Approaches on Uncertainty Expression in Nuclear Material Accounting

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Implementation of IAEA Safeguards in the ROK (before SLA)



* IAEA, INFCIRC/153 (Corr.)



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Implementation of IAEA Safeguards in the ROK (under SLA)



* IAEA, Safequards Glossary 2022



Legal basis for national safeguards inspection and MBE



NSSC notification No. 2017-83

- (Article 4) National safeguards inspection includes
- Book examination
- Verification of declared information
- Verification of accounting equipment
- Verification of C/S system
- Verification of records
- Design information verification (DIV)
- Examination of MBAs and KMPs
- Material balance evaluation (MBE)
- Examination of accounting process
- Verification of other required processes

% nsic.mssp.go.kr/nsic.do?nsicKey=300101

Need to perform an independent MBE (MUF evaluation) to satisfy domestic notification



- Practical requirements for an MBE in national safeguards inspection
 - Accumulation of cumulative MUF for a series of MBPs in domestic MBAs
 - MUF is not significant for a single MBP
 - Cannot identify the key accounting process for the MUF accumulation





Need to conduct an independent MBE (MUF evaluation) to evaluate the accounting system as well as to detect diversion



• What is MBE (MUF evaluation)?





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Uncertainty expression in MBE

- MUF is calculated using the inventory of individual items(X_i) $MUF = f(X_1, X_2, ..., X_n)$
- An item(X_i) is calculated using the individual measurement(x_{ij}) $X_i = f(x_{i1}, x_{i2}, ..., x_{in})$





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Characteristics of uncertainty expression methods

	Top-down method (ANOVA)	Bottom-up method (GUM)
Requirements	 Pair-wise difference data for a number of grouped items Mathematical adjustments (DODGRU, CELEX) for negative variances 	 Detailed facilities' accounting information to identify, quantify, and propagate individual uncertainty components (Bayesian statistics)
Advantages	 Do not require facilities' detailed accounting information (Can maintain independency) 	 Can analyze the contribution of individual uncertainty components (Have high traceability)
Disadvantages	 Cannot analyze the contribution of individual uncertainty components (Have low traceability) Cannot modify the IAEA's adjustments 	 Assumptions on facilities' accounting information in individual uncertainty components (Cannot maintain independency)
Application	 IAEA and national inspection(back-up) Target: all BHFs in member states Purpose: diversion detection 	 National inspection (KINAC) Target: domestic BHFs Purpose: diversion detection & evaluation of accounting system



• Governing equation for MUF in a LEU fuel conversion & fabrication plant

 $M = \sum_{l=PB,X,Y,PE} A_l \sum_{i=1}^{I} \sum_{j=1}^{J} (p_j f_{U,ij} w_{235,ij} \sum_{k=1}^{K} (m_{ijk}))$

- Individual measurement uncertainty components
 - Weighing (m) with EBAL
 - EBAL indicator (X), buoyancy factor (f_b) , and calibration factor (f_c)
 - Sampling (p) for destructive analysis ($p \sim N(1, \delta_p^2)$)
 - U concentration analysis (f_U) with GRAV
 - Oxygen to Uranium ratio (O/U)

> Mass ratio (m_i/m_f) , impurity concentration (w_I, w_F) , and ²³⁵U enrichment (w_{235})

- -²³⁵U enrichment (w_{235}) with TIMS
 - Isotopic ratio $(R_{234}/R_{238}, R_{235}/R_{238}, R_{236}/R_{238})$

Sample meas. ratio $(RS(m)_{23x/238})$, cert. meas. ratio $(RC(m)_{23x/238})$, certificate ratio $(RC(c)_{23x/238})$, BKG $(RB_{23x/238})$, det. eff. $(\delta(Y), \delta(L), \delta(F))$

 A_l : type of physical inventory (+1 (PB, X), -1 (PE, Y),) I: number of stratum for an inventory (i = 1, 2, ..., I), J: number of lots in a stratum (j = 1, 2, ..., J), K: number of items in a lot (k = 1, 2, ..., K).

Individual uncertainty

Uncertainty components



- (IAEA) ANOVA-based uncertainty quantification (1/4)
 - Setup a pair-wise difference statistics & separate random and systematic components
 - * IAEA, IAEA-SG-PR-2016
 - 1. Establish a database of pair-wise differences for a number of groups of samples
 - 2. Let x_{gi} and y_{gi} be the facilities' and inspectors' measurement results for an item whose group is g and ID is i
 - 3. Let m_g and G be the number of items in group g and the number of groups.
 - 4. Let d_{gi} and V_{gd} be the pair-wise difference $x_{gi} y_{gi}$ and its variance for items in group g
 - 5. Estimate the random variance $(V_{rd} \ (= \ \widehat{\sigma_{rd}}^2))$ of the pair-wise differences $\widehat{\sigma_{rd}}^2 = \frac{\sum_{g=1}^G (m_g 1) V_{gd}}{\sum_{g=1}^G (m_g 1)}$
 - 6. Estimate the systematic variance $(V_{sd} (= \hat{\sigma_{sd}}^2))$ of the pair-wise differences

$$\widehat{\sigma_{sd}}^2 = \left(\frac{\sum_{g=1}^G \left(\sum_{i=1}^m \frac{d_{gi}}{m_g}\right)}{G}\right)^2 - \frac{\left(\frac{\sum_{g=1}^G \left(\frac{1}{m_g}\right)}{G}\right) \widehat{\sigma_{rd}}^2}{G}$$





(IAEA) ANOVA-based uncertainty quantification (2/4)

- Separate operator's and inspector's variance

* IAEA, IAEA-SG-PR-2016

• Estimate the random variance of an operator $(V_{rx} (= \hat{\sigma_{rx}}^2))$ and inspector $(V_{ry} (= \hat{\sigma_{ry}}^2))$ using the Grubbs' method

$$\widehat{\sigma_{rx}}^2 = \frac{\sum_{g=1}^G (m_g - 1) \widehat{\sigma_{rgx}}^2}{\sum_{g=1}^G (m_g - 1)} , \ \widehat{\sigma_{ry}}^2 = V_{rd} - \widehat{\sigma_{ry}}^2$$



 $\widehat{\sigma_{rgx}}^2$: operator's random variance for items in group g

 v_{gx} : operator's variance for items in group g

 v_{gxy} : operator's and inspector's co-variance for items in group g



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• (IAEA) ANOVA-based uncertainty quantification (3/4)

- Separate operator's and inspector's variance

* IAEA, IAEA-SG-PR-2016

- If impossible ($V_{rx,ry} < 0$), estimate the random variance of a facility based on the DODGRU (DOD and GRUbbs' estimator) method

$$\widehat{\sigma_{rx}}^2 = \mathrm{S}\frac{I_0}{I_1}$$

DODGRU parameters





- The estimated results have low traceability



• (IAEA) ANOVA-based uncertainty quantification (4/4)

- Separate operator's and inspector's variance
 - * IAEA, IAEA-SG-PR-2016
- Estimate the systematic variance of a facility ($V_{sx}(=\widehat{\sigma_{sx}}^2)$)) based on an assumption ($\widehat{\sigma_{sx}}^2 = \widehat{\sigma_{sy}}^2$) $\widehat{\sigma_{sx}}^2 = \frac{1}{2} (\widehat{\sigma_{sd}}^2)$



- (National Inspection) GUM-based uncertainty quantification (1/5)
 - Setup an equation to quantify a measurement result
 - $X = f(x_1, x_2, x_3)$

X₂

- Establish standard accounting procedures
 - 1. Identify initial characteristics of a sample (x_1, x_2, x_3)
 - 2. Measure the sample using an accounting system with the initial characteristics (X)
- Identify individual uncertainty components

$$x_{1} = f\left(x_{1r_{1}}, \dots, x_{1r_{n}}, x_{1s_{1}}, \dots, x_{1s_{n'}}\right), x_{2} = f\left(x_{2r_{1}}, \dots, x_{2r_{m}}, x_{2s_{1}}, \dots, x_{2s_{m'}}\right), x_{3} = f\left(x_{3r_{1}}, \dots, x_{3r_{k}}, x_{3s_{1}}, \dots, x_{3s_{k'}}\right)$$

Propagate them based on their characteristics

Equation for the mesurand X

$$X = f(x_1, x_2, ..., x_n)$$
Apply Taylor series

$$X = X_o + \sum_{i=1}^n \frac{\partial X}{\partial x_i} (x_i - x_{i0}) + \sum_{k=1}^n \sum_{j=1}^n \frac{1}{2!} \frac{\partial^2 X}{\partial x_j x_k} (x_j - x_{j0}) (x_k - x_{k0}) + \cdots$$

$$Independent factors
(Random components) Correlation factors
(Systematic components) (Systematic comp$$



(National Inspection) GUM-based uncertainty quantification (2/5)

(Example) measurement uncertainty for U concentration analysis using GRAV method

- Setup an equation to quantify U concentration (f_U)

 $f_U = \frac{A_U}{A_U + A_O(O/U)}$

• Consider A_U and A_O as a constant, O/U as the only uncertainty source

- Setup an equation to quantify the oxygen-to-uranium ratio (O/U)

 $O/U = \frac{\left[(1 - w_I)(m_i/m_f) - F_S(1 - w_F)\right]A_U}{F_S(1 - w_F)A_O} \qquad F_S = \frac{3A_U}{3A_U + 8A_O}, A_U \cong w_{235}A_{U-235} + (1 - w_{235})A_{U-238}$

• Consider A_0 , F_S as constants and m_i , m_f , w_I , w_F , w_{235} as uncertainty sources



(National Inspection) GUM-based uncertainty quantification (3/5)

(Example) measurement uncertainty for U concentration analysis using GRAV method

- Establish standard accounting procedures
 - 1. Calibrate electric balance (EBAL) before measurement
 - 2. Measure sample mass before oxidation (m_i) using the EBAL $(m_i = m_i(gross) m_i(tare))$
 - 3. Identify ²³⁵U enrichment (w_{235}) and impurity concentration before oxidation (w_I) using the QC paper
 - 4. Oxidize the sample using a thermogravimetric analyzer (TGA)
 - 5. Measure sample mass change (Δm) inside TGA and calculate sample mass after oxidation (m_f) ($m_f = m_i + \Delta m$)
 - 6. Identify impurity concentration after oxidation (w_F) using the QC paper
 - 7. Calculate O/U ratio using the identified m_i , m_f , w_I , w_F , w_{235}
 - 8. Calculate f_U using the calculated O/U ratio



(National Inspection) GUM-based uncertainty quantification (4/5)

(Example) measurement uncertainty for U concentration analysis using GRAV method

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 Identify individual uncertainty components $u(f_c) = f(m_{std}, X_{std}, \varepsilon_{lin}, \varepsilon_{res})$ $u(X_s) = f(x_{s1}, \dots)$ $u(m_i) = f(m_g, m_t)$ \leftarrow $u(m_{g,t}) = f(X_s, f_b, f_c)$ \leftarrow $u(f_b) = f(x_{b1}, ...)$ 1. Calibrate electric balance (EBAL) before measurement 2. Measure sample mass before oxidation (m_i) using the EBAL * $u(w_{235}) = a(w_{235})/\sqrt{3}$ Identify ²³⁵U enrichment (w_{235}) and impurity concentration before exidation (w_I) 3. $u(w_I) = a(w_I)/\sqrt{3}$ using the QC paper Oxidize the sample using a thermogravimetric analyzer (TGA) 4. $u(\Delta m) = f(\Delta m_{TGA}, drift, buo.)$ 5. Measure sample mass change (Δm) inside TGA and calculate $u(m_f) = f(m_i, \Delta m)$ $u(\Delta m_{TGA}) = f(x_{\Lambda 1}, ...)$ sample mass after oxidation (m_f) $(m_f = m_i + \Delta m)$ $u(drift) = f(x_{d1}, ...)$ Identify impurity concentration after oxidation (w_F) using the QC paper 4 $u(w_F) = a(w_F)/\sqrt{3}$ 6. Calculate O/U ratio using the identified $m_i, m_f, w_I, w_F, w_{235}$ $u(buo.) = f(x_{b1},...)$ 7. Calculate f_U using the calculated O/U ratio 8. $u(O/U) = f(m_i, m_f, w_I, w_F, w_{235})$ $u(f_U) = f\big(u(O/U)\big)$



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(National Inspection) GUM-based uncertainty quantification (5/5)

(Example) measurement uncertainty for U concentration analysis using GRAV method

- Propagate individual uncertainty components based on their characteristics

U concentration $(u(f_U))$





- Quantifying $u(f_U)$ using previous inspection data for two methods
 - Results of U concentration analysis for pure UO₂ pellets in KO1R
 - 6 groups, 53 items
 - Sampled between 2020 ~ 2023
 - Both KNF and KINAC analyzed U concentration using GRAV method

G	iroup	Item	KNF (x_gi)	KINAC (y_gi)	d	Gr	oup	Item	KNF (x_gi)	KINAC (y_gi)	d
	P0011	1			1.200E-03	11/11/1		1			3.700E-03
	(2020)	2			-1.700E-03		B0077-78	2			-4.470E-02
	(2020)	3			6.600E-02		(2022)	3			-3.000E-02
1000	B0012	1			7.700E-03	1115		4			-1.200E-03
	(2020)	2			-1.880E-02	3		1			2.900E-02
1	(2020)	3			1.110E-02		B0089-90	2			-1.520E-02
	P0016	1			-6.500E-03		(2022)	3			3.460E-02
	(2020)	2			5.800E-03			4			-9.700E-03
	(2020)	3			8.000E-04		B0100	1			3.600E-02
1	D0017	1			-1.090E-02		B0104	1			2.800E-02
	(2020)	2			-1.700E-03	4	B0107	1			-1.400E-02
	(2020)	3			/ 1.260E-02		B0112	1			-1.400E-02
	B0022	1			4.260E-02		P0115	1			2.500E-02
	(2021)	2			3.030E-02		BUITS	2			-1.400E-02
	B0023	1			4.590E-02	E	R0119	1			-1.150E-01
	(2021)	2			3.490E-02	5	DOTTO	2			2.450E-01
	B0024	1			4.740E-02		B0124	1			2.000E-02
	(2021)	2			3.850E-02		00124	2			-2.300E-02
	B0026	1			4.040E-02		B0126	1			1.800E-02
	(2021)	2			3.080E-02		B0131	1			3.900E-02
2	B0028	1 /			1.900E-02	6	B0132	1			-1.600E-02
2	(2021)	2			2.670E-02		B0133	1			1.500E-02
	B0029	1			3.420E-02		B0137	1			4.300E-02
	(2021)	2			3.980E-02						
and the	B0045	1			2.200E-02						
	(2021)	2			-1.400E-02						
	B0047	1			-1.200E-02						
1111	(2021)	2			2.600E-02						
	B0051	1			9.000E-03						
	(2021)	2			-9.000E-03						



• Quantifying $u(f_U)$ for the ANOVA method

- Estimate variances for pair-wise differences

Group	G	m_G	1/m_G	m_G-1	V_gd	(m_G-1)*Vgd	(o_r)^2	Avg(d_g)	Avg(d_g)^2	V(d)	(σ_s)^2
1	6	12	0.0833	11	0.00044	0.00489	0.00197	5.467E-03	2.988E-05	1.323E-04	1.217E-04
2		18	0.0556	17	0.00038	0.00648	σ_r	2.514E-02	6.320E-04		σ_s
3		8	0.1250	7	0.00073	0.00514	0.0444	-4.187E-03	1.754E-05		0.0110
4		4	0.2500	3	0.00072	0.00215	δ_r (%)	9.000E-03	8.100E-05		δ_s (%)
5		6	0.1667	5	0.01437	0.07183	0.0504	2.300E-02	5.290E-04		0.0125
6		5	0.2000	4	0.00055	0.00221	12-1/5	1.980E-02	3.920E-04		

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- Estimate operator's random & systematic variances using PADCEL ($V_y < 0$)

Group	G	m G	m G-1	sum(x a)	sum(v a)	sum(x a^2)	sum(v a^2)	sum(x a*v a)	V ax	V av	V axv	(σ rax)^2	rax)^2*(m a	(σ rav)^2	rav)^2*(m a-	(σ rx)^2	(σ rv)^2	(σ sx)^2	(σ sv)^2	
1	6	12	11	1057	1057	93186	93174	93180	8.291E-04	1.046E-03	7.151E-04	1.141E-04	1.255E-03	3.309E-04	3.640E-03	4.852E-05	1.924E-03	7.726E-05	7.726E-05	
2		18	17	1587	1586	139849	139769	139809	1.069E-05	4.115E-04	2.045E-05	-9.758E-06	-1.659E-04	3.910E-04	6.648E-03					
3		8	7	705	705	62149	62155	62152	1.143E-04	5.312E-04	-4.414E-05	1.584E-04	1.109E-03	5.753E-04	4.027E-03					
4		4	3	353	353	31079	31073	31076	1.667E-06	6.590E-04	-2.767E-05	2.933E-05	8.800E-05	6.867E-04	2.060E-03					
5		6	5	529	529	46618	46594	46606	1.067E-06	1.439E-02	1.507E-05	-1.400E-05	-7.000E-05	1.438E-02	7.190E-02				1118911	
6		5	4	441	441	38848	38831	38840	5.800E-06	5.272E-04	-1.035E-05	1.615E-05	6.460E-05	5.376E-04	2.150E-03					
		DOI	DGRU parameter	'S					DODGRU M	IATRIX(nu_x(g,h))					DODGF	RU MATRIX(n	u_y(g.h))		
S_0	V1	V2	S_1	Rev(S_0)	V_x0	V_y0	m_g^(-1)	0.083333333	0.0555556	0.125	0.25	0.16666667	0.2	m_g^(-1)	0.083333333	0.05555556	0.125	0.25	0.16666667	0.2
-1.571E-04	1.323E-04	1.972E-03	9.433E-06	9.433E-06	2.153E-04	1.961E-04	Avg(x_g)	88.1219	88.1441	88.1400	88.1465	88.1457	88.1456	Avg(x_g)	88.1219	88.1441	88.1400	88.1465	88.1457	88.1456
$DOD(\sigma_g x)^2$	2	DOD(o_gy)^2					Avg(y_g)	88.1164	88.1190	88.1442	88.1375	88.1227	88.1258	Avg(y_g)	88.1164	88.1190	88.1442	88.1375	88.1227	88.1258
4.938E-06		4.495E-06						1	2	3	4	5	6		1	2	3	4	5	6
							1	-4.043E-06	2.153E-04	-9.254E-05	3.542E-05	2.025E-04	1.632E-04	1	-1.603E-04	-1.588E-04	-6.631E-05	-3.579E-04	-2.953E-04	-3.399E-04
							2	_	2 6055 06	5 500E 05	2 660E 05	7.054E 06	1.0175.05	2		1 0605 04	10615.04	1 4445 04	2 0085 04	2 2765 04
				R	(f)					2	(f)						f) 3)		05
	$o(J_U)$					$\boldsymbol{o}_{\boldsymbol{r}}(\boldsymbol{j}_{\boldsymbol{U}})$				$\boldsymbol{O}_{\boldsymbol{S}}(\boldsymbol{J}_{\boldsymbol{U}})$				04						
			0.00015				0.000070				04									
0.00015				0.000079				0.00012												



• Quantifying $u(f_U)$ for the GUM-based method



Replaced to the KINAC's repeated measurement process (Standard U concentration analysis using GRAV(TGA))

$\boldsymbol{\delta}(f_U)$	$\boldsymbol{\delta_r}(f_U)$	$\boldsymbol{\delta_s}(f_U)$	
0.00038	0.00038	0.000014	

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Analysis of uncertainty components in accounting process level

- Estimated $u(f_U) : u_r(m_i/m_f)$

δ(f_U)	f_U	u(f_U)	δ(O/U)	O/U	u(O/U)	u_r(mi/mf)	u_s(mi/mf)	u_r(w_l)	u_r(w_F)	u_r(w_235)
3.8317E-04	8.8130E+01	3.3768E-02	3.2279E-03	2.0027E+00	6.4647E-03	3.6782E-04	1.3260E-05	2.1252E-05	5.9525E-06	3.1220E-05
δ_r(f_U)	nu(f_U)	u_r(f_U)	δ_r(O/U)	nu(O/U)	u_r(O/U)	c(mi/mf)	c(mi/mf)	c(w_l)	c(w_F)	c(w_235)
3.8292E-04	5.0640E+04	3.3747E-02	3.2259E-03	5.0640E+04	6.4605E-03	1.7535E+01	1.7535E+01	-1.6873E+01	1.6873E+01	7.2002E-03
δ_s(f_U)		u_s(f_U)	δ_s(O/U)	c(O/U)	u_s(O/U)	frac_r(mi/mf)	frac_s(mi/mf)	frac(w_l)	frac(w_F)	frac(w_235)
1.3781E-05		1.2146E-03	1.1610E-04	-5.2235E+00	2.3252E-04	9.9539E-01	1.2936E-03	3.0769E-03	2.4137E-04	1.2091E-09

- Estimated $u_r(m_i/m_f) : u_r(m_f)$

					-	
mi/mf	u(mi/mf)	u_r(mi)	u_r(mf)	u_s(mi_fc)	u_s(mf_fc)	u_s(mf_m_b)
0.96217	3.681E-04	1.9217E-04	E-04 3.4709E-04 6.5		6.5149E-06	1.44339E-05
nu(mi/mf)	u_r(mi/mf)	c(mi)	c(mf)	c(mi)	c(mf)	c(mf)
5.0663E+04	3.678E-04	0.95464	-0.91853	0.95464	-0.91853	-0.91853
	u_s(mi/mf)	frac(u_r(mi/mf)_r	ni ^f rac(u_r(mi/mf)_mf)	frac(u_s(r	mi/mf)_fc)	frac(u_s(mi/mf)_mb)
	1.326E-05	2.4875E-01	7.5125E-01	3.148	1E-04	9.997E-01

- Estimated $u_r(m_f) : u_r(\Delta m)$

mf	u(mf)	u_r(m(C))	u_r(m(C+Pt))	$u_R(m(C+Pt+U))$	u_r(m(C+U_res))	u_s(m(C))	u_s(m(C+Pt))	$u_s(m(C+Pt+U))$	u_s(m(C+U_res))	u(Δm)	u(m_b)	u(drift)
1.0475	3.4745E-04	6.40086E-05	0.000112463	0.000126828	6.40081E-05	2.5556E-05	4.9620E-05	5.6135E-05	2.5556E-05	1.4435E-05	1.4434E-05	2.8868E-04
nu(mf)	u_r(mf)	c(m(C))	c(m(C+Pt))	c(m(C+Pt+U))	c(m(C+U_res))	c(m(C))	c(m(C+Pt))	c(m(C+Pt+U))	c(m(C+U_res))	c(Δm)	c(m_b)	c(Δm)
3.1130E+04	3.4709E-04	1	-1	1	-1	1	-1	1	-1	1	-1	1//
	u_s(mf)	frac(m(C))	frac(m(C+Pt))	frac(m(C+Pt+U))	frac(m(C+U_res))		frac(u	_s(mf))		frac(Δm)	frac(m_b)	$frac(\Delta m)$
	1.5836E-05	3.4009E-02	1.0499E-01	1.3352E-01	3.4009E-02		1.692	25E-01		1.7296E-03	8.3075E-01	6.9174E-01



Drift effect is the most significant uncertainty component in GRAV





- Quantifying uncertainty with different expression methods
 - Both method satisfied target $\delta(f_U)$ in ITV 2020 * IAEA, IAEA-STR-368 (rev.1.1)

	$\boldsymbol{\delta}(f_U)$	$\boldsymbol{\delta_r}(f_U)$	$\boldsymbol{\delta_s}(f_U)$
ITV 2020	0.0007	0.0005	0.0005
ANOVA	0.00015	0.000079	0.00012
GUM	0.00038	0.00038	0.000014

Comparison between two uncertainty expression methods

Methods	ANOVA	GUM
Future works to check	 Too small δ_r(f_U), need to check whether sample analysis is for the QC and adopt nominal values Need to pile up more pair-wise 	 Too many assumptions in estimating facilities' accounting process Need to reflect facilities' detailed
	differences	accounting process



• KINAC has been developing an MBE method to strengthen the technical capability of SSAC as well as to solve cumulative MUF issue

- We are considering to adopt a GUM-based method for domestic MBE since it can analyze contribution in accounting process level
- Two uncertainty expression methods were examined for U concentration analysis using the GRAV method for previous national inspection results
- Results indicated the both method satisfy the value in ITV 2020
- However, we need more detailed information of facility to achieve more realistic value

Thank you for your attention!

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