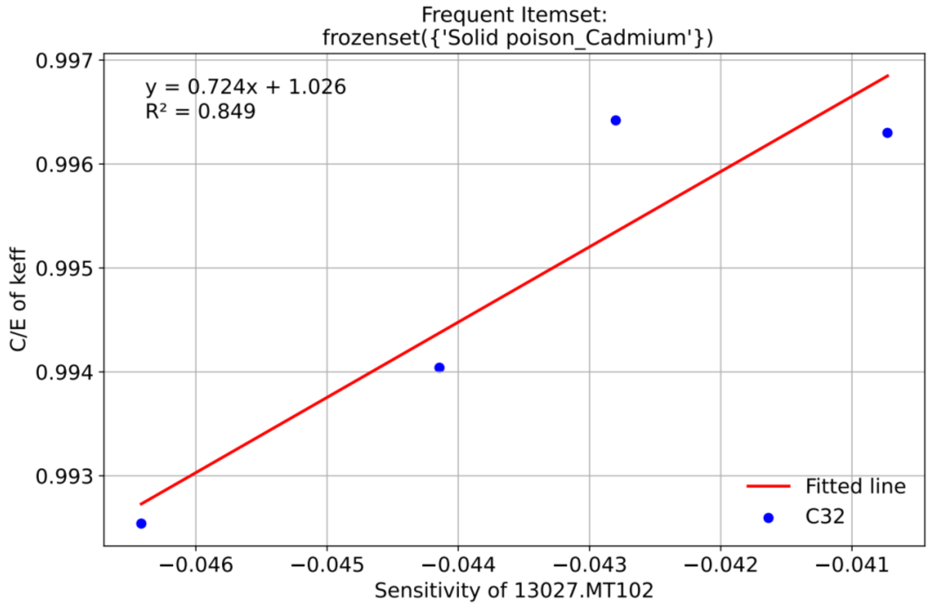
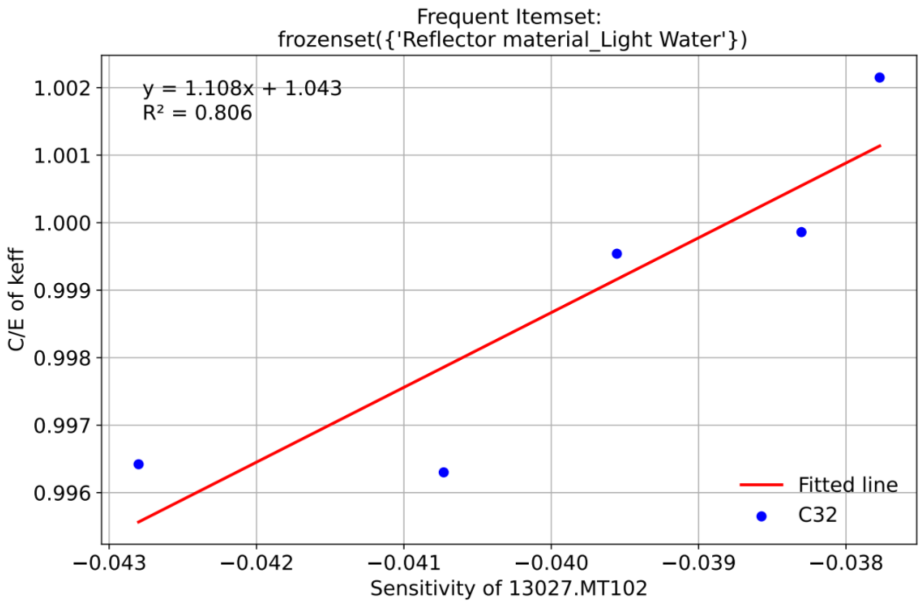
☐ Solid poison_Cadmium

HMT006_17-20



☐ Reflector material_Light Water

HMT006_19-23

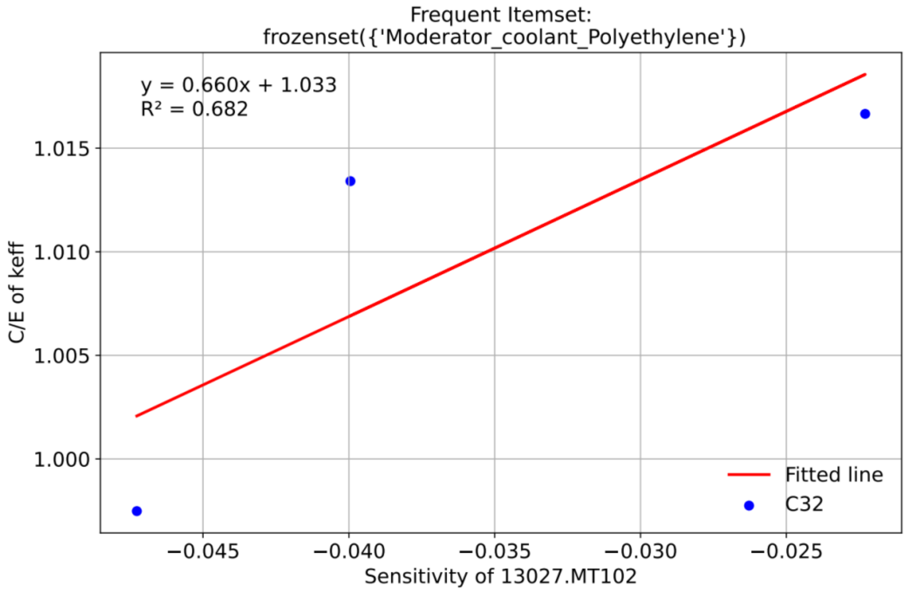


True trend: The devices are similar, and there is a positive linear correlation between C/E values and ^{27}Al(n,g).

3.1.3 Al-27(n,g)

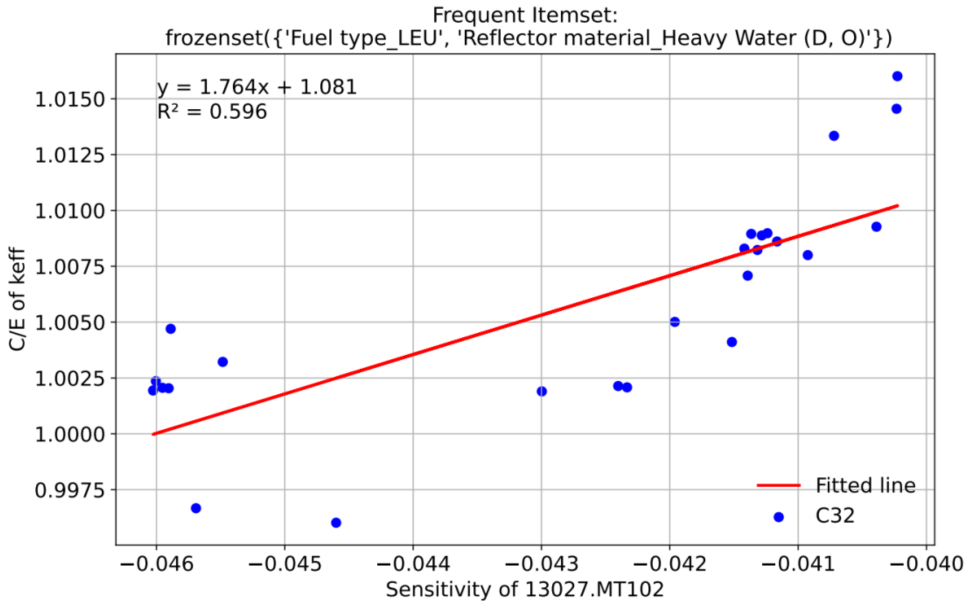
- **Moderator_coolant_Polyethylene**

HMT006_01, HMT008_01S, HMT012_01D



- **Fuel type_LEU, Reflector material_Heavy Water (D, O)**

LMT002_01-12，LMT015_01-LMT015_13



True trend: The devices are similar, and there is a positive linear correlation between C/E values and $^{27}Al(n,g)$.

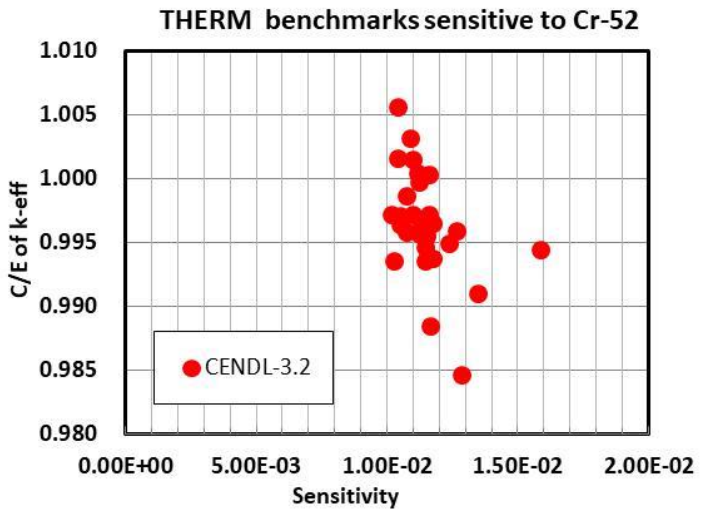
Summary of Al-27

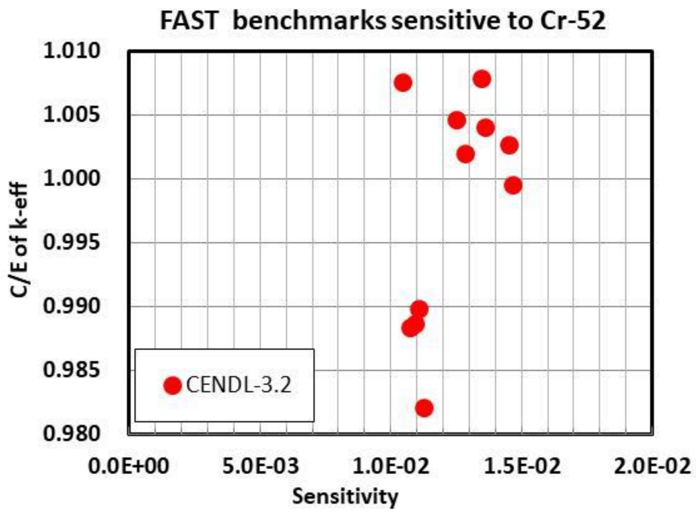
- There are linear trends positively correlated with the sensitivities of the ^{27}Al(n,el) reaction in the 0.1-3 MeV energy range and the (n,g) reaction in the thermal energy range, indicating that the ^{27}Al(n,el) and (n,g) cross sections need to be improved.
- No linear positive trend correlated with the sensitivity of the ^{27}Al(n,inl) reaction was found.
- There are spurious trends caused by mathematical coincidences or nuclide-reaction competition.

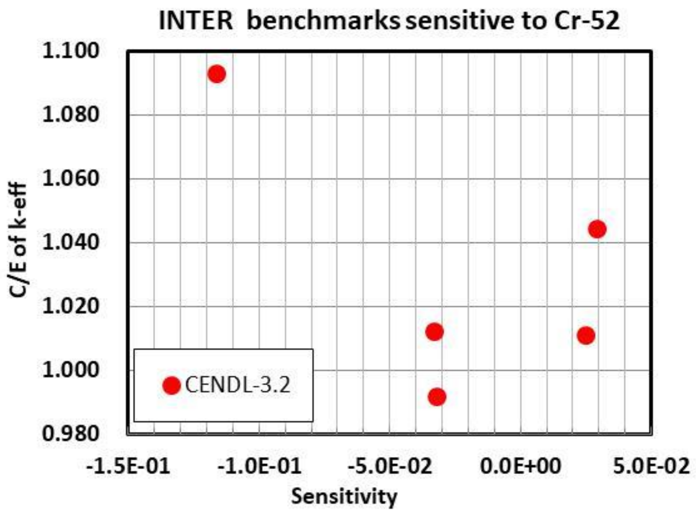
3.2 Cr-52,53

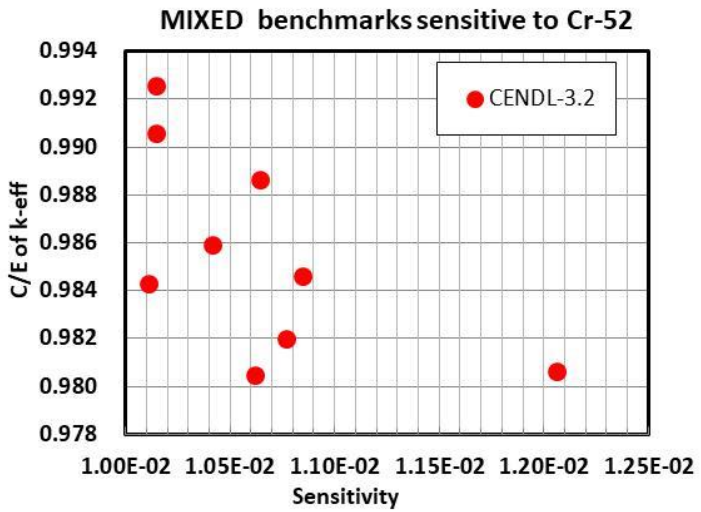
Testing results for the benchmarks sensitive to Cr-52

- Again, it is difficult to identify the relationship between k_{eff} deviations and nuclear data when conducting nuclide sensitivity analysis by energy spectrum classification.





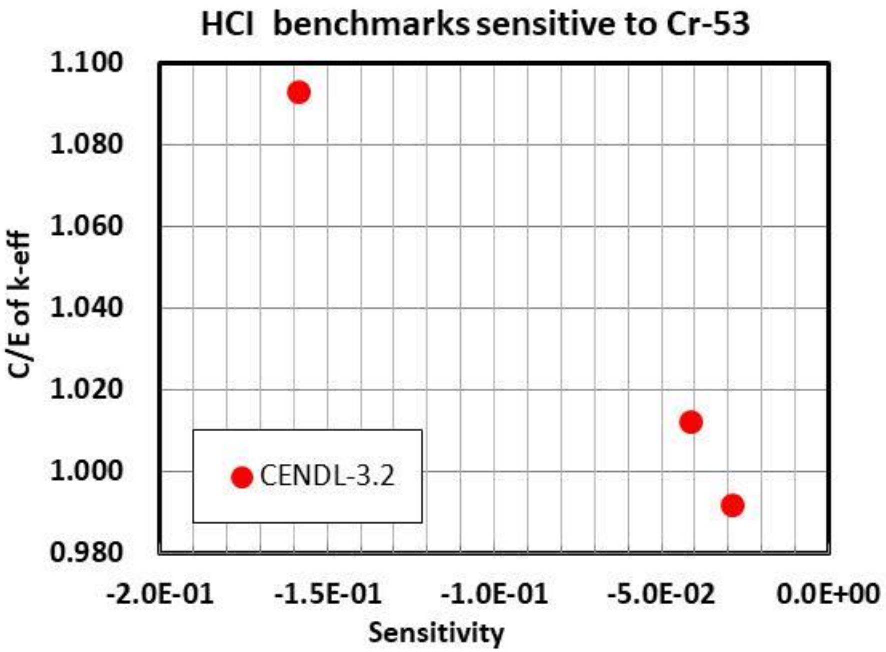


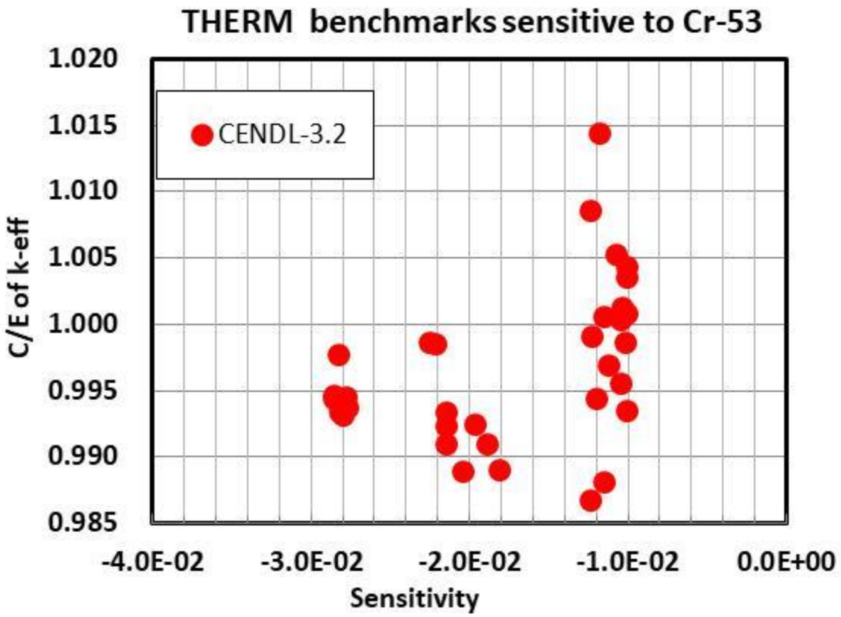


3.2 Cr-52,53

□ Testing results for the benchmarks sensitive to Cr-53

- **It is difficult to identify the relationship between k_{eff} deviations and Cr-53 data when the result of all thermal benchmarks sensitive to Cr-53 is analyzed.**





3.2.1 Cr-52(n,tot)

No.	Frequent Itemset	Support	R^2	Cases
1	['Form_MET']	0.1538	0.890	HMF061_01, HMF075_01, MMF011_01-4, PMF033_01, PMI002_01
2	['Spectrum_FAST', 'Moderator_coolant_Water (Heavy Water), Water (Light Water)']	0.0769	0.737	HCF003_02, HCF003_21-23
3	['Spectrum_FAST', 'Reflector material_Water (Light Water)']	0.0962	0.648	HCF003_01, HCF003_02, HCF003_21-23

3.2.1 Cr-52(n,tot)

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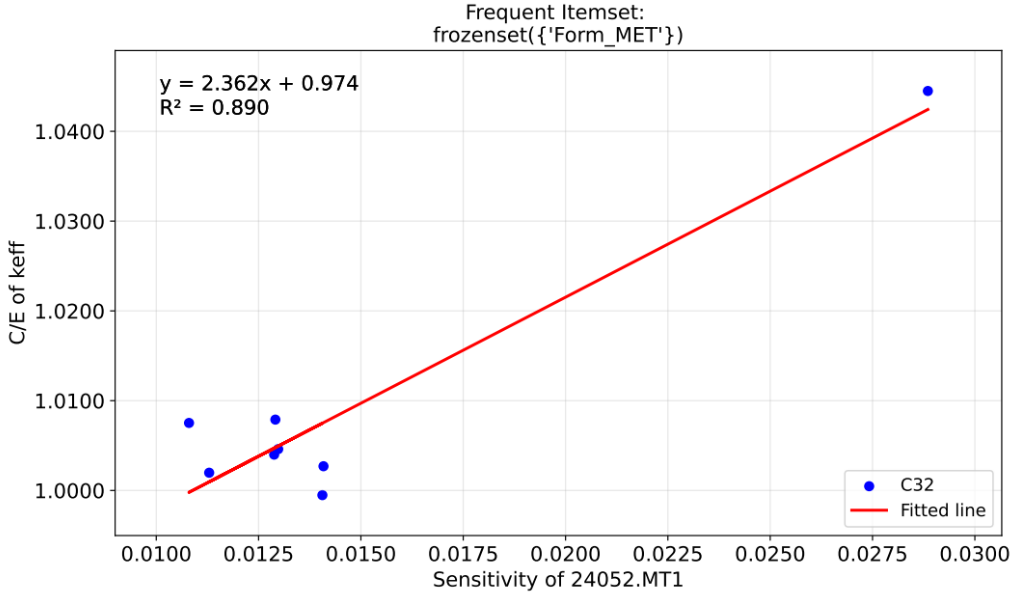
◻ Form_MET

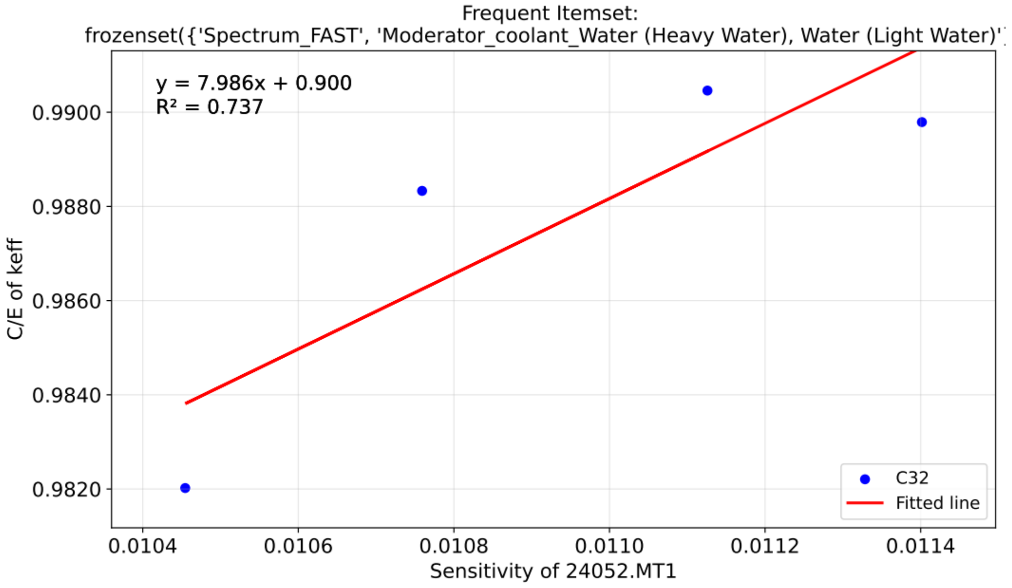
HMF061_01, HMF075_01, MMF011_01-4, PMF033_01, PMI002_01



Spurious trend: It may merely be a mathematical coincidence.

◻ Spectrum_FAST, Moderator_ coolant_ Water (Heavy Water), Water (Light Water)

HCF003_02, HCF003_21-23

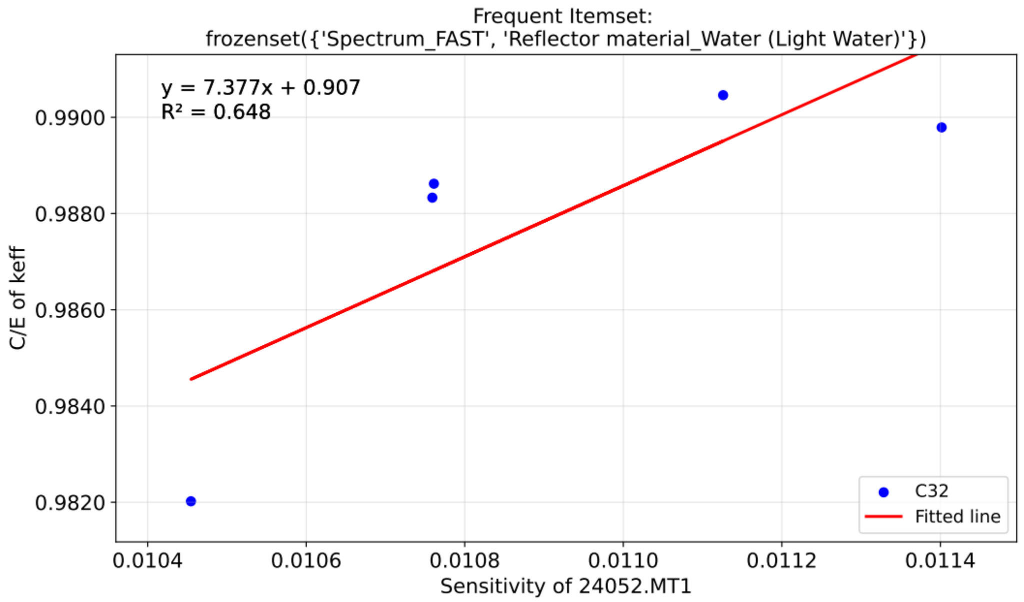


True trend: The benchmarks are similar, and there is a positive correlation between C/E values and ^{52}Cr(n,tot).

3.2.1 Cr-52(n,tot)

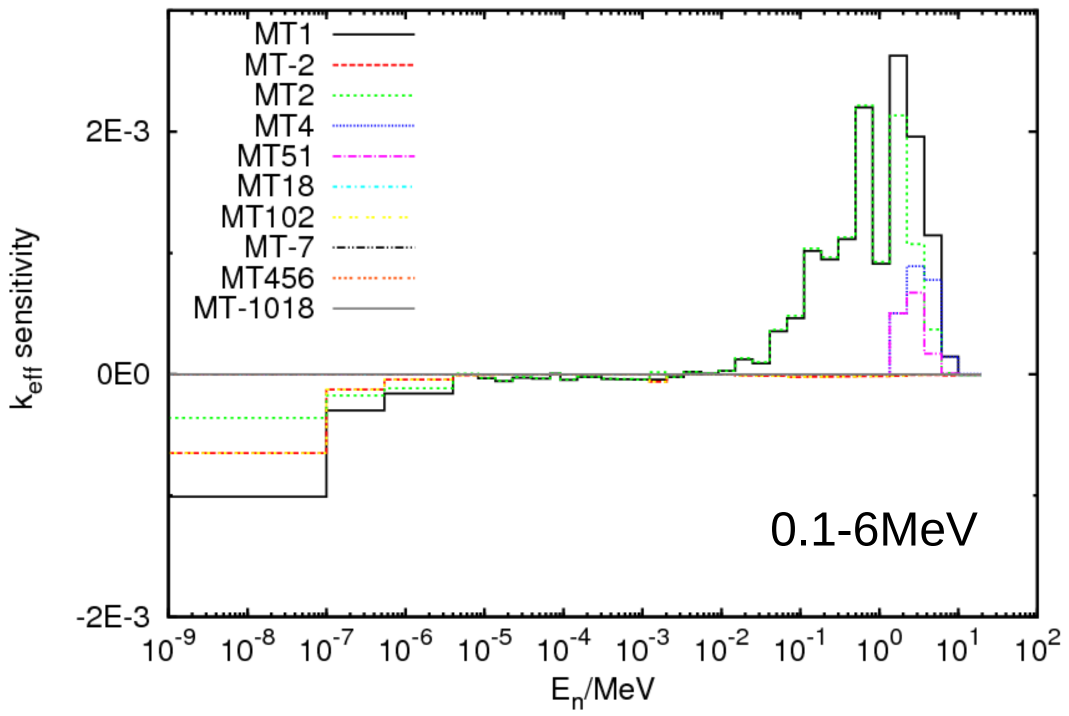
◻ Spectrum_FAST, Reflector material_Water (Light Water)

HCF003_01-02, HCF003_21-23



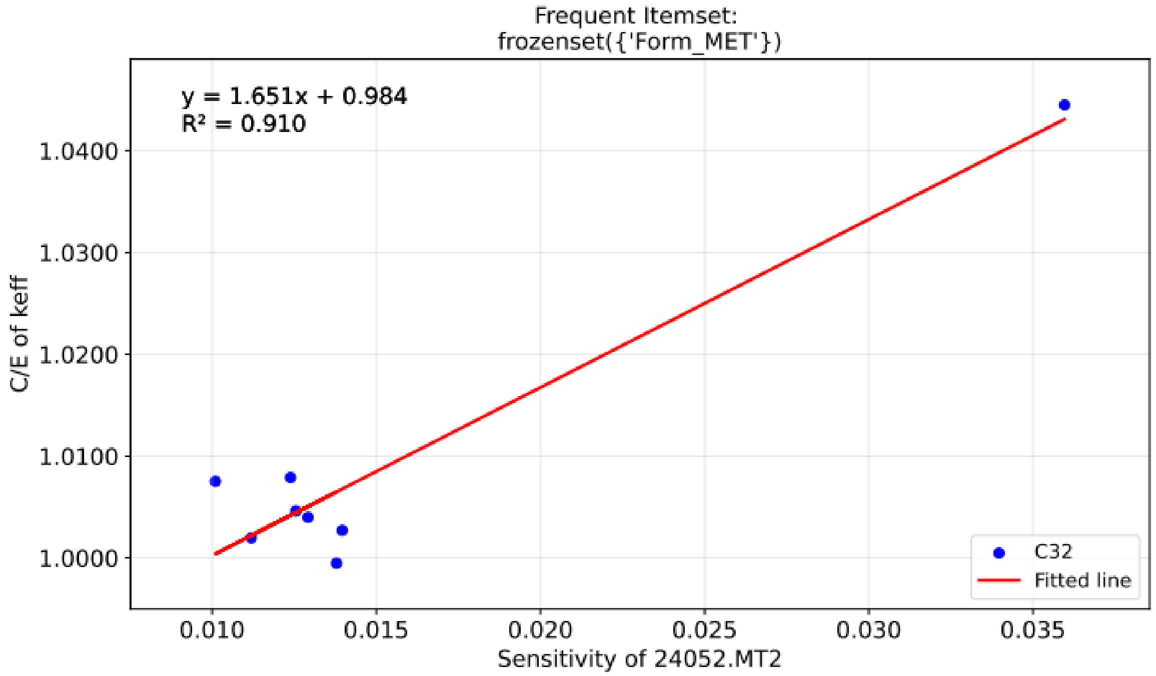
True trend: The benchmarks are similar, and there is a positive correlation between C/E values and ^{52}Cr(n,tot).

HEU-COMP-FAST-003-021(alias: HEU-COMP-MIXED-002-021),24052.00c



3.2.2 Cr-52(n,el)

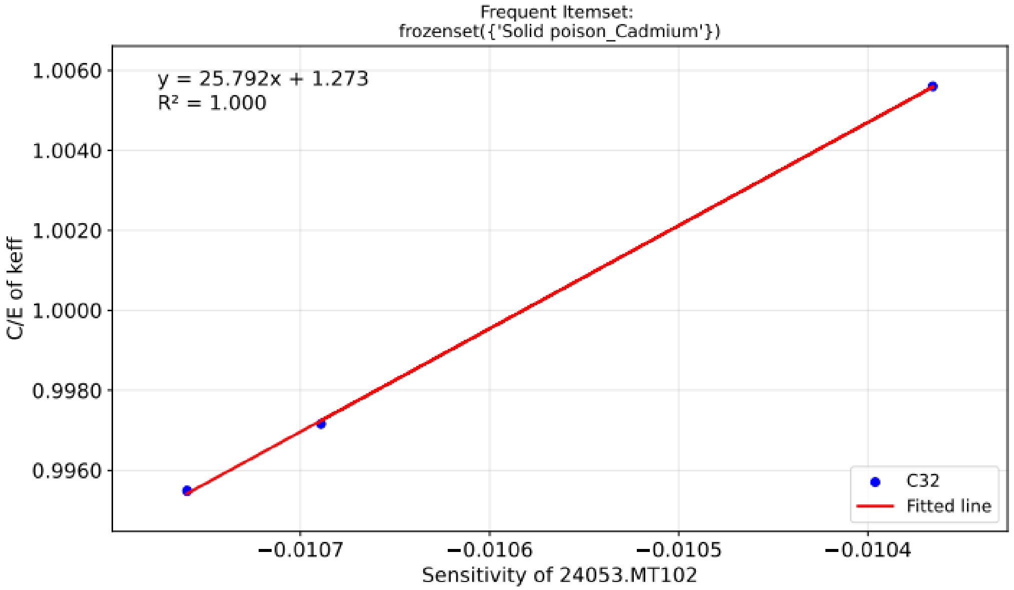
No.	Frequent Itemset	Support	R^2	Cases
1	['Form_MET']	0.242	0.910	HMF061_01, HMF075_01, MMF011_01-04, PMF033_01, PMI002_01

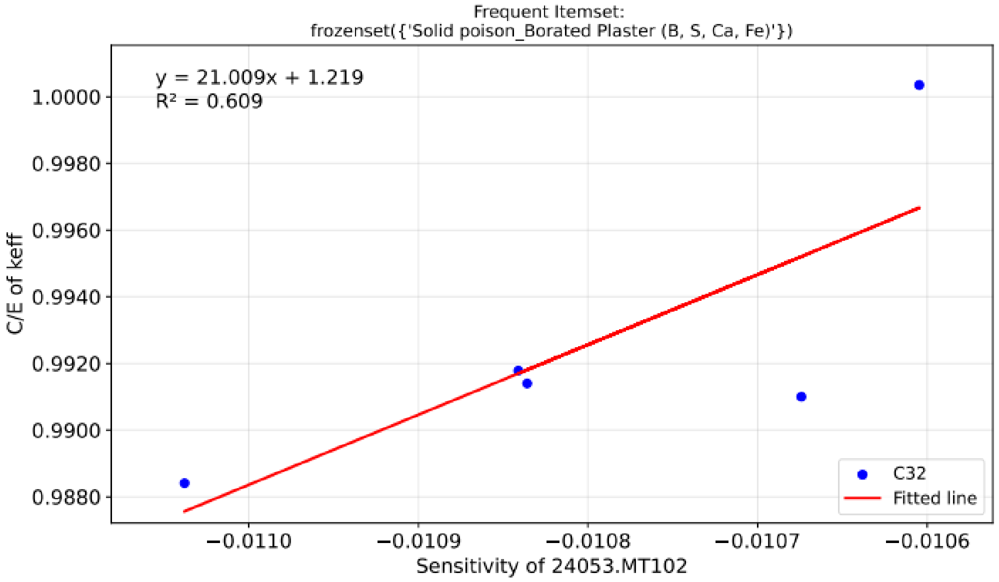


Spurious trend: It may merely be a mathematical coincidence.

3.2.3 Cr-53(n,g)

No.	Frequent Itemset	Support	R^2	Cases
1	['Solid poison_Cadmium']	0.0303	1.000	HST033_07S,08S, ICT002_05
2	['Solid poison_Borated Plaster (B, S, Ca, Fe)']	0.0758	0.609	HST033_13S-14S,17S-19S





True trend: The benchmarks are similar, and there is a positive correlation between C/E values and ^{53}Cr(n,g) sensitivity.

3.2 Cr-52,53

Summary of Cr

- There is **a linear trend positively** correlated with the cross-section sensitivity of ^{52}Cr(n,tot); sensitivity analysis indicates that the total cross-section from 0.1 to 6 MeV energy range may need to be improved.
- There is **a linear trend positively** correlated with the cross-section sensitivity of ^{53}Cr(n,g), and this cross-section needs to be improved.
- The linear trend positively correlated with the cross-section sensitivity of ^{52}Cr(n,el) may be a spurious trend.

4 Summary

- The Apriori machine learning algorithm was applied to establish a trend analysis method for criticality benchmark tests based on nuclide-reaction channel sensitivities, enabling automated analysis.
  - The granularity of trend analysis reaches the reaction channel level.
  - The efficiency of trend analysis is significantly improved, though the results still require supplementary expert judgment.
- It was found that the data related to the ^{27}Al(n,el) and (n,inl) reactions, as well as the (n,γ) cross-section, need to be improved.
- It was also determined that the cross-sections of ^{52}Cr(n,tot) and ^{53}Cr(n,γ) need to be improved.

Thank you for your attention！