Quality of Physicochemical Data on Nanomaterials: an Assessment of Data Completeness and Variability

Daniele Comandella[1], Stefania Gottardo[1], Iria Maria Rio-Echevarria[1,2], Hubert Rauscher[1]

1 European Commission, Joint Research Centre (JRC), 21027 Ispra (VA), Italy (Hubert.RAUSCHER@ec.europa.eu)

2 Present address: European Commission, Research Executive Agency (REA), 1049 Brussels, Belgium

Introduction

- Full characterisation of nanomaterial (NM) physicochemical properties is fundamental for identification, prediction and grouping
- Harmonised Excel® templates for data logging were developed in NANoREG[1] and extended in GRACIOUS[2] to ensure comparison, reproducibility and re-use of test results (Fig. 1)
- Here, a procedure for collection and completeness evaluation of existing data on NM physicochemical properties using the templates is presented. Data generated in previous EU-funded research projects were retrieved from the eNanoMapper database[3]

Sample Information					Sample Preparation					Method and Instrument					Results					SOP
I1	I2	I3	…	In	I1	I2	I3	…	In	I1	I2	I3	…	In	I1	I2	I3	…	In	I
R1																				
R2																				
R3																				
R4																				
…																				
Rn																				

Fig. 1: Structure of an Excel® template for data logging. Each template refers to a specific property (e.g. size) and technique (e.g. DLS) and requires reporting of several information items (I1 to In) for each experiment, including (meta)data describing sample, method, protocols, results, and uncertainty. All (meta)data for one experiment are reported in the same row (R1 to Rn).

Data collection

Procedure to retrieve existing data from the eNanoMapper database:

1. **Data extraction**: the database was queried by project (NANoREG, MARINA) and property (e.g. size, shape) and resulting records filtered for NM names (e.g. Ag, SiO_2) and techniques (e.g. TEM, DLS)
2. **Data cleaning**: extracted data records were corrected (e.g. typos, inappropriate values) and duplicates removed, if needed
3. **Transfer to templates**: cleaned data were re-organised according to the corresponding templates (Fig. 2)

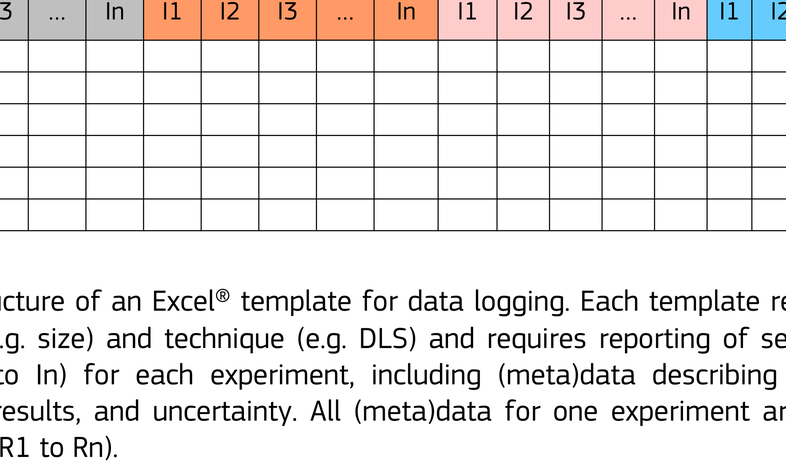

Fig. 2: Number of data rows in the templates for each property. Data refer to representative test materials and physicochemical properties selected in GRACIOUS

Data evaluation

Data transferred in the templates were evaluated in terms of:

- **Data availability and gaps**: data rows contained in every template were counted and gaps identified for each combination of NM/property/technique
- **Data completeness score CS_i**: reported (meta)data were compared with the information items requested by the template to verify their degree of compliance (completeness score) (Fig. 3)[4]
- $CS_i = \frac{number\ of\ items\ reported\ in\ row\ i}{number\ of\ required\ items}$

Property	Technique	Ag	$BaSO_4$	CeO_2	MWCNT	SiO_2
Composition	CHN	0.65	0.65			
	EDX			0.54		
	ICP-MS	0.09			0.18	
	ICP-OES	0.3	0.6	0.57	0.26	
	XRF		0.14	0.14		
Shape	TEM	0.45		0.42		0.45
Particle size	CLS					0.21
	DLS	0.24	0.26	0.26	0.23	0.26
	TEM	0.33		0.33		0.37

Fig. 3: Portion of the summary table visualising gaps and completeness scores. Red cells indicate no data availability. Green cells indicate data availability. The associated score (0 to 1) indicates the degree of compliance of the available data with the information items required by the correspondent template.

- Completeness scores are an important component of data quality. They can refer to selected items and be weighted, involving expert judgement.

Conclusions

- Standardised schemes for reporting test results are effective tools to increase (meta)data completeness in existing repositories
- In this study, NANoREG and GRACIOUS templates were not only used as spreadsheets for data logging but also as checklists to assess the completeness of the (meta)data stored in them
- The calculation of the completeness score is easy and can be implemented in any database as an automatic functionality

References

[1] Totaro et al. 2017, EUR 28137 EN, doi: 10.2787/505397

[2] Gottardo et al. 2019, EUR 29848 EN, doi:10.2760/142959, JRC117733.

[3] Jeliazkova et al. 2015, Beilstein Journal of Nanotechnology, doi: 10.3762/bjnano.6.165

[4] Comandella et al., 2020, Nanoscale, 12, 4695

Acknowledgment

This study was funded by the European research project GRACIOUS, "Grouping, Read-Across, CharacterIsation and classificatiOn framework for regUlatory risk assessment of manufactured nanomaterials and Safer design of nano-enabled products", Horizon 2020, Grant Agreement ID: 760840, 2018-2021, https://cordis.europa.eu/project/rcn/212339/factsheet/en