DEVELOPMENT AND IMPROVEMENT OF THERMODYNAMIC UNDERSTANDING FOR USE IN NUCLEAR WASTE DISPOSAL SAFETY CASE

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OUTLINE

1 Objective and targets

2 Framework

3 Work Package breakdown

4 Timeline

OBJECTIVE AND TARGETS

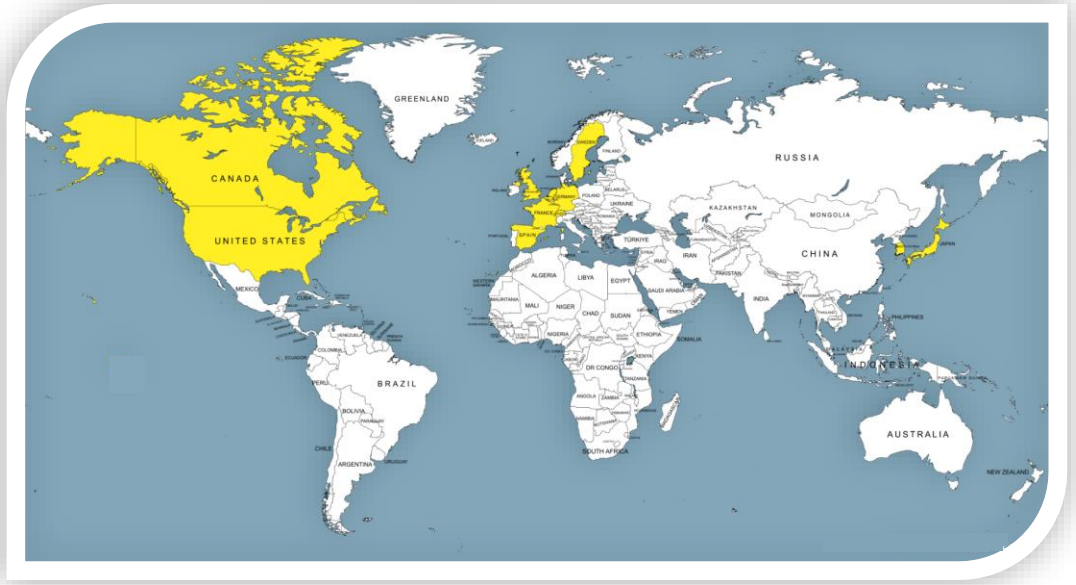
- **To assess current thermodynamic understanding in support of the Radioactive Waste Disposal Safety Case, with special focus given to a transversal understanding**
  - **State-of-the-Art report** (SOTA) documenting the scientific basis supporting the use of thermodynamic approaches in the safety case (SC) and how these are implemented in safety analysis.
  - Complementarity / synergies with **on-going thermodynamic projects**, e.g., NEA-TDB, ThermoChimie, THEREDA, PSI/Nagra TDB, JAEA-TDB, etc.
  - In close collaboration with the End User Group, identify, **critically assess and prioritize data gaps** of relevance to the SC
  - Definition of **technical approaches** and possible scientific strategies to fill in the identified gaps.
  - **Collaborative work** and scientific awareness will be organized through surveys, exchange meetings, open workshops and training courses
  - **White paper** summarizing the outcomes of the integral assessment and promoting new valuable R&D actions to further support/improve the use of thermodynamics in the SC.

FRAMEWORK

- **Type: Strategic Study**

- **Actors:**
  - EU Partners: **12**
  - Non-EU Associated Partners: **6**
  - End Users: **9 (+2)** – still under discussion

- **Duration: 24 months**
- **Resources: c.a. 60 PME in total**



ONDRAF/NIRAS

KIT Karlsruher Institut für Technologie

AMPHOS 21 an RSK company

IMT Atlantique Bretagne-Pays de la Loire École Mines-Télécom

sck cen Exploring a better tomorrow

JÜLICH Forschungszentrum

Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

cea

BGE BUNDESGESELLSCHAFT FÜR ENDLAGERUNG

Géosciences pour une Terre durable brgm

GRS global research for safety

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

PARTNERS

ANDRA

SKB

nagra.

KORAD KOREA RADIOACTIVE WASTE AGENCY

Nuclear Waste Services

nwmo NUCLEAR WASTE MANAGEMENT ORGANIZATION

enresa

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

U.S. DEPARTMENT OF ENERGY | OFFICE OF ENVIRONMENTAL MANAGEMENT

END-USER GROUP
(to be confirmed)

PSI

Empa Materials Science and Technology

KAIST KOREA ADVANCED INSTITUTE OF SCIENCE AND TECHNOLOGY 1971 한국과학기술원

Lawrence Livermore National Laboratory

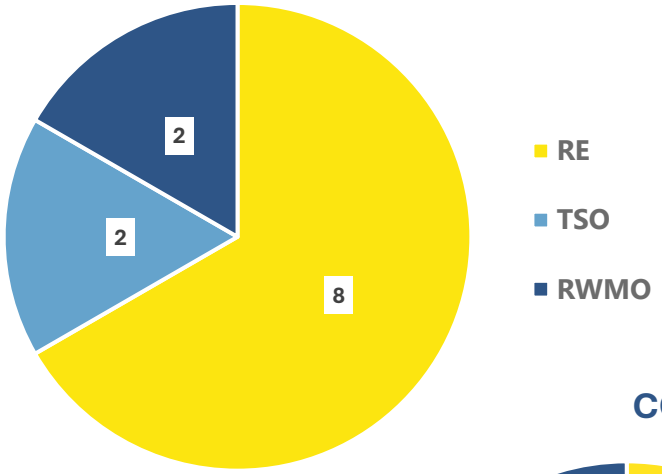
KYOTO UNIVERSITY KYOTO JAPAN FOUNDED 1897

Sandia National Laboratories

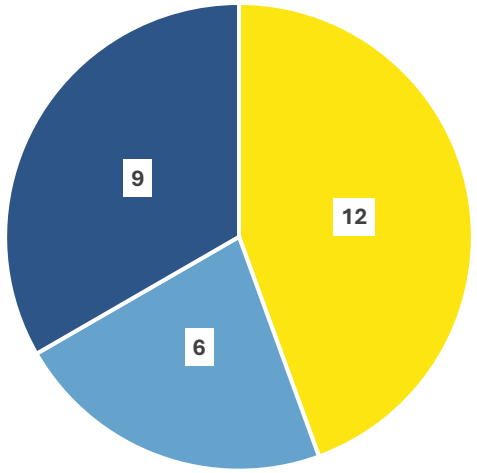
ASSOCIATED PARTNERS

STATISTICS

PARTNERS AND ASSOCIATED PARTNERS

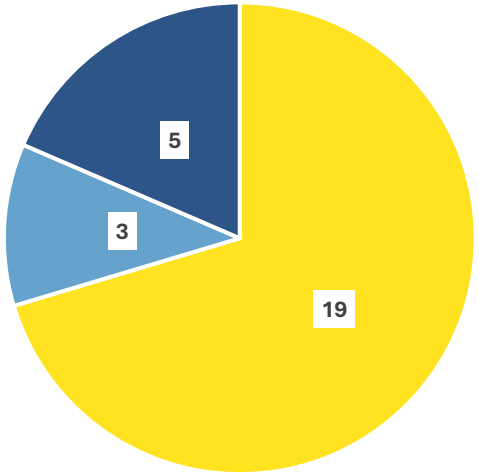


DITUSC WP AND END USERS

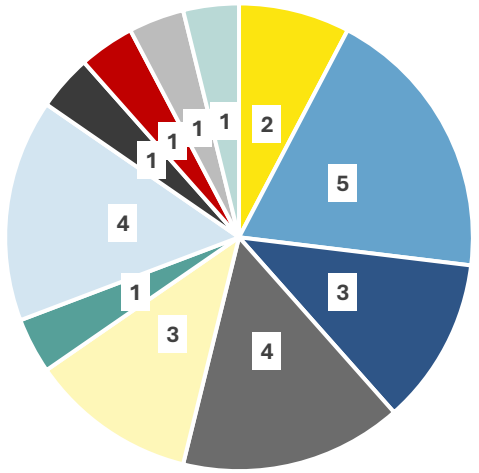


End-User Group still under discussion

CONTINENT



COUNTRIES



DITUSC WP BREAKDOWN

- **Task 1 - Management / Coordination of the WP – ONDRAF/NIRAS & KIT**
  - T1.1. S/T coordination
  - T1.2. Dissemination / outreach / impact
  - T1.3. Quality control
- **Task 2 - Knowledge Management – JFZ**
  - T2.1. Knowledge capture
  - T2.2. Knowledge transfer
- **Task 3 - Thermodynamics: data gaps, solid-solutions, interlink with kinetics, and Safety Case – A21 & PSI**
  - T3.1. Thermodynamic data gaps for RNs and organics
  - T3.2. Perturbed systems (high saline systems and high temperature)
  - T3.3. Thermodynamics of solid-solutions
  - T3.4. Interplay of thermodynamics and kinetics
  - T3.5. Thermodynamics and Safety Case

T1: MANAGEMENT / COORDINATION OF THE WP

T1.1. S/T coordination
T1.2. Dissemination / outreach / impact
T1.3. Quality control

Deliverable (1):

D1.1: outcome/impacts report to Member States and End Users → analysis and integration of the WP results

T2: KNOWLEDGE MANAGEMENT

T2.1. Knowledge capture
T2.2. Knowledge transfer

T2.1: KNOWLEDGE CAPTURE

Capture all relevant information to the work package

- existing knowledge and use in the Safety Case (prior to EURAD 2)
- critical evaluation
- possible ways for improvement and prioritization

Deliverables (3):

D2.1. State-of-the-Art report

D2.3. White paper (first full draft)

D2.4. White paper (final)

T2.1: KNOWLEDGE TRANSFER

Interactions with other Eurad 2 Work Packages

- **WP8** Release of safety relevant radionuclides from spent nuclear fuel under deep disposal conditions (**SAREC**)
- **WP9** Innovative and new container/canister materials under disposal fields conditions: manufacturing feasibility and improved durability (**INCOMAND**)
- **WP12** Radionuclide mobility under perturbed conditions (**RAMPEC**)
- **WP14** Near-surface disposal optimisation based on knowledge and understanding (**SUDOKU**)
- **WP16** High fidelity numerical simulations of strongly coupled processes for Repository systems and design optimisation with physical models and machine learning (**HERMES**)

Interactions with key actors of previous EC projects :

e.g. FUNMIG, RECOSY, SKIN, CEBAMA, FUTURE, …

Interactions with on-going thermochemical database projects:

- NEA-TDB
- ThermoChimie
- Thereda
- Nagra/PSI TDB
- JAEA-TDB
- Thermodderm
- CEMDATA…

T2.1: KNOWLEDGE TRANSFER

3 SPECIAL WORKSHOPS: open to any interested parties

November 2024 (Spain)

(i) Exhange with on-going Thermochemical database programs

(ii) Introduction to DITUSC Survey

AMPHOS 21 an RSK company

Summer-Fall 2025 (France)

(i) Thermodynamics and kinetics

(ii) Thermodynamics and OM

(iii) Thermodynamics of solid-solutions

(iv) Feedback survey

IMT Atlantique
Bretagne-Pays de la Loire
École Mines-Télécom

Spring 2026 (Belgium)

(i) Review of the achievements

(ii) Identification and prioritization of knowledge gaps and current limitations of use in the Safety Case

ONDRAF/NIRAS

TRAINING COURSE: Education and increase awareness of students and young professional on the use of Thermodynamics in the Safety Case

→ Coupled to NEA-TDB annual course (in conjunction to the next Migration conference - September 2025)

DEVELOPMENT AND IMPROVEMENT OF THERMODYNAMIC UNDERSTANDING FOR USE IN NUCLEAR WASTE DISPOSAL SAFETY CASE

European Partnership on Radioactive Waste Management

1st OPEN WORKSHOP
Exchange with on-going TDB projects
14&15 November 2024
Barcelona

DITUSC

Non copyrighted image

FIRST OPEN WORKSHOP (14&15 NOVEMBER 2025 – BARCELONA, SPAIN)

- **Content:**
  - Introduction to EURAD-2 DITUSC Strategic Study
  - Presentations on **on-going TDB projects**:
    - NEA-TDB
    - THEREDA
    - ThermoChimie
    - PSI/Nagra TDB
    - CEMDATA
    - JAEA-TDB
    - WIPP TDB
    - Thermoddem
    - Prodata
  - Focus on **TDB status / Systems covered / Priorities / Future plans**
  - **Data gaps:** identification and methodologies to cover them
  - Introduction to **DITUSC Survey**

T3: THERMODYNAMICS: DATA GAPS, SOLID-SOLUTIONS, INTERLINK WITH KINETICS, AND SAFETY CASE

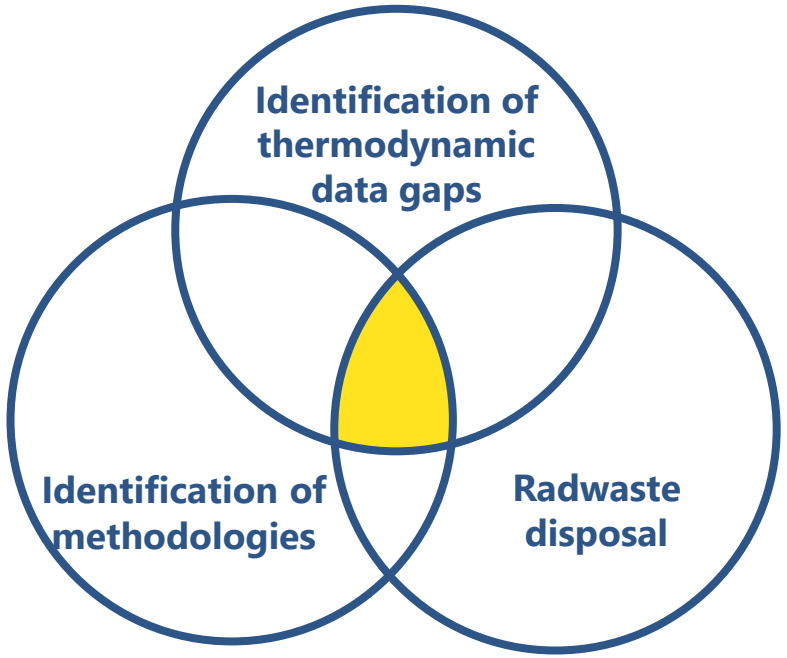
T3.1. Thermodynamic data gaps for RNs and organics
T3.2. Perturbed systems (high saline systems and high temperature)
T3.3. Thermodynamics of solid-solutions
T3.4. Interplay of thermodynamics and kinetics
T3.5. Thermodynamics and Safety Case

T3.1: THERMODYNAMIC DATA GAPS FOR RN AND ORGANICS

Focused on the identification of data gaps related to the use of thermodynamic approaches

▶ Identification of data gaps ▶ Identification of the methodologies ▶ Specific relevant example

Radionuclides



- **Exchanges with on-going thermodynamic database projects (Specific workshop)**
- **Comprehensive surveys**
- **Literature review**
- **Case Studies:**
  - Use of Linear Free Energy Relationships (LFERs) to cover data gaps
  - Ln(III) and An(III) analogies
  - Interaction between multicharged anionic species of actinides with alkaline earths

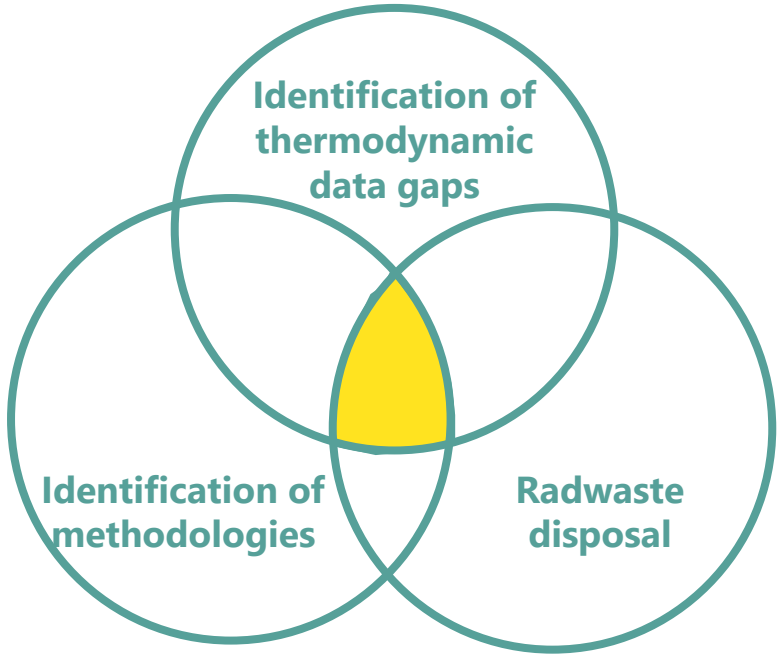
- **SAREC**
- **INCOMAND**
- **RAMPEC**
- **SUDOKU**
- **HERMES**

3.1: THERMODYNAMIC DATA GAPS FOR RN AND ORGANICS

Focused on the identification of data gaps related to the use of thermodynamic approaches

▶ Identification of data gaps ▶ Identification of the methodologies ▶ Specific relevant example

Organics



- **Synergies with on-going thermodynamic-related projects (Specific workshop in November)**
- **Specific workshop for high molecular weight organics**
- **Comprehensive surveys**
- **Literature review**
- **Case Studies:**
  - Applicability of group additivity schemes
  - Interaction of An(III) with hydrosoluble degradation products
  - Thermal degradation of solid organic matter

- **SAREC**
- **INCOMAND**
- **RAMPEC**
- **SUDOKU**
- **HERMES**

T3.2: PERTURBED SYSTEMS

Analyzing the thermodynamic description of relevant systems under perturbed conditions.

Explore strategies to close existing data gaps by estimation methods

HIGHLY SALINE SYSTEMS

(Nitrate, chloride and sulfate plumes)

- **Analyzing and comparing ion interaction theories.**
  - Identify missing data
  - Assess what is achievable today

- **Definition of the relevant conditions**
- **Identification of thermodynamic data gaps for relevant radionuclides and cement phases**
- **Evaluation of existing approaches to estimate missing ion interaction coefficients.**

TEMPERATURE

(Up to 200 °C)

- **Identification of missing data for geochemical modelling (including cement and high saline conditions)**
- **Identification of systems for which experimental data at elevated T are reported but lack adequate model.**
- **Description and benchmark of various estimation methods for transition metals.**

!!!! Avoiding redundances with NEA TDB SOTA reports on high temperatures & high ionic strengths systems

- **SAREC**
- **INCOMAND**
- **RAMPEC**
- **SUDOKU**
- **HERMES**

T3.3: THERMODYNAMICS OF SOLID-SOLUTIONS

Understanding the benefits of using solid solution (SS) models

▶ Approaches and guidelines to include SS in the Safety Case ▶ Identify potential pitfalls

Cement hydrates

- Focus on relevant cases concerning C-S-H, LDH/Afm solid solutions
- Emphasis on end-members incorporating anionic species and radionuclides

Zeolites

- Use of SS models in zeolites
  - Evolution of cementitious materials
  - Cement/clay interaction
  - Uptake of radionuclides

Sulfates/Carbonates

- Role of sulphates and carbonates in retention of safety relevant radionuclides
  - Ra, Tc, Se, I…

- SAREC
- INCOMAND
- RAMPEC
- SUDOKU
- HERMES

T3.4: INTERPLAY OF THERMODYNAMICS AND KINETICS

Assess the interplay of thermodynamics and kinetics

Solid phase transformation

- **M(II), M(III) and M(IV)**
- **Hydroxides, hydrous oxides**
  - Literature search
  - Exploring methods and techniques of solid phase characterization
  - General kinetic interpretation of solubility equations
  - Collection of reaction constants

Redox phenomena

- **Inorganic redox reactions frequently modelled using kinetics**
  - analysis of the source of the data
  - identification of limitations
  - improvement possibilities

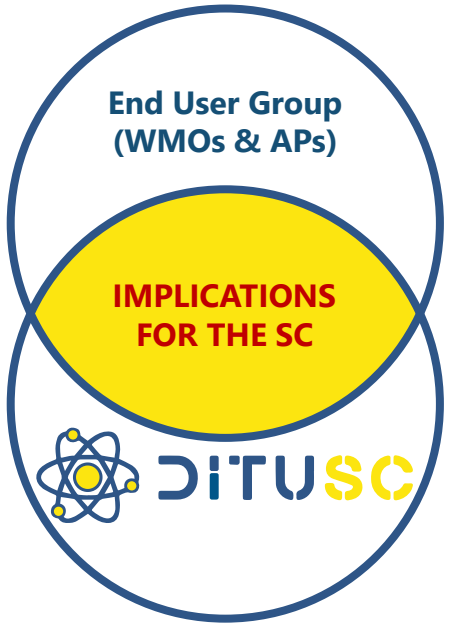
Applications

- **Example: Spent fuel dissolution under reducing conditions**
  - comparison between solubility controlled and dissolution controlled by the forward/backward rate
  - evaluation of the impact of the stoichiometry

- **SAREC**
- **INCOMAND**
- **RAMPEC**
- **SUDOKU**
- **HERMES**

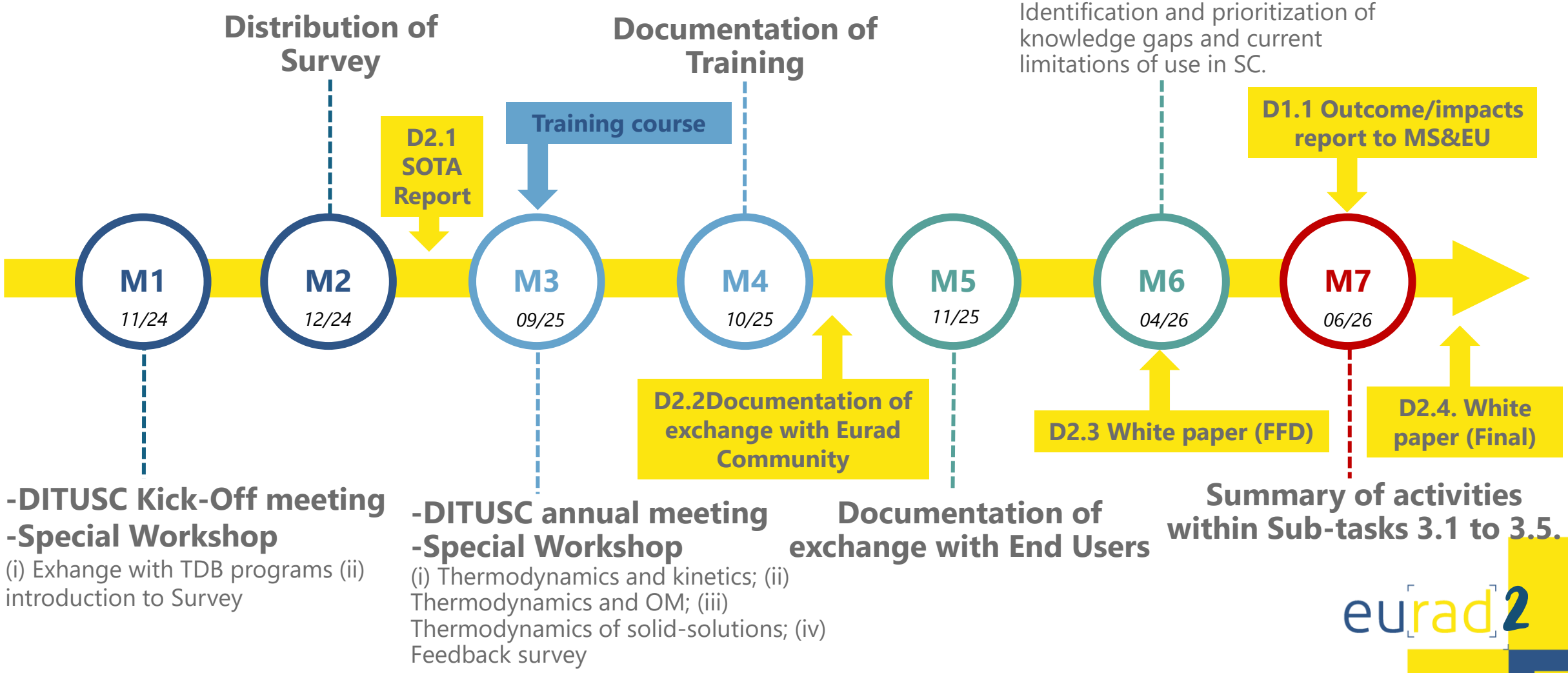
T3.5: THERMODYNAMIC AND SAFETY CASE

- Documenting how thermodynamic approaches are currently implemented in the Safety Case (SC)
- Assessing possible improvements in the use of thermodynamic models in Safety Analysis and Performance Assessment



- **Close interactions with End Users from WMOs & Associated Partners involved in the Safety Case**
  - Comprehensive survey
  - Closure Workshop on output of DITUSC
- **Thermochemical database and the Safety Case**
  - International TDBs and their role in the SC
  - Evaluation of the technical achievements of Sub-task 3.1 to 3.4
  - Identification and prioritization of remaining data/knowledge gaps
- **Use of Thermodynamic approaches in the Safety Case**
  - Summary of the use of Thermodynamic approaches in SC
  - Evaluation of the possible ways of improvement
  - Prioritization of the remaining knowledge gaps

TIMELINE


Distribution of Survey
Documentation of Training
-DITUSC closure meeting
-DITUSC Final Workshop
(i) Review achievements (ii) Identification and prioritization of knowledge gaps and current limitations of use in SC.
D2.1 SOTA Report
Training course
D1.1 Outcome/impacts report to MS&EU
M1 11/24
M2 12/24
M3 09/25
M4 10/25
M5 11/25
M6 04/26
M7 06/26
D2.2Documentation of exchange with Eurad Community
D2.3 White paper (FFD)
D2.4. White paper (Final)
-DITUSC Kick-Off meeting
-Special Workshop
(i) Exhange with TDB programs (ii) introduction to Survey
-DITUSC annual meeting
-Special Workshop
(i) Thermodynamics and kinetics; (ii) Thermodynamics and OM; (iii) Thermodynamics of solid-solutions; (iv) Feedback survey
Documentation of exchange with End Users
Summary of activities within Sub-tasks 3.1 to 3.5.