Nuclear Data:
An personal overview

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for Nuclear Data

Summary

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- What does “nuclear data” and “evaluation” mean
- History
- Evaluation projects
- Working Party on International Nuclear Data Evaluation Co-operation
- Experimental data (EXFOR)
- EC/Euratom
- IAEA
- Overview of UK/International links
- Examples of validation

Nuclear Data

- A definition: "Parameters required to model the nuclear physics of an applied/industrial process to give engineering relevant quantities."
  - Smallest possible number of parameters that preserve the needed physics, but not necessarily all underlying physics.
  - Simplified, if possible, to allow easy use.
  - Best possible agreement with differential measurements and underlying theory.
  - Complete dataset including all required data.
  - Must be self-consistent and agree with physical constraints.
  - Produced in a standard format so can easily be understood and used.
  - Frozen version that can be referenced.
  - Validated for standard benchmarks.

Industrial Nuclear Data

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- Principle applications
  - Criticality.
  - Reactor operation (static and transient response).
  - Reactor accident studies.
  - Neutron transport/shielding.
  - Radiation damage.
  - Spent fuel composition (chemistry, radiations, heat, …)
  - Fuel cycle calculations.
  - Waste management.
  - Geological disposal.
- New needs
  - Proton transport; medical applications, transmutation etc.

Simple example of ND measurement

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- Measure decay properties of radionuclide
  - Need quality of radionuclide and detector setup
  - Measure characteristic gamma-ray emission
    Count rate, $C\gamma = n\lambda I\gamma$ (assuming detector efficiency is 1.0)
  - Measure $C\gamma \pm \Delta C\gamma$ equivalent to $(n\lambda I\gamma) \pm \Delta(n\lambda I\gamma)$
  - Measure decay over time to determine $\lambda \pm \Delta\lambda$ and thus $I\gamma \pm \Delta I\gamma$ can be determined. If independent determination of n is made, i.e. $n \pm \Delta n$

- Evaluated file needs $\lambda \pm \Delta\lambda$ and $I\gamma \pm \Delta I\gamma$
  - Note as you drill down to components the uncertainty increases.

Simple example of ND simulation

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- If you have n atoms of the radio nuclide in a sample or container, how many gamma-rays emitted.
- Reverse of experiment and analysis.
- Want the number of emitted gamma-rays from a specific number of atoms $E\gamma \pm \Delta E\gamma$, simply $E\gamma = n\lambda I\gamma$
- But if calculate uncertainty based upon Δn, $\Delta\lambda$ and $\Delta I\gamma$ will over estimate uncertainty.
- To get true estimate of uncertainty need to consider covariance terms- possible in this example, but what if λ is determined from a number of different types of experiment?

Time of flight total cross-section measurement

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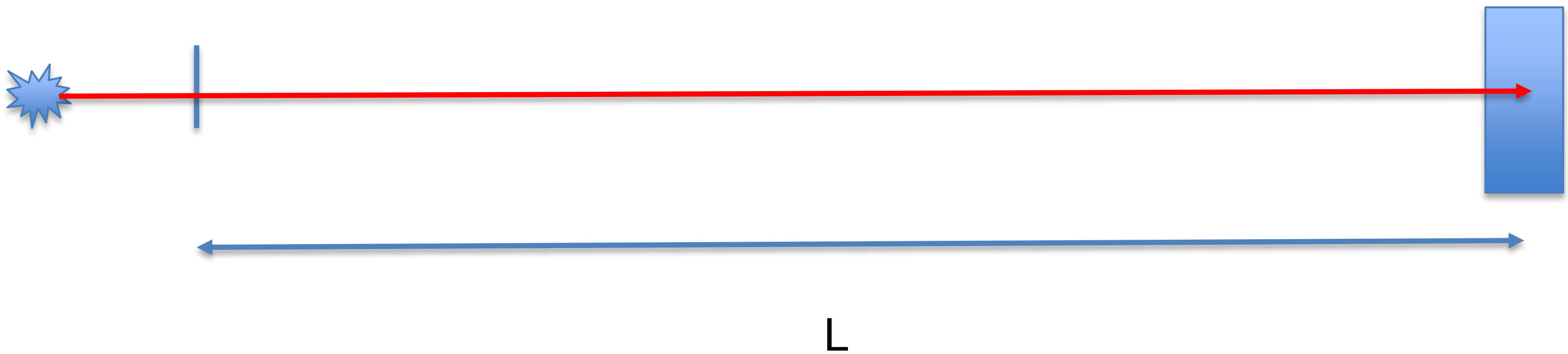
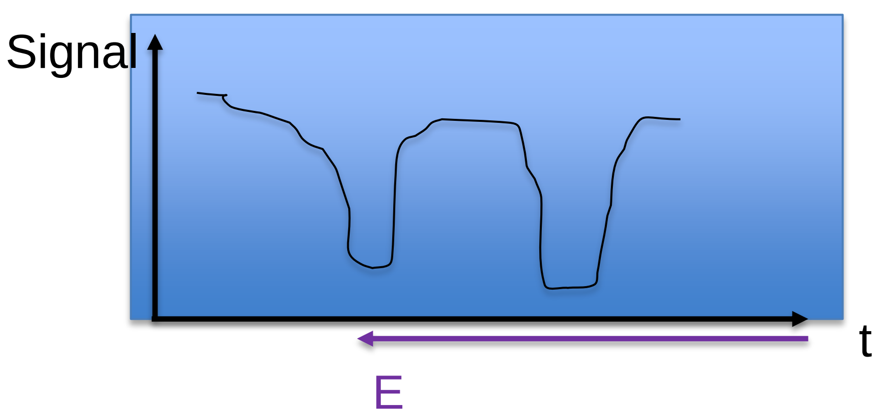
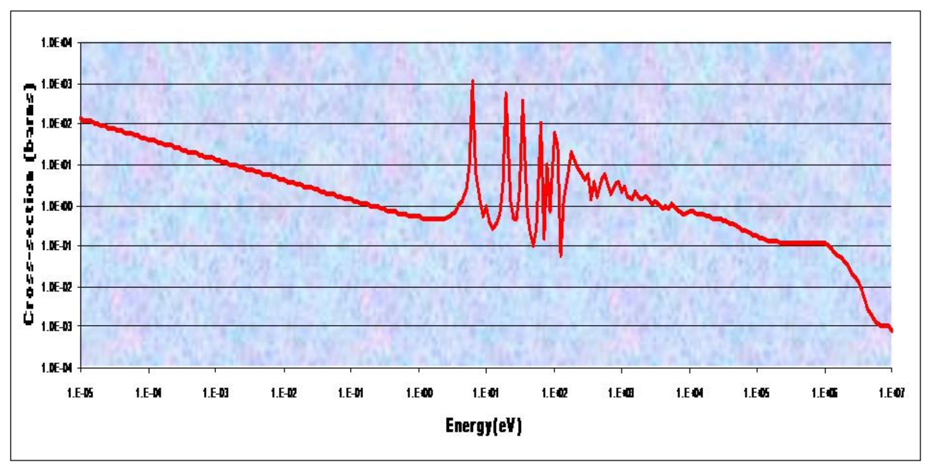


Classically

$E = ½ mv^2 = 0.5\ Mn\ (L/t)^2$





Time of flight cross-section analysis

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- Complex to extract the total cross-section using standards, analysis of self-shielding of target, resonance fitting, … .
- But similar to before want capture, fission, and other cross-sections for the evaluated file and simulations which are often more difficult to measure.
- Have good estimate of total, often with less accurate components.
- Again component uncertainties correlated.
- Currently can consider covariance for single component reaction with energy, but rarely between reactions or between different nuclides.

Nuclear Data Evaluation

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Inputs

- Consider all differential measurements available
- Corrections from measurement analysis
- Physics theory and approximations (if any)
- Physical constraints (conservation of energy, charge etc.)

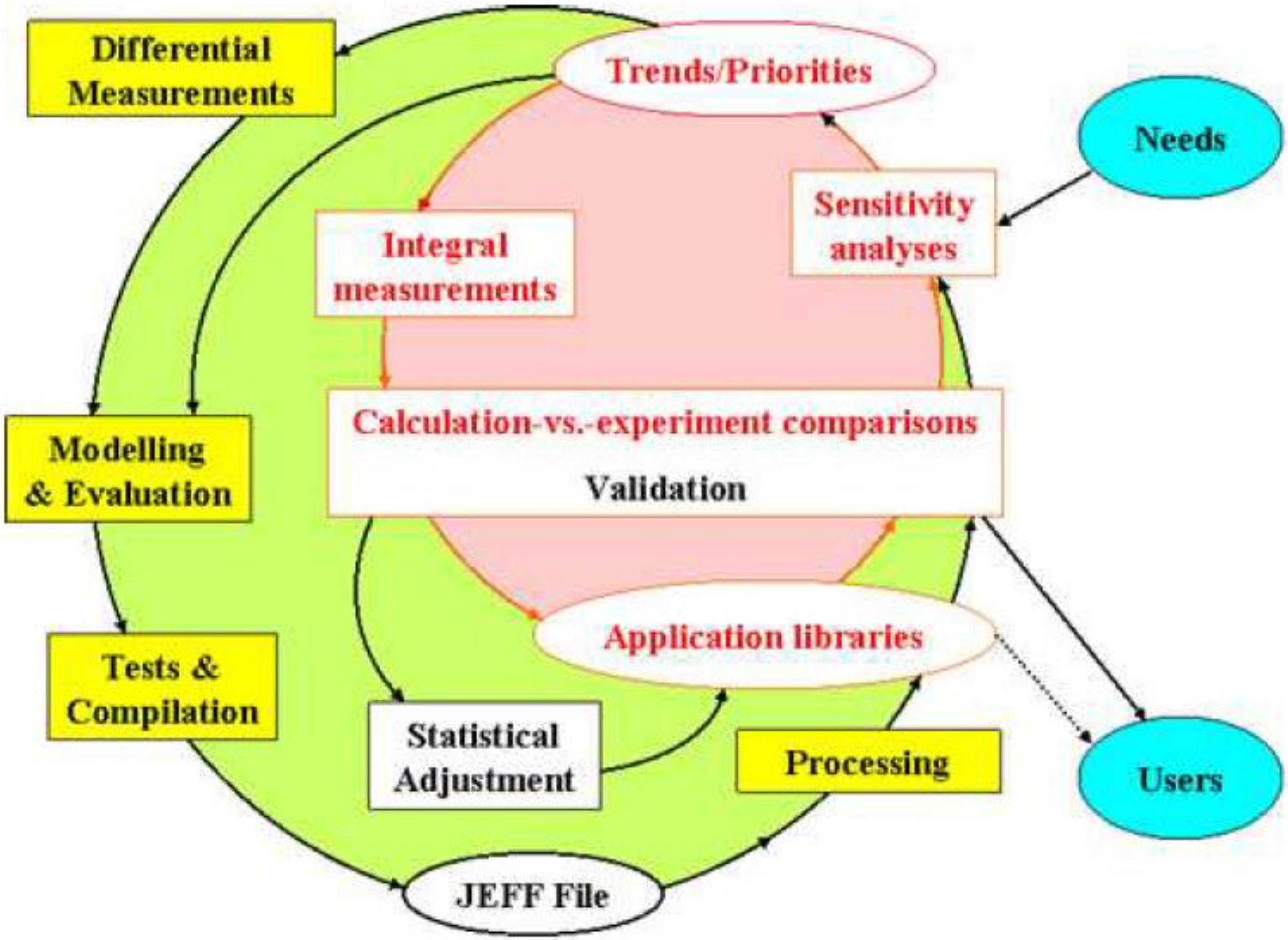
Process

- “Best fit” to inputs (measurements/theory)
- Generate complete datasets – “fill gaps”
- MUST conserve physical constraints.

Outputs

- Frozen version in standard format
- Tested against integral benchmarks
  - array of pins that go critical
  - volume of sphere that goes critical
  - insertion of absorber in reactor …

Nuclear Data Cycle



History

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- In 1940s/50s nuclear data needed for calculations of engineering parameters.
  - Measurements limited by technology; timing, energy resolution etc.
  - Results limited by calculation methods.
- In 1960s/70s computer codes developed that could handle large amounts of computer readable nuclear data allowing improved representation.
  - Improved detectors energy resolution and faster response
- In 80s to present day
  - Large detector arrays, storage of all results
  - Improved analysis
  - Improved simulation codes

History

- Initially each country developed its own data and formats overseen by local technical committees.
- International collaboration resulted in extension of data and adoption of a single (evolving) format, ENDF (Evaluated Nuclear Data Format). Currently on ENDF-6.
- Number of projects reduced as efforts become merged, now Evaluated Nuclear Data File [ENDF] (Americas), JEFF (Europe, Korea,…), JENDL (Japan), CENDL (China), BROND/ROSFOND (Russia + former Soviet Union states), …

JEF/JEFF

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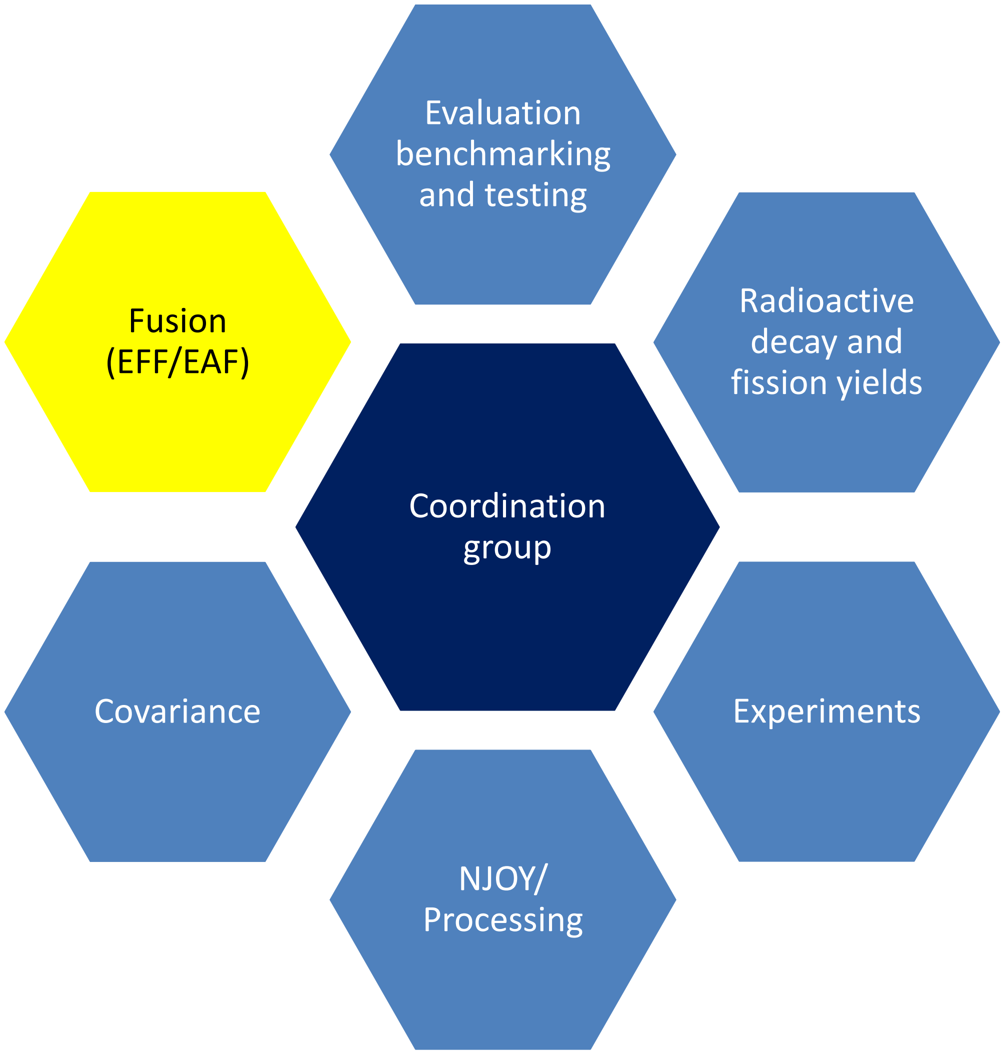
- Joint Evaluated File (JEF) started in the 1980s around a core of European efforts.
- Become Joint Evaluated Fission Fusion file (JEFF) around 2000 with closer links with the European Fusion File project.
- Volunteer project- partners need to obtain own funding for work.
- Split into sub-groups
  - Sub-groups meet (if needed) during 6 monthly meetings.
  - Any bona fide engineers and scientists from NEA Data Bank countries can attend, present or contribute data.
- Managed by Coordination group
  - Nominated country representatives and sub-group chairs.

JEF/JEFF


Evaluation benchmarking and testing
Fusion (EFF/EAF)
Radioactive decay and fission yields
Coordination group
Covariance
Experiments
NJOY/ Processing

Working Party on International Evaluation Cooperation (WPEC)

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- The Working Party on International Nuclear Data Evaluation Co-operation manages co-operation activities involving the following evaluation projects: ENDF (United States), JENDL (Japan), ROSFOND/BROND (Russia), JEFF (other Data Bank member countries) and CENDL (China) in close co-operation with the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

- It was established to promote the exchange of information on nuclear data evaluations, measurements, nuclear model calculations, validation, and related topics, and to provide a framework for co-operative activities between the participating projects. The working party assesses nuclear data improvement needs and addresses these needs by initiating joint evaluation and/or measurement efforts.

Working Party on International Evaluation Cooperation (WPEC)

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- Organised by the Nuclear Energy Agency (NEA) under the Nuclear Science Committee.
  - Membership limited to small number of project representatives and sub-group monitor and coordinators.

- Technical work in subgroup either permanent (formats, processing, high priority request list) or short-lived single purpose tasks (2 or 3 years).
  - Open to any interested bona fide scientists and engineers who agree with NEA charter.
  - All work open and published by OECD/NEA when complete.
  - Volunteer project – no funding available, need to obtain funds for work locally.

Working Party on International Evaluation Cooperation (WPEC)

- Current sub-groups 37-41 are:
  - 37 Improved fission product yield evaluation methodologies Co-ordinator: R.W. Mills
  - 38 Beyond the ENDF format: A modern nuclear database structure Co-ordinator: D. McNabb
  - 39 Methods and approaches to provide feedback from nuclear and covariance data adjustment for improvement of nuclear data files Co-ordinator: G. Palmiotti and M. Salvatores
  - 40 Collaborative International Evaluated Library Organisation (CIELO) Pilot Project Co-ordinator: M. Chadwick
  - 41 Improving nuclear data accuracy of Am-241 and Np-237 capture cross-sections Co-ordinator: H. Harada

- For more details or to become involved see https://www.oecd-nea.org/science/wpec/

Working Party on International Evaluation Cooperation (WPEC)

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- High Priority request list
- No new accepted proposals since 2008
  - Very high bar related to general purpose applications
  - Applicable to neutron transport, reactor modelling and criticality.
  - Requests must show sensitivity studies showing one element of nuclear data needs new measurements.
  - Review by modellers and experimentalists
  - Measurement must be credible and POSSIBLE
    - Want/need +/- 1%, best currently +/- 10%, can measurement achieve desired result?
- New Special Purpose Requests (SPR) category
  - Not as rigorous sensitivity studies required.
  - Decay data (e.g. Decay heat nuclides/TAGS), Fission yields, Thermal scattering data, …

EXFOR

- EXFOR or the “exchange format” is designed to allow transmission of nuclear data measurements between the Nuclear Reaction Data Centres, from whose web-sites it can then be obtained by evaluators and other interested parties. These include
  - IAEA Nuclear Data Section, Vienna, Austria.
  - OECD NEA Data Bank Paris, France.
  - US National Nuclear Data Center, Brookhaven, USA.
  - Russian Nuclear Data Center, Obninsk, Russian.
- The local web-site is http://www.oecd-nea.org/janisweb/search/exfor

EXFOR

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- EXFOR is the main source of data for evaluators.
  - Only reported (usually published) data is included.
  - Try to cover all major journals where nuclear data is reported.
  - Each entry tries to pull together all relevant documents (journal papers, lab reports, theses, conference papers) to report the final result of work.
- <u>PLEA TO EXPERIMENTALISTS</u>

  Please put your numeric data somewhere (e.g. appendix of thesis, internal report, ...) as reading data from a small 5x5 cm figure in a journal (often log-log!) will never show the accuracy you have worked so hard to achieve!

Other international activities

- ENDSF – Evaluated Nuclear Structure File
  - Less interest for applications, but good source for experimental data to aid decay data evaluations.
- EURATOM H2020 calls [Partially EC funded]
  - Specific tasks put out to contract via bids for European consortiums.
  - Tasks previously determined by commission, but now from a review of member country needs.
- IAEA Collaborative Research Projects
  - IAEA has broader remit that NEA.
  - Tend to be more general than WPEC or Evaluation projects.
  - Funding for travel and subsistence at meetings, some small research contract funding available.
  - IAEA/NEA coordinate activities to avoid direct duplication.

Links

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New Ideas/
Basic Science

Universities

National labs

Industrial R&D
Government/
Commercial

Implementation

Industrial
/Government

Experiment/Theory

Evaluation

Application

Experiment

Academic institutions with access to international facilities (EPSRC/STFC funding)

UK wide (e.g. UKNSF)

Industry, Regulators, Data/Code developers, Academics

-Peer review
-Advise on nuclear data and international links

[previously DTI/HSE funded]

Local evaluation projects

Contribute work,

Collaborate to solve problems and develop standards

e.g. JEFF

Worldwide Activities

IAEA
NEA
WPEC

Adverts

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- Nuclear Data Meeting calendar
  - https://www.oecdnea.org/science/wpec/calendar.html
- JEFF sub-groups
  - Letters of support for measurement and evaluation activities.
- WPEC sub-groups
- Nuclear Data for Science and technology (ND2016), Sept 2016, Bruges, Belgium. *www.**nd2016**.eu/*

Adverts

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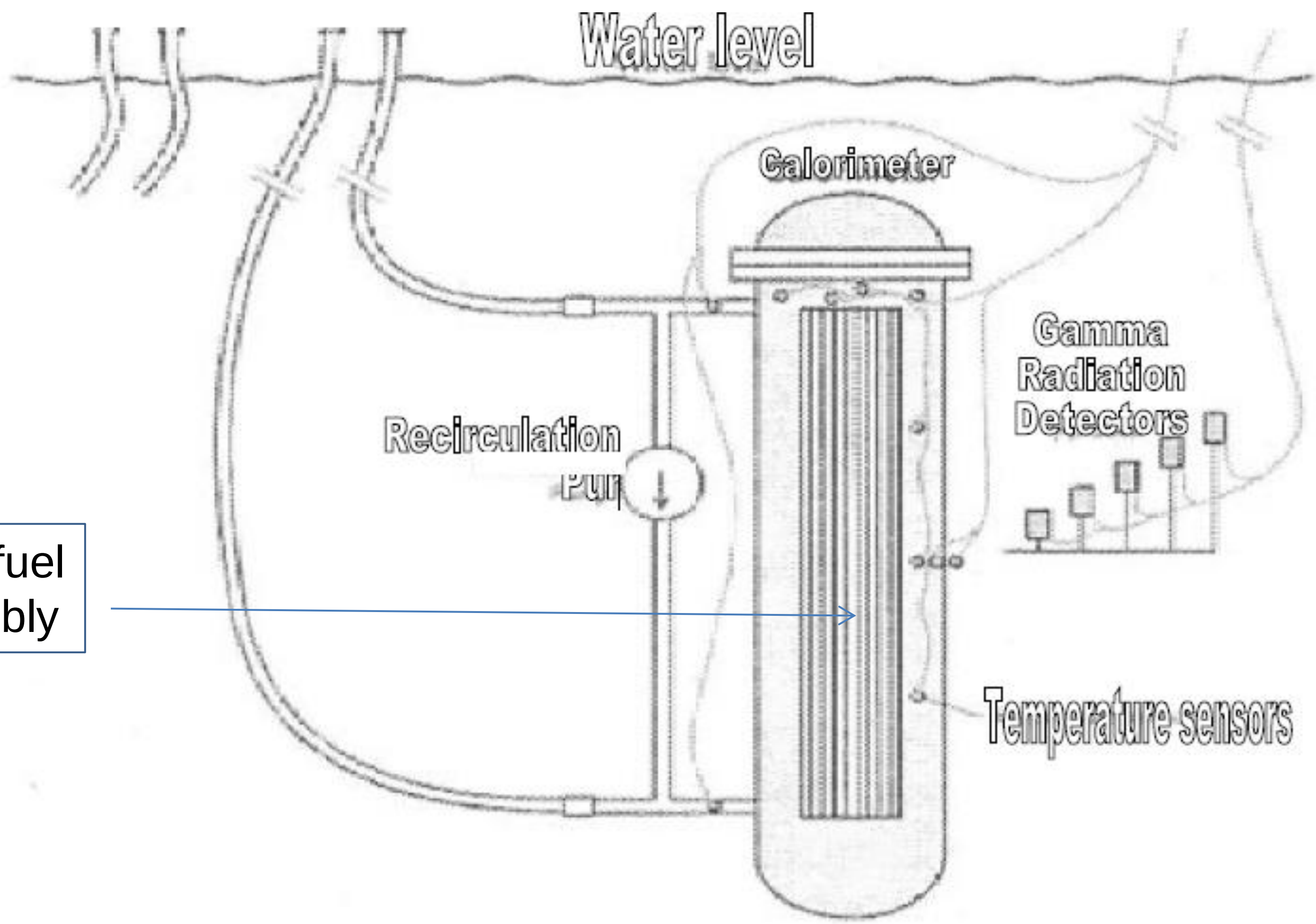
- <u>UK Nuclear Data Network</u>
  - Funded by STFC
  - Managed by Universities of Manchester, Surrey and York, and National Laboratories (NPL and NNL).
  - Started 1st April 2016 and will run for 4 years.
  - Designed to fund nuclear data measurements which benefit the UK (INDUSTRIAL INPUT! NEEDS!).
  - Will offer grants to Universities to prototype measurements or travel to facilities to make measurements.
  - Will fund UK Nuclear Science Forum chairman; forum to act as industrial peer review for proposals.
  - Fund UK subscriptions to nToF at CERN and Geel.
  - Interested in industrial need.

Validation

"The strongest arguments prove nothing so long as the conclusions are not validated by experience."

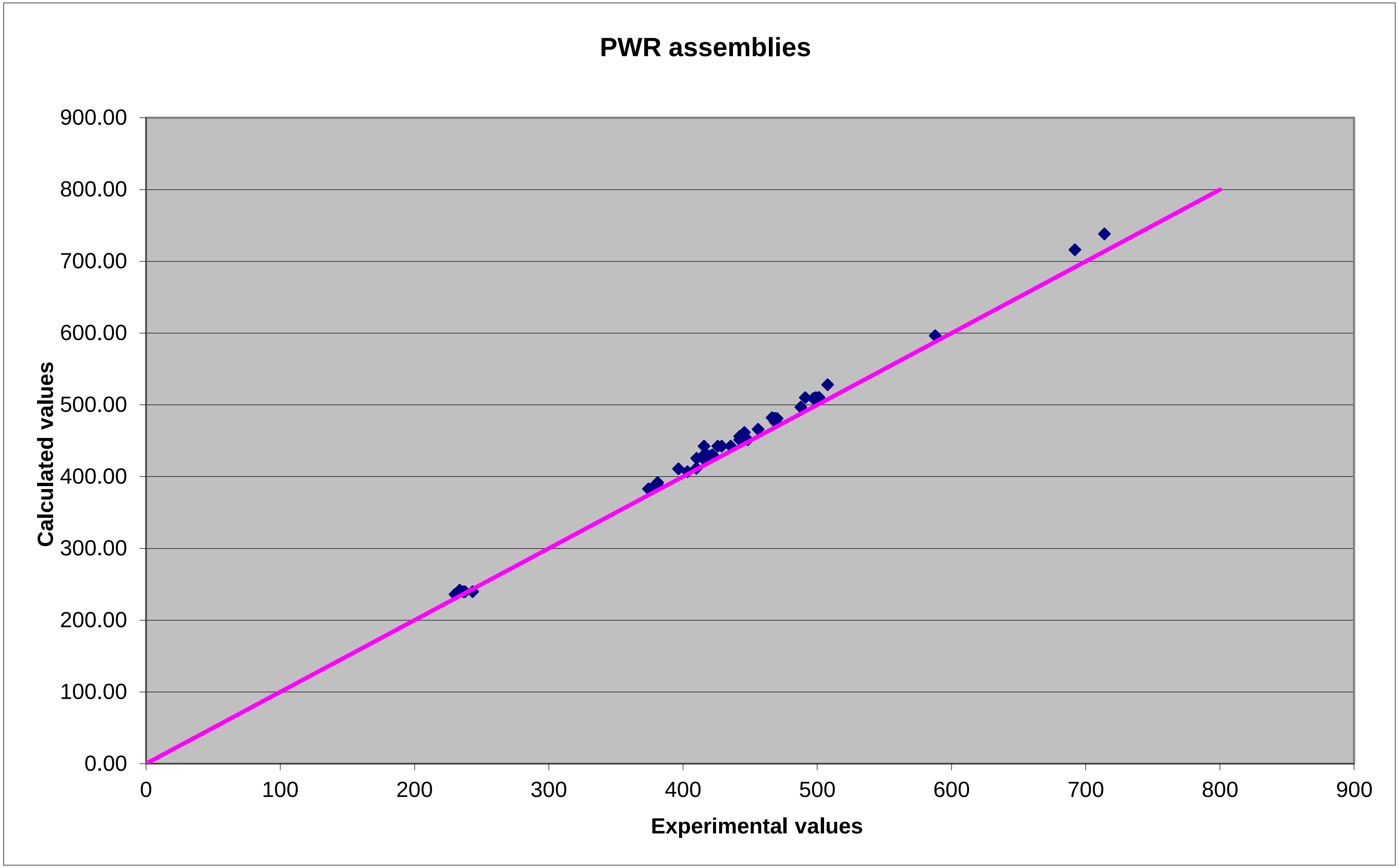
Roger Bacon,
Franciscan Friar
Born Ilchester ~1220
Died Oxford ~1294

Decay Heat Measurement at CLAB, Oskarshamn, Sweden



Spent fuel assembly

Decay Heat Example
Validation against SKB data



Decay Heat Example
Validation against SKB data

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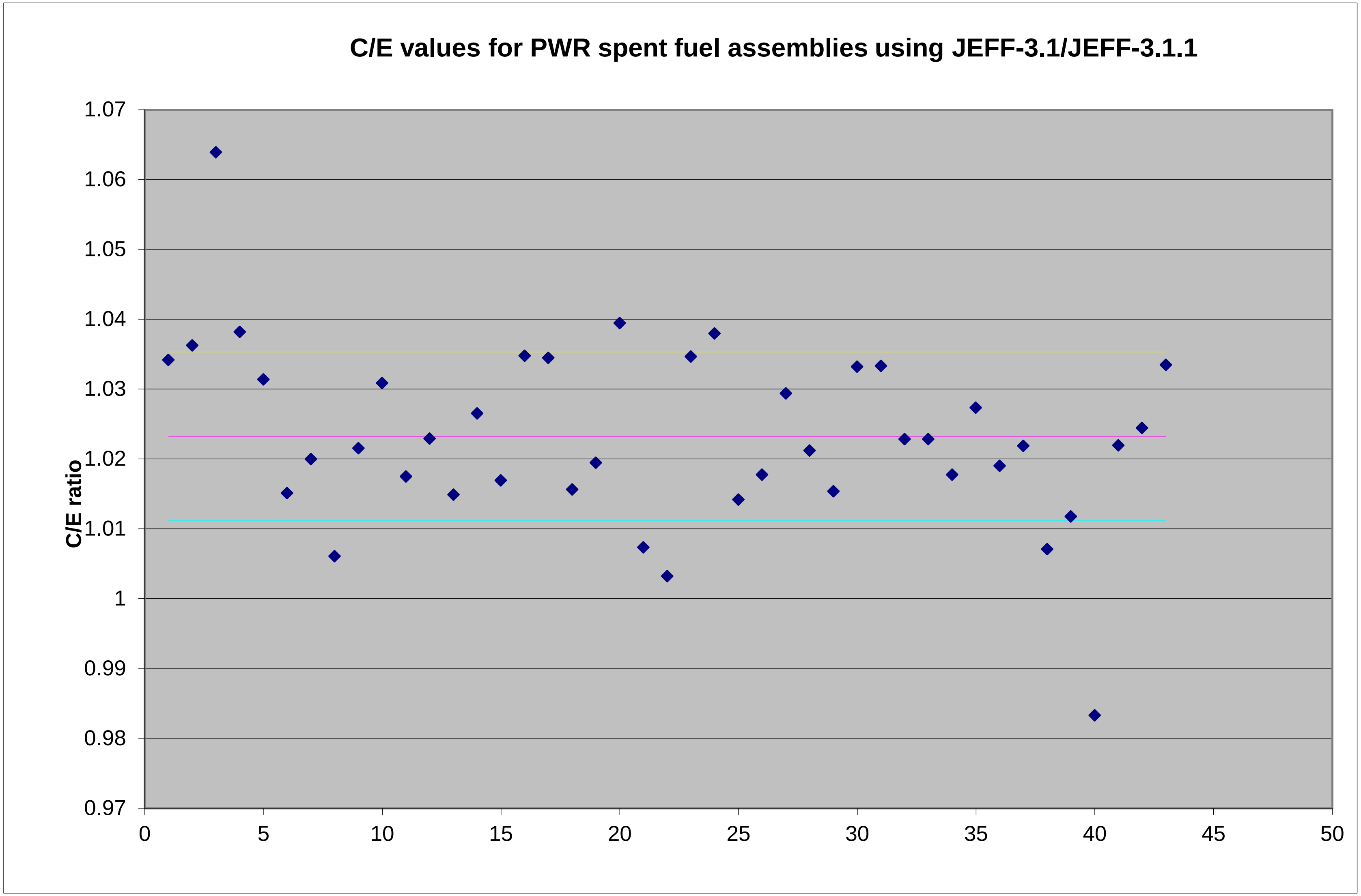

Decay heat
Using PIE to predict future heat

Can estimate decay heat biases and uncertainties by

- Comparing measurements of heating to calculation, or
- Alternatively, understanding radionuclide biases and uncertainties from radiochemical measurements and validation
  - Need validation for similar fuel to that being modelled

Expected heat from nuclide i, $\mathbf{h_i = N_i(expected)\ \lambda_i\ E_i}$

where

$$\mathbf{N_i(expected) = N_i(calc) / (C/E\ bias\ for\ i)}$$

and

$$\mathbf{Expected\ Heat,\ H = \sum h_i}$$

Decay heat
Goesgen PIE C/E from ARIANE

Nuclide	GU1	GU3'	GU3	GU4	JEFF-3.1 Mean ; SD	JEF-2.2 Mean ; SD
Sr90	0.77	1.03	0.98	0.99	0.94 ; 0.12	0.96 ; 0.12
Mo95	1.00	0.88	0.95	0.98	0.95 ; 0.05	0.95 ; 0.05
Tc99	1.01	0.90	1.01	1.26	1.04 ; 0.15	1.05 ; 0.15
Ru101	1.06	0.87	0.95	0.97	0.96 ; 0.08	0.96 ; 0.08
Ru106	1.08	0.86	0.47	0.85	0.81 ; 0.25	0.80 ; 0.25
Rh103	1.13	1.16	1.18	0.96	1.11 ; 0.10	1.11 ; 0.10
U234	1.16	1.38	1.43	1.40	1.34 ; 0.12	1.34 ; 0.12
U235	1.45	1.16	1.28	1.07	1.24 ; 0.16	1.24 ; 0.17
U236	1.01	0.99	0.98	0.99	0.99 ; 0.01	0.99 ; 0.01
U238	1.00	1.00	1.00	0.99	0.996 ; 0.001	0.996 ; 0.001
Np237		0.85	0.79	0.70	0.78 ; 0.07	0.78 ; 0.07
Pu238	0.99	0.92	0.85	1.00	0.94 ; 0.07	0.94 ; 0.07
Pu239	1.20	1.07	1.07	1.10	1.11 ; 0.06	1.11 ; 0.06
Pu240	0.96	0.96	0.93	0.97	0.96 ; 0.02	0.96 ; 0.02
Pu241	1.16	1.08	1.06	1.08	1.09 ; 0.04	1.09 ; 0.04
Pu242	0.83	0.91	0.83	0.94	0.88 ; 0.06	0.87 ; 0.06
Pu244	0.68	0.52			0.60 ; 0.11	0.60 ; 0.11
Am241	1.24	1.27	1.25	1.05	1.20 ; 0.10	1.20 ; 0.10
Am242m	1.27	0.94			1.11 ; 0.23	1.10 ; 0.23
Am243	1.01	1.03	0.79	1.00	0.96 ; 0.11	0.95 ; 0.11
Cm242	0.99	0.93			0.96 ; 0.04	0.95 ; 0.04
Cm243	3.12	1.17			2.14 ; 1.38	2.11 ; 1.35
Cm244	0.90	0.82	0.56	0.76	0.76 ; 0.15	0.76 ; 0.15
Cm245	0.98	0.76	0.50	0.73	0.75 ; 0.20	0.74 ; 0.19
Cm246	0.62	0.62			0.62 ; 0.00	0.62 ; 0.01
$Pu^{\dagger}$	1.07	1.03	1.01	1.06	1.04 ; 0.03	1.04 ; 0.03

Decay heat
Using PIE to predict future

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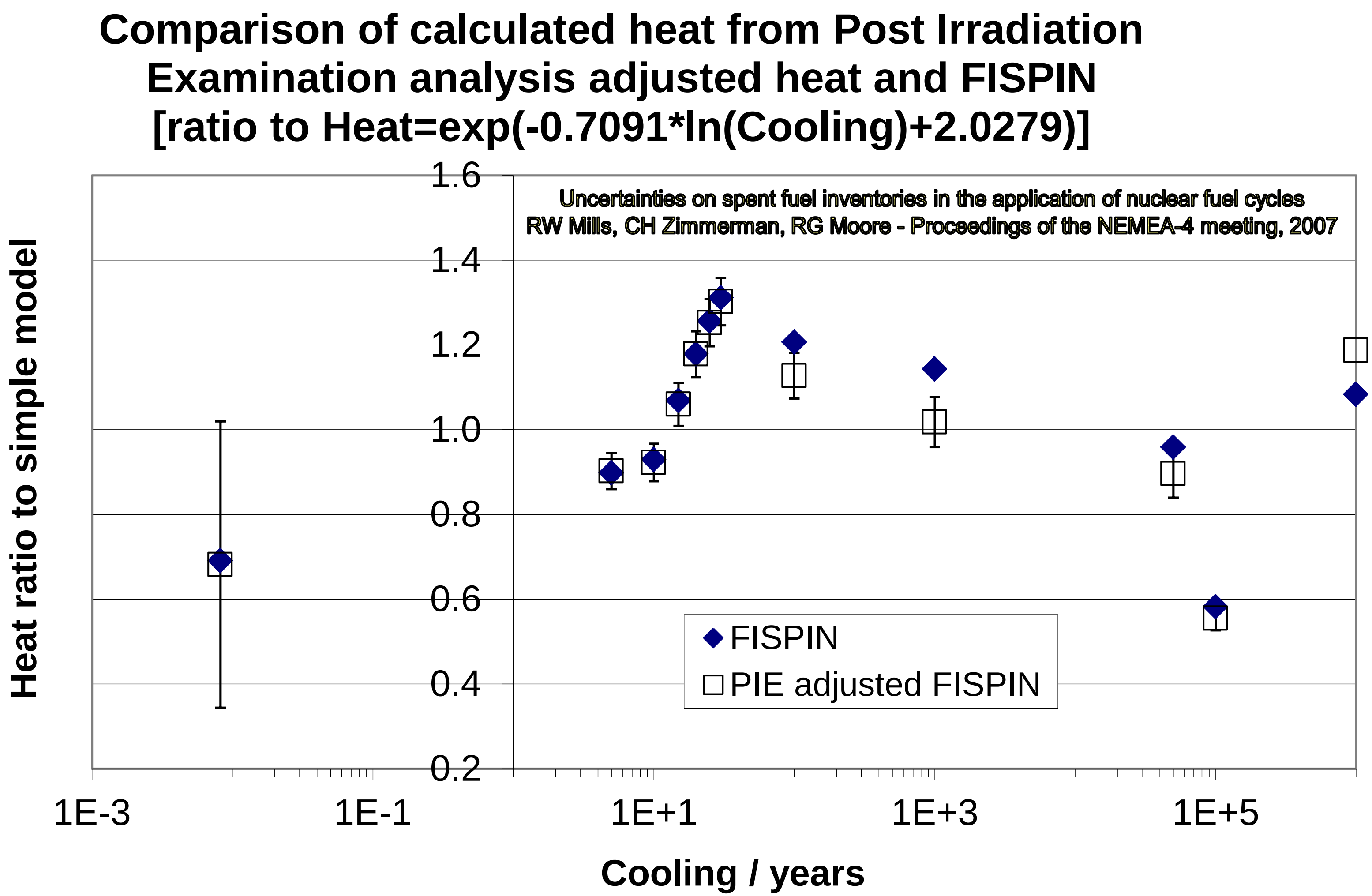

Current situation and way forward?

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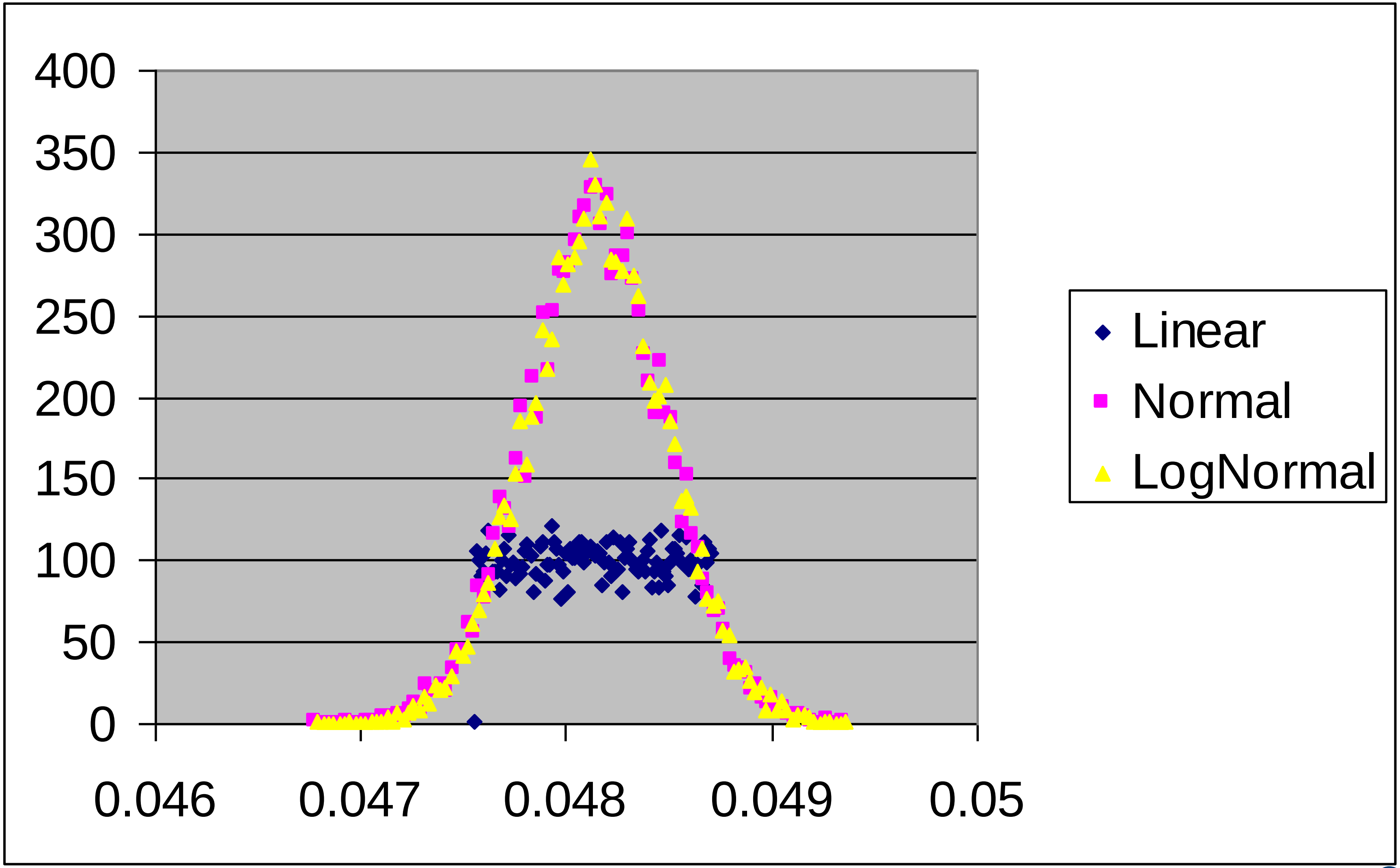
- Current methods for determining uncertainties on spent fuel inventory calculations rely upon validation against experimental measurements.
  - Due to the difficulties of such measurements and their costs the range of validated nuclides, and quantities, are small and the number of measurement limited.
- Taking advantage of the measurements of basic nuclear data and their uncertainties offer the possibility of generating uncertainty estimates for a much wider range of nuclides and global properties such as decay heat etc.
  - Options include sensitivity methods and "Total Monte Carlo" but these result in new fundamental questions on evaluated nuclear data and its evaluation. (WPEC-37)

Sampling probability distributions



Simple "Total Monte Carlo" for practical decay data example

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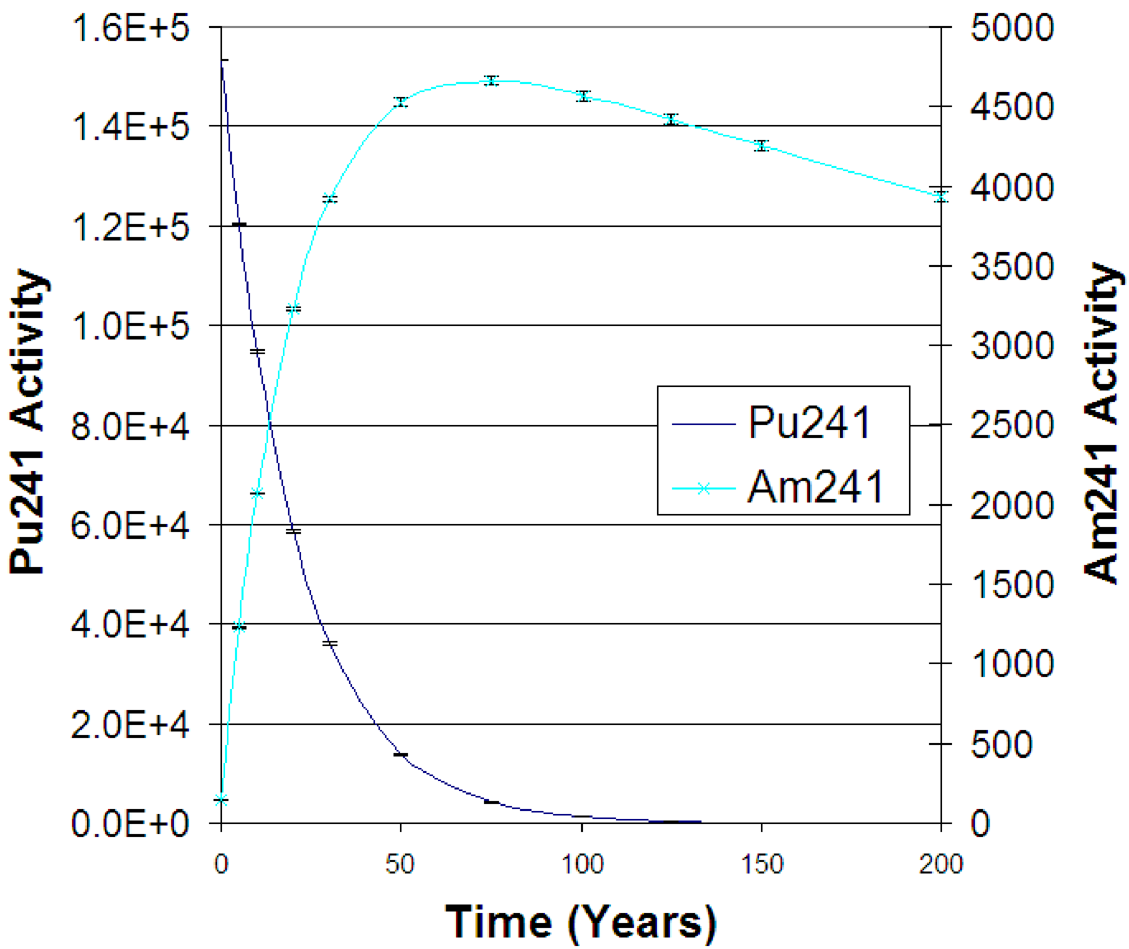
- Consider a mass of plutonium containing an initial activity of ^{241}Pu and ^{241}Am. How do these vary with time and what are their uncertainties?
- Given the decay constants are $4.8134 \times 10^{-2} \pm 3.342 \times 10^{-4}$ per year and $1.6019 \times 10^{-3} \pm 1.852 \times 10^{-6}$ per year respectively.
- The "best estimate" result can easily be calculated.
- If we sample the decay constants from different probability distributions with the required mean and standard deviation, run each for 10000 times and then analyse the results we get ….

Result



Activities at 200 years

PDF	^{241}Pu	^{241}Am
Normal	10.13 ± 0.68	3933 ± 28
Linear	10.12 ± 0.67	3933 ± 28
Log Normal	10.13 ± 0.68	3933 ± 27

Fission Product decay heat following a fission pulse

- TENDL-2010 included FPY and decay data files with up to 1000 randomly perturbed data libraries for used in uncertainty propagation but physical constraints are correct.
- Using these FPY libraries, the UK spent fuel inventory code FISPIN was used to calculate decay heat from a fission pulse with each library.
- The unperturbed JEFF-3.1.1 decay data library was used and thus the uncertainties from energy release per decay and half-lives are not considered. Although some published Algora/Tain TAGS data was included extending JEFF-3.1.1.
- The results were compared Tobias (1989).

^{239}Pu total energy release

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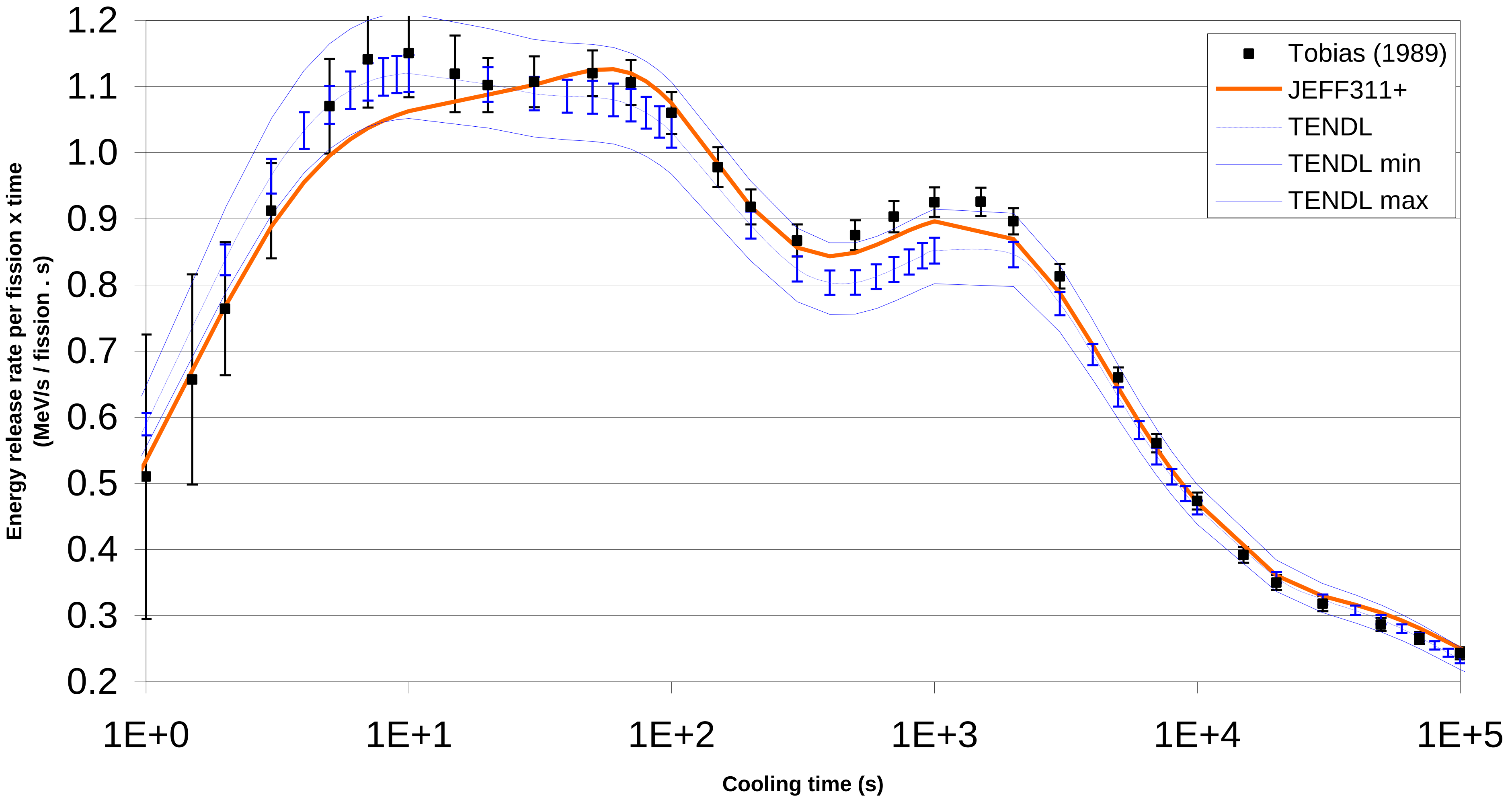

Examples of C14 in irradiated graphite

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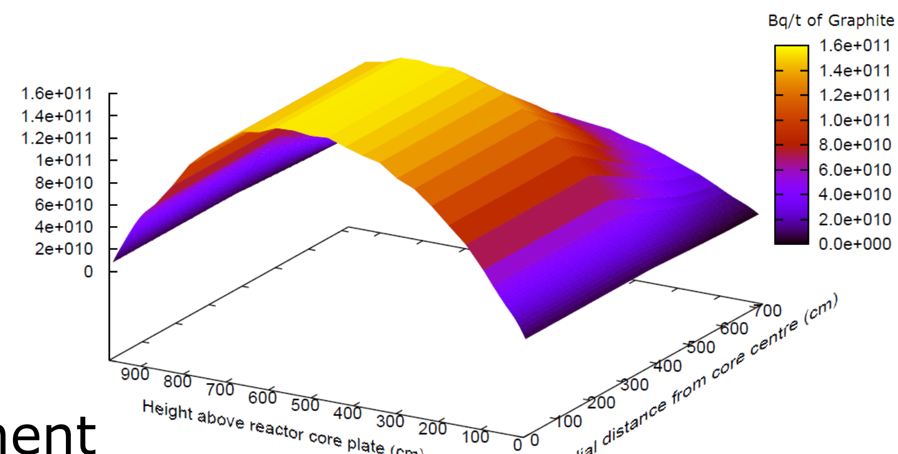
- C14 production in graphite (Magnox) reactors
  - EURATOM CARBOWASTE project and IAEA's i-graphite.
  - NNL measurement of C14 in samples and benchmarked using nuclear data in the FISPIN modelling code.
  - Review of cross-section data
  - Estimation of whole core C14 in Oldbury 2 (ENC2012 paper)
    - Found reflector is ILW from C14 alone
  - Testing of C14 mass balance using reactor discharge data (Annals of Nuclear Energy, 2014/5)



  - Investigating new measurement of C13(n,γ)C14 through University of Manchester at n_ToF as ~50% between measurements.

Effect on cumulative yield uncertainties

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- The following shows the JEFF-3.1.1 file data and a calculation of cumulative yields from independent yields and their uncertainty without the covariance terms (assuming independent uncertainties).

Quantities	^{85}Ge	^{85}As	^{86}Ga	^{86}Ge	^{86}As	^{85}Se	^{85}Br	^{85m}Kr	^{85}Kr	^{85}Rb
JEFF-3.1.1 Y^i	2.44e-5	1.41e-3	1.82e-6	2.85e-6	4.42e-4	9.58e-3	2.19e-3	1.12e-5	4.85e-5	3.30e-8
JEFF-3.1.1 Y^i 1FPY	9.08e-6	4.69e-4	6.65e-11	1.04e-6	1.59e-4	9.47e-4	7.14e-4	4.18e-6	1.81e-5	1.23e-8
JEFF-3.1.1 Y^c	2.44e-5	1.43e-3	1.82e-10	2.85e-6	4.45e-4	1.08e-2	1.30e-2	1.30e-2	2.86e-3	1.31e-2
JEFF-3.1.1 Y^c 1sd	9.06e-6	4.19e-4	6.66e-11	1.04e-6	1.55e-4	2.10e-4	1.19e-4	1.19e-4	2.10e-4	1.19e-4
Calculated Y^c	2.44e-5	1.43e-3	1.82e-10	2.85e-6	4.45e-4	1.08e-2	1.30e-2	1.30e-2	2.86e-3	1.31e-2
Calculated Y^c 1sd	9.08e-6	4.69e-4	6.65e-11	1.04e-6	1.59e-4	1.02e-3	1.24e-3	1.24e-3	2.68e-4	1.24e-3
Y^c ratio file/calc	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Y^c 1sd file/calc	0.998	0.893	1.000	1.000	0.978	0.206	0.096	0.096	0.785	0.095

- The results show that without the covariance terms many of the cumulative yield uncertainties are over-predicted.

Conclusions

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- Still strong activity on nuclear data, but reducing, international community for nuclear data through NEA, IAEA etc.

but

- UK must engage if it wishes to use these resources to solve UK issues, or go it alone at much higher cost.

- UK has strong history of nuclear data and some remaining expertise in nuclear data, but we must act NOW if these do not become history.

Acknowledgements

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