

Sorption Data Management for Radioactive Waste

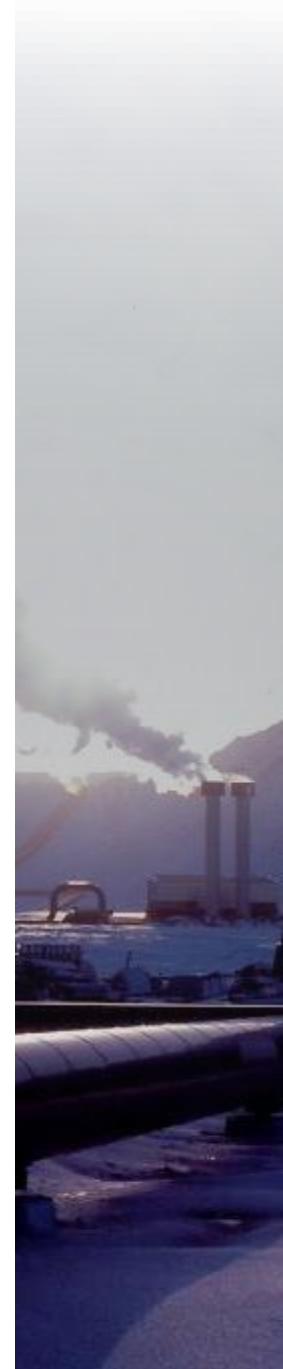
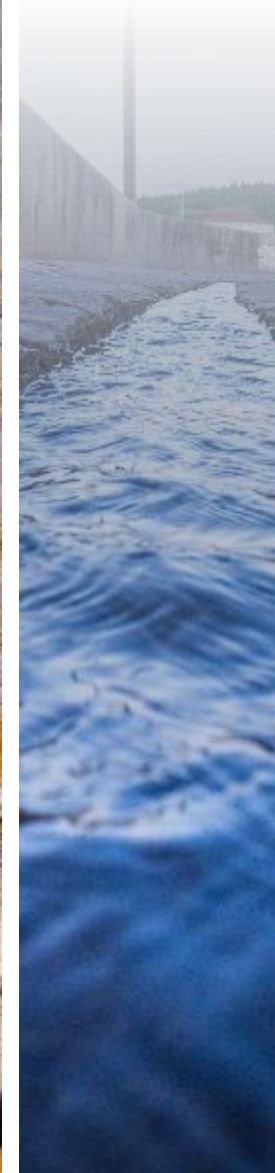
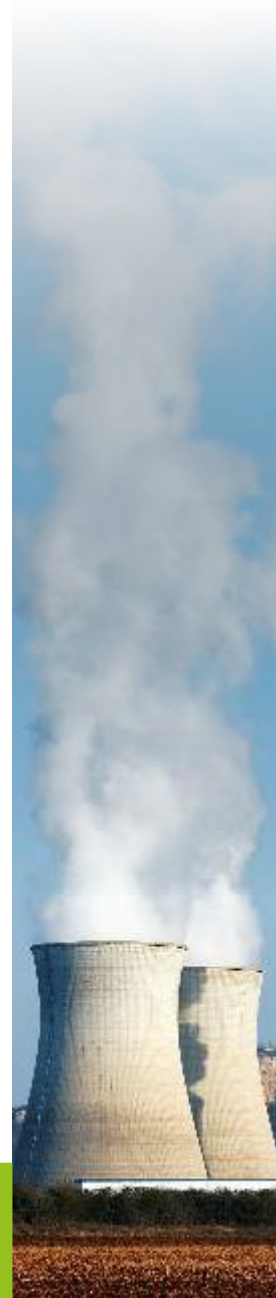
Dr. David García

Nuclear Market Director

Amphos 21

Eurad-2 Annual Event, Dublin

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SORPTION DATA MANAGEMENT FOR RADIOACTIVE WASTE

David García⁽¹⁾, Stéphane Brassinnes⁽²⁾, Mavrik Zavarin⁽³⁾, Vinzenz Brendler⁽⁴⁾, Seonggyu Choi⁽⁵⁾, Jeonghwan Hwang⁽⁵⁾, Dan Miron⁽⁶⁾, Liesbeth Van Laer⁽⁷⁾, Susan Britz⁽⁸⁾, Delphine Durce⁽⁷⁾, Florian Bocchese⁽²⁾, Soo-Gin Kim⁽⁹⁾, Benoît Madé⁽¹⁰⁾, Tammy Yang⁽¹¹⁾ and Jose Luis Leganés⁽¹²⁾

- (1) Amphos 21, Spain*
- (2) ONDRAF/NIRAS, Belgium*
- (3) LNNL, USA*
- (4) HZDR, Germany*
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- (6) PSI, Switzerland*
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- (8) GRS, Germany*
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- (10) Andra, France*
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- (12) ENRESA, Spain*



Take home message

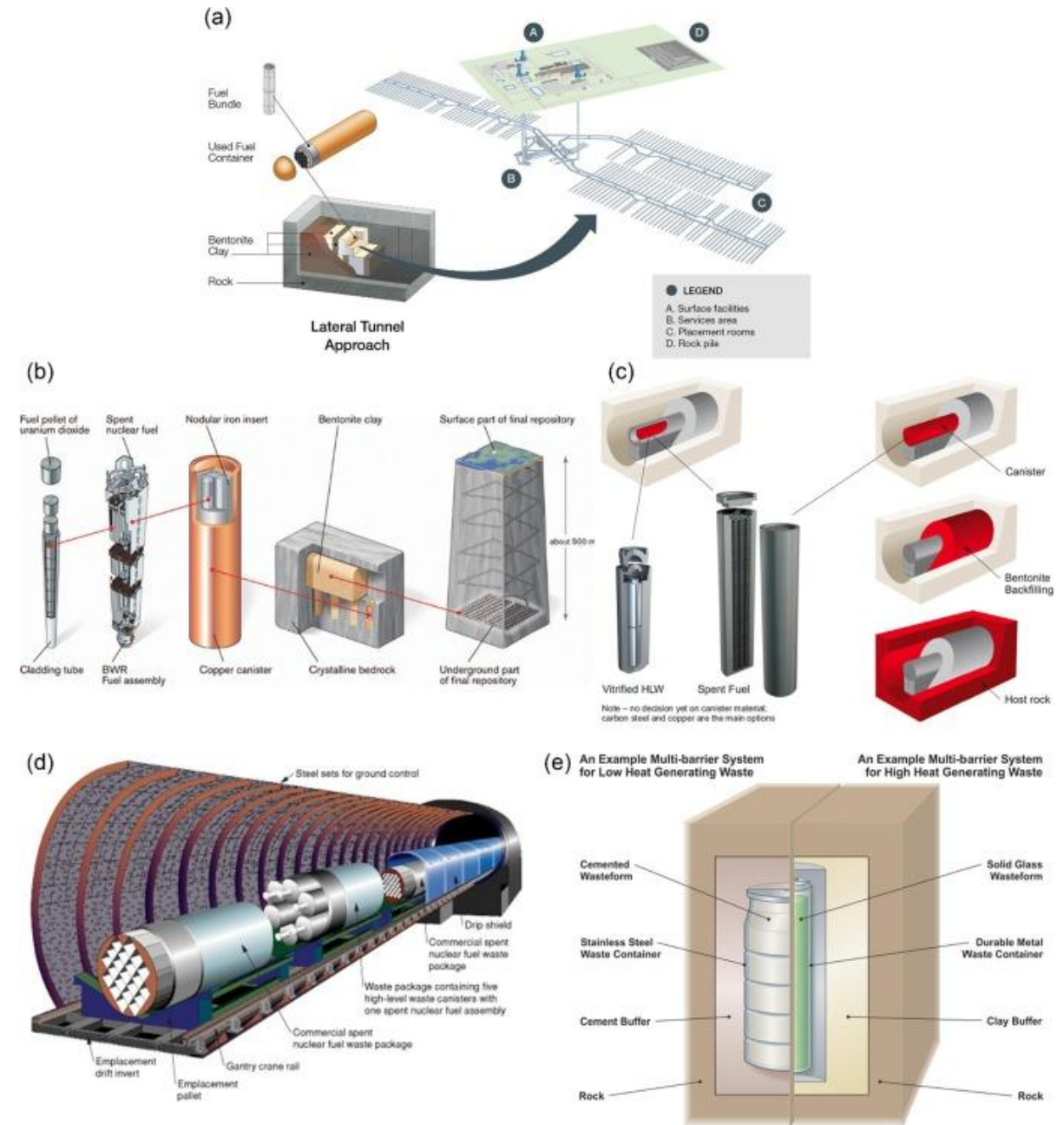
 No database is sufficiently extensive (to our knowledge) to answer all kinds of purposes...

what do we need?



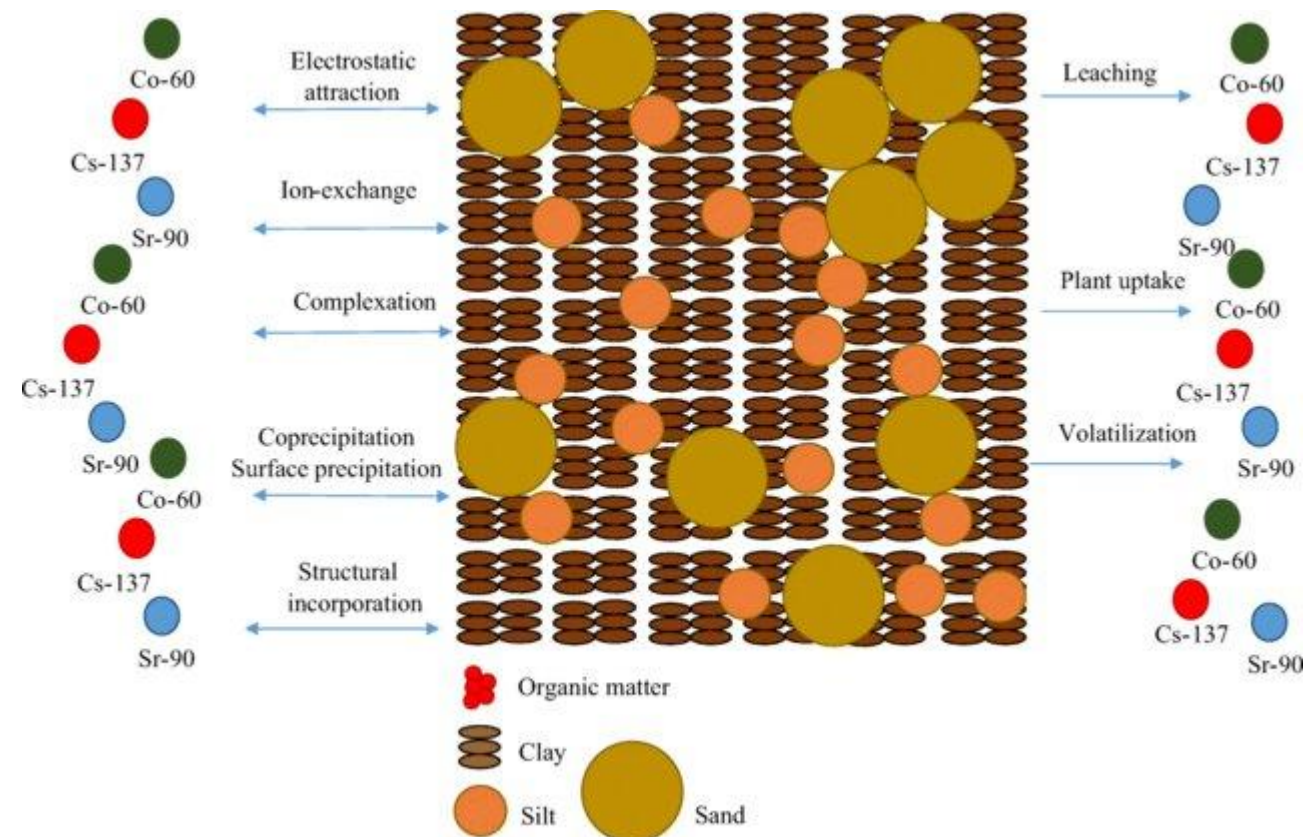
Databases

- In radioactive waste management, **geochemical-thermodynamic modelling** is used in support of various applications, including pre-disposal activities (e.g., waste characterization, conditioning and packaging, (e.g., Small et al., 2018; Wieland et al., 2020)), site selection and safety assessment for near surface and deep geological disposal facilities (e.g., Ma et al., 2022; Hennig and Kühn, 2022), decommissioning of nuclear facilities or management of contaminated land and legacy waste (e.g., Joseph et al., 2019; Balboni et al., 2022).



Databases

- Sorption encompasses various mechanisms, including adsorption, co-precipitation, ion exchange, and surface complexation. These processes govern the extent to which radionuclides are retained by geological and engineered barriers. **Sorption databases** store valuable information on sorption coefficients (K_d values), distribution ratios, and kinetic parameters. The ability to access and analyze experimental data enables nuclear waste management agencies to make informed decisions regarding site selection, waste form design, and containment strategies.



Databases

Within the context of safety assessments of waste disposal facilities, the databases provide support for various fields of application, including:

- Evaluation of **speciation, sorption and solubility of radionuclides** and chemotoxic elements in ground waters and pore waters including derivation of radionuclide solubility limits (e.g., Grivé et al., 2010; Berner, 2014),
- Assessment of **effects of organic ligands** – either present in the waste itself, or derived by degradation of organic materials present in the wastes, the engineered barriers (e.g. superplasticisers in cementitious materials), or in the host rocks (i.e., natural organic matter (NOM) particularly in clay formations such as Opalinus Clay, Callovo-Oxfordian claystone or Boom Clay) – on **radionuclide solubility and mobility** (e.g., Stern et al., 2016; Garcia et al., 2018),
- Definition of **pore water geochemistry**, for example, in bentonite buffers (e.g., Wersin et al., 2016), in cementitious barriers (e.g., Lothenbach and Winnefeld., 2006; Miron et al., 2022) or in clay rock formations (e.g., Mäder and Wersin, 2023), and
- Assessment of the **geochemical evolution** of the repository near field, addressing, for example, formation of **secondary phases** due to waste canister corrosion (e.g., Wilson et al, 2016; Mon et al., 2017) or geochemical **interactions at barrier interfaces** such as cement-clay interactions (e.g., Marty et al., 2014; Idiart et al., 2020)

1st Workshop on Sorption Database Development

Organized in Barcelona, 2024, pivoting on 4 different topics:

- ❑ Session I: State-of-the-art knowledge on Sorption
- ❑ Session II: Current research trends in this field of research
- ❑ Session III: RWMOs views
- ❑ Session IV: Knowledge management

Outcome compiled in a NIRAS/ONDRAF Technical Report:

Brassinnes et al. (2025) NIROND 2025-09 E



**Proceedings of the workshop on
Sorption data management and
database development for
radioactive waste management**

Belgian Agency for Radioactive Waste and Enriched Fissile Materials
NIROND-TR 2025-09 E 03 September 2025

Key points

- 
- Sorption Data gaps
 - Confidence building
 - Experimental considerations
 - Know-how in the long-term
 - Data Structure, Documentation and Record
 - Long-term preservation of key datasets
 - Scientific knowledge and update of the Safety Case?
 - Use of literature data in SA/PA
 - Dispersed to consolidated systems
 - Use of chemical analogues to fill data gaps / knowledge transfer from one system to another
 - Time-evolving chemical systems
 - Over-conservatism in envelope scenarios and loss of realism

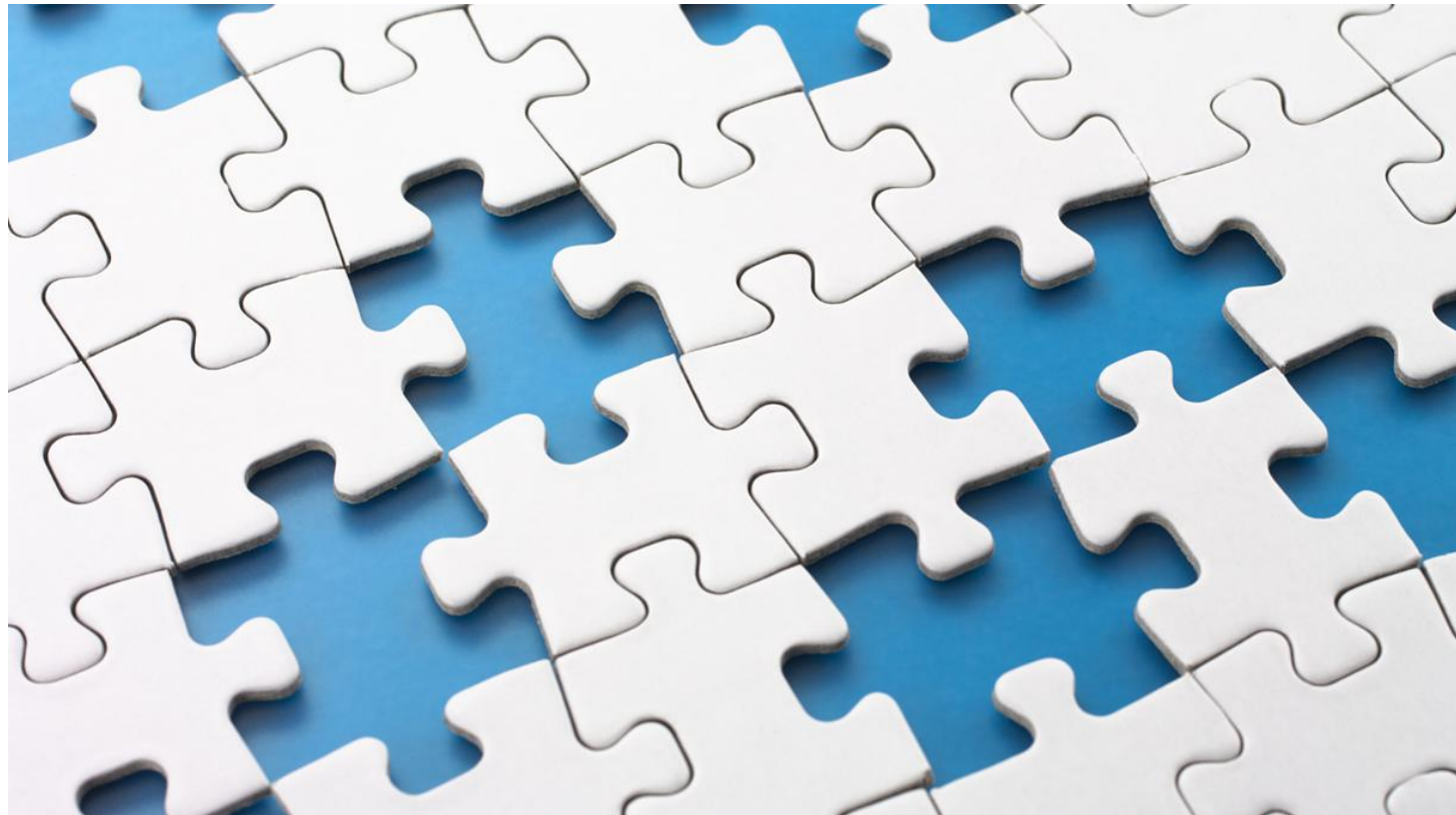


Key points

Scientific needs in support to radioactive waste disposal

■ Sorption Data gaps

- New systems to be investigated?
- Site/design specific materials?
- Effect of perturbations?
- Which RNs/CTs?
- Priorities



Key points

Sorption data management

- **Long-term preservation of key datasets**
 - Approach?
 - Accessibility
 - Done internally (i.e., own SDB project) or externally (e.g., open literature)
 - Are there new data processing tools on the horizon ?

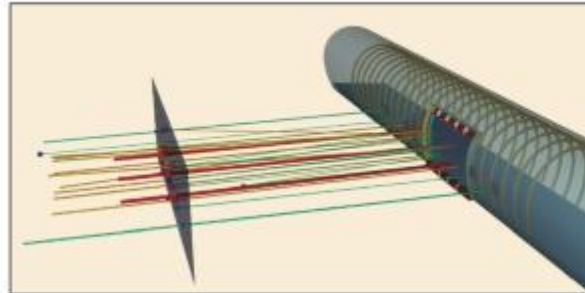


Key points

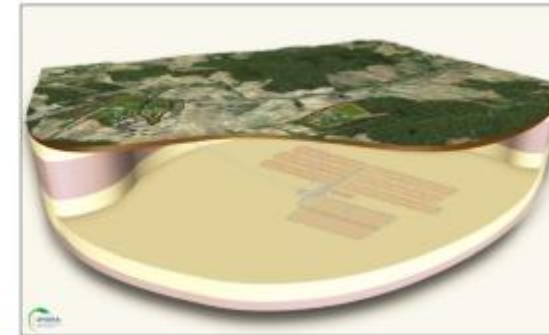
Use of sorption data & knowledge in SA and PA

- **Dispersed to consolidated systems**
 - Upscaling
 - Taken for granted?
 - Accessibility to sorption site
 - Methodologies to select representative S/L
 - Consistency between retention and transport

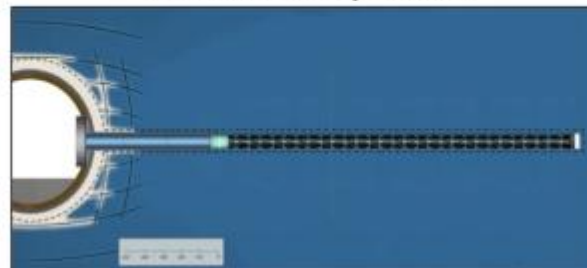
Meso-scale TED Experiment (Calibrated Against Data)



Repository-scale Modeling



Full-scale ALC Experiment



Blind Prediction and
Comparison Against ALC

Blind Prediction and Comparison
Against Other Modeling Teams

2nd Workshop on Sorption Database management and database development for RWM

The event will be hosted by NIRAS-ONDRAF and take place at Brussels, Belgium, from November 17th to November 18th 2026. 4 different topics:

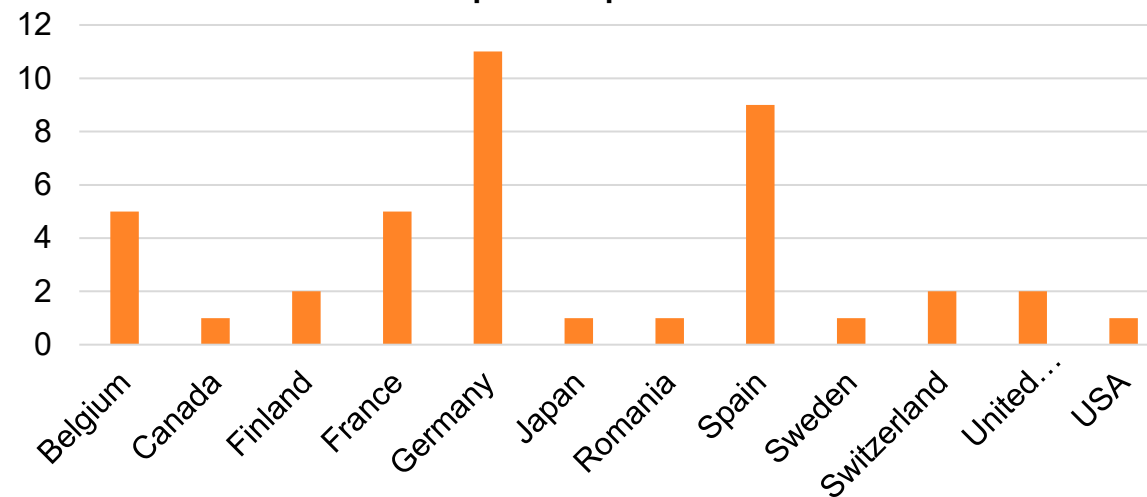
- ❑ *Session A:* Lessons learnt from the Sorption Community: Initiatives, Experimental Capacity and Harmonization Needs
- ❑ *Session B:* Advanced Methodologies for Sorption Experiments
- ❑ *Session C:* From Data to Impact: Linking mechanistic modeling, uncertainty analysis and Safety Cases
- ❑ *Session D:* Database Structures, FAIR (Findable, Accessible, Interoperable, Reusable) Principles & Quality Control

❖ **42 participants**

❖ **24 organisations**

❖ **12 countries**

Countries represented per number of participants



AMPHOS²¹

an **RSK** company

PERÚ

Av. Primavera 781-785, Int. 201,
San Borja, 15037 LIMA
Tel.: +51 1 592 1275

City Center, Of. 1605
Urb. Teresa de Jesús
AREQUIPA 04014

CHILE

Avda. Nueva Tajamar, 481
WTC – Torre Sur – Of 1005
Las Condes, SANTIAGO
Tel.: +562 2 7991630

ESPAÑA

C. Venezuela, 103, 2ª planta
08019 BARCELONA
Tel.: +34 93 583 05 00

C. Raquel Meller, 7, plta. baja.
Ciudad Lineal, 28027 MADRID
Tel.: +34 911 235 562

www.amphos21.com

www.rskgroup.com



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